

Exact Dimensional Reduction of Linear Dynamics: Application to Confined Diffusion

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In their stochastic versions, dynamical systems take the form of the linear dynamics of a probability distribution. We show that exact dimensional reduction of such systems can be carried out, and is physically relevant when the dimensions to be eliminated can be identified with those that represent transient behavior, disappearing under typical coarse graining. Application is made to non-uniform quasi-low dimensional diffusion, resulting in a systematic extension of the “classical” Fick-Jacobs approximate reduction to an exact subdynamics.

KEY WORDS: diffusion, Fick-Jacobs equation, dimensional reduction, mapping.

1. INTRODUCTION

A crucial objective along the path to understanding the dynamical behavior of a complex system lies in the development of tools allowing us to shift back and forth between different levels of resolution. In particular, we would like to be able to recognize coarse-grained objects obeying a coarse-grained dynamics that actually represents a swath of trajectories of the mother system. In the best of all possible worlds, these objects would themselves be experimental observables, but at the very least we would know that the trajectories they represent provide an informative sample of those of the original system. Examples of this strategy are not in great supply, except in various limiting cases. Sometimes,⁽¹⁾ one can indeed find “similarity solutions,” in which only the dynamics of a small finite

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number of variables is required. And approximate solutions as functionals of a primitive, self-consistently obtained, dynamics are the key to Bogoliubov's graded time-scale analysis⁽²⁾ of many-body dynamics. More often, some variant⁽³⁾ of Zwanzig's projection method⁽⁴⁾ is used, shifting the complexity in principle to a non-local time development with a decaying memory. Of course, special situations, such as the prototype that follows, are also handled by more specialized methods.⁽⁵⁾

The major context of this communication is that of dimensional reduction of systems that are highly confined in some of the dimensions they inhabit, which we would therefore like to eliminate from the description, producing a kind of low-resolution picture. A now classical prototype is that of the diffusion of a single particle in a container of "small" non-uniform cross-section $A(x)$ normal to the one-dimensional longitudinal direction x . Assuming that the density does not vary in the transverse direction allows one to conclude that if the diffusion equation $\dot{\rho}(\mathbf{r}, t) = D\nabla^2\rho(\mathbf{r}, t)$ is satisfied in the interior, then the integrated density $p(x, t) = \int \rho(x\mathbf{r}_\perp, t) d\mathbf{r}_\perp$ satisfies the simple (Fick-Jacobs)⁽⁶⁾

$$\dot{p}(x, t) = D\partial_x(A(x)\partial_x(p(x, t)/A(x, t))). \quad (1)$$

In recent work, the Bogoliubov strategy was used to extend the applicability of (1), resulting⁽⁸⁾ in an expansion starting in the case of one transverse dimension, as

$$\begin{aligned} \dot{p} = \partial_x \left\{ A - \frac{1}{3}AA'^2 - \frac{1}{45}AA' [2A(AA'' + A'^2)\partial_x \right. \\ \left. + AA'A'' + A^2A''' - 7A^3] + \dots \right\} \partial_x p/A. \end{aligned} \quad (2)$$

Conversely, the corresponding 2D density $\rho(\mathbf{r}, t)$ (representing the high-resolution picture) can be calculated from the 1D density $p(x, t)$ by the formula

$$\rho(x, y, t) = \left(1 + \left(\frac{y^2}{2A} - \frac{A}{6} \right) A' \frac{\partial}{\partial x} + \dots \right) \frac{p(x, t)}{A}. \quad (3)$$

Here, we will observe that (2) is an example of a reduction process *with no approximation*, valid in principle for all linear systems, and hence for the probability distributions serving as typical descriptive formats.

We now want to consider conclusions such as (2) in a much more general context. It must of course be emphasized that in the type of problem before us, the system and the observer are of equal importance: the latter chooses the compressed data used to represent the system at suitably defined low resolution. When the system development is fully determined by its initial state, it is in general not true that the initial observation, bearing highly reduced information, will determine its own future propagation. But what we will soon show is that there exists a large class of "trajectories" of the full probability distribution for which the time development of the mapping onto the observer's space is indeed

uniquely determined by a suitable dynamical equation on the reduced space. This begs the question of how special the full space trajectories must be, and we will see how the existence of a physically motivated small parameter biases the flow in the required direction. Since this parameter appears most naturally as a temporal scaling, it will also be necessary to transform from spatial confinement to temporal compression to obtain such as (2), but this is more of a technical issue.

2. BASIC FORMULATION

To avoid deeper questions that must ultimately be addressed, we start with the “high-resolution” time-local, i.e., Markovian, linear dynamics

$$\dot{\eta} + M\eta = 0, \tag{4}$$

where η belongs to the finite-dimensional vector space S , of dimension d , M is a $d \times d$ matrix, and we seek the behavior of the reduced dimension vector

$$\xi = P\eta, \tag{5}$$

where P maps S onto S' , of dimension $d' < d$. The question we now pose, an inversion of the usual query, is whether there exists a time-local dynamics

$$\dot{\xi} + Q\xi = 0, \tag{6}$$

any solution of which generates one of (4) under a suitable dimension-raising map W :

$$\eta = W \xi, \tag{7}$$

the existence of which is expected according to the relation (3) and will be verified in the following study of the spectral structure of the transformation.

Equations (4–7) are deceptively simple in appearance, but nonetheless serve to mirror in formal detail the physically realistic situations under study. The answer to the question posed is also deceptively simple, involving rather pedestrian linear algebra.

For (7) to be consistent with (5), we require $\xi = PW \xi$ for all ξ , i.e., $PW = I'$, the identity on S' . Then if (6) holds, we have $\dot{\eta} = W\dot{\xi} = -WQ \xi$, which satisfies (4) if $WQ \xi = -M\eta = -MW \xi$ for all ξ (since it must also hold initially), and so

$$MW = WQ$$

where

$$PW = I', \tag{8}$$

a simple traditional extension of the linear algebra concept of similarity, see e.g. Wedderburn.⁽⁷⁾ If the pair (8) is satisfied by W and Q , our objective is accomplished: Eq. (8) and definition (7) lead directly back from (6) to (4). Indeed, this

remains the case if $\partial/\partial t$ in (4) is replaced by any linear operator on time, e.g. a discrete jump.

Equation (8) can also be combined into a more compact form. Applying P to the first line of (8), and using the second line of (8), we have the identification of the subdynamics

$$Q = PMW, \quad (9)$$

so that (8) implies $MW = WPMW$, and of course $M^2W = MWPMW$. If we define $\Omega = MW$, we then have the simple

$$Q = P\Omega$$

where

$$M\Omega = \Omega P\Omega. \quad (10)$$

In fact, if M is invertible and $\dot{\xi} = -Q\xi$, then Eq. (10) implies Eq. (4): we set $\eta = M^{-1}\Omega\xi$, so that $\dot{\eta} = M^{-1}\Omega\dot{\xi} = -M^{-1}\Omega Q\xi = -M^{-1}(\Omega P\Omega)\xi = -\Omega\xi = -M\eta$.

3. STRUCTURE OF TRANSFORMATION

The brevity of (9,10) conceals the internal nature of our reduction. Let us uncover this, still at a somewhat abstract and formal level. An initial surprise, perhaps, is that our problem, as stated, is very solvable. In fact, it has many solutions, thus offering both an opportunity and a challenge—the former because one has many options, the latter because one wants the class of trajectories selected to have discernible physical relevance.

Suppose for simplicity (but not necessity) that M is hermitian positive definite, so that all solutions of (4) decay in time, and that the eigenvalues $\{\lambda_\alpha\}$ of M are nondegenerate. Then the solutions of (4) are linear combinations of the linearly independent set $\{\chi_\alpha(t) = \psi_\alpha e^{-\lambda_\alpha t}\}$, where ψ_α is the normalized eigenvector belonging to λ_α . Hence, $\{\xi_\alpha(t) = P\psi_\alpha e^{-\lambda_\alpha t}\}$ spans the solution space of (6). It follows from (5) and (6) that the d' eigenvalues of Q are a subset of the d eigenvalues of M . For convenience, order them as $\{\lambda_1, \dots, \lambda_{d'}\}$, so that the corresponding eigenvectors of Q are $\{\varphi_\alpha = P\psi_\alpha, \alpha = 1, \dots, d'\}$. The $\{\varphi_\alpha\}$ are in general not even orthogonal, but it is easy to see that the

$$\{\varphi_\alpha^+ = \psi_\alpha^T W, \quad \alpha = 1, \dots, d'\} \quad (11)$$

are biorthogonal to the $\{\varphi_\alpha\}$, and that

$$Q = \sum_{\alpha=1}^{d'} \lambda_\alpha \varphi_\alpha \varphi_\alpha^+ \quad (12)$$

on the space S' .

Conversely, suppose that $\{\lambda_1, \dots, \lambda_{d'}\}$ is a set of d' eigenvalues of M , and choose the basis $\{\psi_1, \dots, \psi_{d'}, \psi_{d'+1}, \dots, \psi_d\}$ of eigenvectors of M to represent the full space S . Then $\{\varphi_\alpha = P\psi_\alpha, \alpha = 1, \dots, d'\}$ will be non-vanishing linearly independent for typical choices of $\{\lambda_1, \dots, \lambda_{d'}\}$. Choose $\{\varphi_\alpha^+\}$ as biorthogonal to $\{\varphi_\alpha\}$, and *define*

$$\begin{aligned}
 W &= \sum_{\alpha=1}^{d'} \psi_\alpha \varphi_\alpha^+ \\
 Q &= \sum_{\alpha=1}^{d'} \lambda_\alpha \varphi_\alpha \varphi_\alpha^+.
 \end{aligned}
 \tag{13}$$

It follows that $WQ = \sum_1^{d'} \lambda_\alpha \psi_\alpha \varphi_\alpha^+ = MW$, as well as $PW = \sum_1^{d'} \varphi_\alpha \varphi_\alpha^+ = I'$, as desired.

In other words, what we have established is that the reduction from $\dot{\eta} + M\eta = 0$ to $\dot{\xi} + Q\xi = 0$ is not merely a dimension-reducing linear map, but is rather one that cleverly chooses a subset of normal modes, with their characteristic time dependence, to construct a dynamical mirror on a smaller “low resolution” vector space. This leaves very much unaddressed the nature and physical justification of the particular subset—specified by the mode frequency subset $\{\lambda_1, \dots, \lambda_{d'}\}$ - that is to be selected.

4. TRANSIENT ELIMINATION

Which subset $\{\lambda_1, \dots, \lambda_{d'}\}$ would we want to choose? If our objective is to operate at reduced temporal resolution, the choice is clear. We want to eliminate the high λ eigenvalues responsible for transients, and so “project” onto the space of low-lying eigenvectors, which we can refer to as quasi-steady. The extent to which this is accomplished is a function of circumstance, and should be verified in each case. However, the physics behind the crucial choice of the reduction P is often apparent. For example, and this is relevant to most of our intended applications, suppose that

$$M = M_0 + \Delta/\epsilon,
 \tag{14}$$

where M is positive definite, Δ non-negative, and ϵ a small parameter. Then, as $\epsilon \rightarrow 0$, the spectrum of M is expected to separate into dominantly low λ and dominantly high λ segments, and we want to set up our formulation so that only the former are retained. If, furthermore P is such that

$$P\Delta = 0,
 \tag{15}$$

then it is just the high eigenvalue segment that P eliminates when $\epsilon \rightarrow 0$, and indeed, away from this limit, (9) reduces to

$$Q = P M_0 W, \tag{16}$$

in which the Δ -dependence is hidden in W .

The parameter ϵ thus regulates the speed of relaxation in the directions that we are going to eliminate. In the case of diffusion, $\epsilon \rightarrow 0$ corresponds to infinitely fast transverse diffusion and therefore to infinitely fast transverse relaxation.

5. EXAMPLE

Let us break the abstractness with a toy example. Consider two hard point particles, x and y , diffusing on a ring of radius 1, i.e. a periodic line segment of length 2π . The fact that y cannot pass x means that we are restricted to the domain $x \leq y \leq x + 2\pi$. Particle x has diffusion constant $D = 1$, but particle y has $D = 1/\epsilon$ for control. We will want eventually to take $\epsilon = 1$, but until then, ϵ allows us to separate out the quasi-steady component of the motion of x , and eliminate the transient part, both generated by the y -interaction. Of course, we have now generalized (4) and (6) to function space. The joint probability density $\rho(x, y, t)$ satisfies (4) with

$$M = -\partial^2/\partial x^2 - (1/\epsilon)\partial^2/\partial y^2, \tag{17}$$

and because the current density is $J = (-\partial\rho/\partial x, -(1/\epsilon)\partial\rho/\partial y)$, no-flux boundary conditions, applied at the boundaries of the y -motion become

$$\partial\rho/\partial x = (1/\epsilon)\partial\rho/\partial y \quad \text{at} \quad y = x \quad \text{and} \quad y = x + 2\pi. \tag{18}$$

The treatment of (17) and (18) is straightforward, and one finds the eigenfunctions and eigenvalues

$$\begin{aligned} \psi_{mn}(x, y) &= \cos(m/2)(y - x) \exp \pm in(x + \epsilon y) \\ \lambda_{mn} &= m^2(1 + \epsilon)/4\epsilon + n^2(1 + \epsilon) \end{aligned} \tag{19}$$

for integers m and n . The transient component, recognized by $\lambda \rightarrow \infty$ as $\epsilon \rightarrow 0$, is given by $m \neq 0$, and so the quasi-steady component is described by

$$\psi_n(x, y) = \exp \pm in(x + \epsilon y), \quad \lambda_n = n^2(1 + \epsilon). \tag{20}$$

In particular, the dimensionally reduced $\psi_n(x) = (1/2\pi) \int_x^{x+2\pi} \psi_n(x, y) dy = C_{n,\epsilon} \exp \pm in(1 + \epsilon)x$, $\lambda_n = n^2(1 + \epsilon)$, yielding the dimensionally reduced diffusion

$$\partial\rho/\partial t = 1/(1 + \epsilon)\partial^2\rho/\partial x^2. \tag{21}$$

Note that a) the coefficient $1/(1 + \epsilon)$ is a power series in ϵ , converging but not absolutely, as $\epsilon \rightarrow 1$, and b) the coefficient $C_{n,\epsilon} \rightarrow 0$ as $\epsilon \rightarrow 1$. Clearly, care must be exercised in taking this limit.

6. SOLUTION OF EQ. (8)

We now examine in detail the reduction of (14), via the formal expansion

$$W = \sum_{s=0}^{\infty} \epsilon^s W_s, \quad Q = \sum_{s=0}^{\infty} \epsilon^s Q_s \tag{22}$$

at fixed P , so that (8) separate at once into the sequence

$$\Delta W_0 = 0, \quad P W_0 = I',$$

and

$$\Delta W_{s+1} + M_0 W_s = \sum_{q=0}^s W_{s-q} Q_q, \quad P W_{s+1} = 0 \quad \text{for } s \geq 0. \tag{23}$$

Applying P to (23) under condition (15), we also have

$$Q_s = P M_0 W_s, \tag{24}$$

which serves as consistency condition for the solvability of (23) for W_{s+1} .

In the limit $\epsilon = 0$, the density $W_0 \xi$ represents the “fine resolution” picture exactly. The infinitely fast transverse relaxation makes the profile flat in the transverse directions, immediately after any change of the “coarse resolution” density ξ . The succeeding terms $W_s \xi$ express s-order corrections, due to finite transverse relaxation speed at $\epsilon > 0$, coupled with the corresponding corrections of the coarse resolution dynamic operator Q .

This is the format we will make use of, but in its function space, e.g. Master equation,⁽⁹⁾ extension. The functions are on the space (x, y) , where x and y denote generalized “longitudinal” and “transverse” coordinate vectors. Then, $P : (x, y) \rightarrow (x)$, so that we can express P formally as $P(x, y, \partial_y) \equiv P(x)$, a y -space operator parametrized by x . Similarly, we have $W = \bar{W}(y, x, \partial_x) \equiv \bar{W}(y)$. In the application about to be studied $M_0 = M_0(y, x, \partial_x) \equiv M_0(y)$ will be non-vanishing only on x -space, $\Delta \equiv \Delta(x, y, \partial_y) \equiv \Delta(x)$ only on y -space, a blatant separation of the dynamics which is however extremely common. It will also be useful to imagine P chosen as a literal projection on y -space:

$$P(x)^2 = P(x). \tag{25}$$

With this somewhat more explicit notation, (23) becomes, applied to the relevant function space $\{f(x)\}$,

$$\begin{aligned}\Delta(x)W_0(y)f(x) &= 0 \\ P(x)W_0(y)f(x) &= f(x)\end{aligned}\tag{26}$$

followed by

$$\begin{aligned}\Delta(x)W_{s+1}(y)f(x) + M_0(y)W_s(y)f(x) &= \sum_{q=0}^s W_{s-q}(y)Q_q f(x), \\ P(x)W_{s+1}(y)f(x) &= 0,\end{aligned}\tag{27}$$

and resulting in

$$Q_s f(x) = P(x)M_0(y)W_s(y)f(x),\tag{28}$$

the set $Q_0 \dots, Q_s$ serving for consistency in solving (27).

Solution of (27) proceeds most directly via construction of Green's operator $G(x) = G(x, y, \partial_y)$ for the inversion of $\Delta(x)$. G is to satisfy

$$\begin{aligned}\Delta(x)G(x)f(x, y) &= f(x, y) \\ P(x)G(x)f(x, y) &= 0\end{aligned}\tag{29}$$

whenever

$$P(x)f(x, y) = 0,$$

for then the general relations

$$\begin{aligned}\Delta(x)a(x, y) &= b(x, y) \\ P(x)a(x, y) &= 0\end{aligned}\tag{30}$$

where

$$P(x)b(x, y) = 0,$$

are indeed solved by

$$a(x, y) = G(x)b(x, y).\tag{31}$$

We will assume that matters have been arranged so that the solution of (30) is unique, i.e. that $\Delta(x)a(x, y) = P(x)a(x, y) = 0$ implies that $a(x, y) = 0$.

In the applications envisioned, we will have

$$\Delta(x)f(x) = 0, \quad P(x)f(x) = f(x),\tag{32}$$

so that (26) is solved, and (28) follows, as

$$\begin{aligned}W_0(y)f(x) &= f(x) \\ Q_0 f(x) &= P(x)M_0(x)f(x).\end{aligned}\tag{33}$$

The set (27), using (31), is then solved sequentially as

$$\begin{aligned} W_1(y)f(x) &= G(x)(Q_0 - M_0(x))f(x), \\ W_2(y)f(x) &= G(x)(Q_1 - M_0(y)W_1(y) + W_1(y)Q_0)f(x), \dots \end{aligned} \tag{34}$$

coupled with

$$\begin{aligned} Q_1 f(x) &= P(x)M_0(y)W_1(y)f(x), \\ Q_2 f(x) &= P(x)M_0(y)W_2(y)f(x), \dots \end{aligned} \tag{35}$$

Example 1. *Transversely Confined Diffusion.* The situation that motivated the above development is the following. We consider isotropic diffusion with coefficient $D = 1$, on the space of longitudinal coordinates x , transverse Y , with confinement in Y -space given by the surface (or surfaces) $B(x, \epsilon^{-1/2}Y) = 0$, bounding the allowed volume $B(x, \epsilon^{-1/2}Y) \geq 0$. Here B is monotone decaying in Y in the sense that the surface $B(x, \epsilon^{-1/2}Y) = K$ lies within the volume $B(x, \epsilon^{-1/2}Y) \leq K' < K$; clearly, Y -space at fixed x has been made to scale as $\epsilon^{-1/2}$.

Diffusion in a region with no-flux boundary conditions at $B = 0$ is equivalent to having a diffusion constant which vanishes in the prohibited region. Rather than the implied requirement of initially vanishing density in the whole prohibited region to establish uniqueness, we simply confine all observations to the allowed region by imagining the projection to be to infinitesimally more than the allowed region:

$$P'(x)f(x, y) = \theta^+(B(x, \epsilon^{-1/2}Y))f(x, y)$$

where $\theta^+(B) = \theta(B + \kappa)$, (36)

($\kappa > 0$, infinitesimal, only required in case of ambiguity), to be applied to all asserted relations; θ is the Heaviside step function.

To make use of the formulation above, we need only replace spatial confinement by enhanced transverse diffusion, which we do by rescaling: $y = \epsilon^{-1/2}Y$, so that diffusion dynamics is now controlled by

$$M = -\partial_x \cdot \theta(B(x, y)) \partial_x - \frac{1}{\epsilon} \partial_y \cdot \theta(B(x, y)) \partial_y, \tag{37}$$

equivalent to $\dot{\rho} - (\partial_x^2 + (1/\epsilon)\partial_y^2)\rho = 0$ inside the surface $B(x, y) = 0$, while $(\partial_x B(x, y)) \cdot \partial_x \rho + (1/\epsilon)(\partial_y B(x, y)) \cdot \partial_y \rho = 0$ on the bounding surface. We now carry out our dimensional reduction by projecting onto the mean density over

available y -space, via

$$P(x)f(x, y) = \frac{1}{A(x)} \int P'(x)f(x, y') dy' \quad (38)$$

where

$$A(x) = \int P'(x) dy' = \int \theta(B(x, y)) dy';$$

note that here, $P(x)^2 = P(x)$, $P'(x)^2 = P'(x)$, but $P(x)P'(x) = P(x)$. We are then ready to apply (32)–(35), in which in the present case

$$\begin{aligned} M_0(y) &= \partial_x \cdot \theta(B(x, y)) \partial_x \\ \Delta(x) &= \partial_y \cdot \theta(B(x, y)) \partial_y. \end{aligned} \quad (39)$$

It is useful to observe, after a few steps of algebra, that

$$P(x)M_0(y)f(x, y) = -\frac{1}{A(x)} \partial_x \cdot \int \theta(B(x, y)) \partial_x f(x, y) dy. \quad (40)$$

Then, carrying out (32)–(35), we have, to start, $W_0(y) = 1$ and $Q_0 f(x) = -(1/A(x))\partial_x \cdot \int \theta(B(x, y)) dy \partial_x f(x)$, or

$$Q_0 = -(1/A(x)) \partial_x \cdot A(x) \partial_x, \quad (41)$$

just the classical Fick-Jacobs dimensional reduction. Continuing, $W_1(y)f(x) = G(x)[(1/A(x))\partial_x \cdot A(x)\partial_x - \partial_x^2]f(x)$, or

$$W_1(y)f(x) = (G(x) \cdot 1)(\partial_x \ln A(x)) \cdot \partial_x f(x), \quad (42)$$

so that

$$Q_1 = -(1/A(x)) \partial_x \cdot \left[\int \theta(B(x, y)) G(x) \cdot 1 dy \right] \partial_x \ln A(x) \cdot \partial_x. \quad (43)$$

We see that, to this order,

$$Q_1 = -(1/A(x)) \partial_x \cdot \left\{ A(x) + \epsilon \int (\theta(B(x, y))G(x) \cdot 1 dy [\partial_x \ln A(x)]) \right\} \partial_x, \quad (44)$$

has precisely the same form as Fick-Jacobs, but with a modified kernel. A similar result has been obtained using a dynamic approximation by Zwanzig,⁽¹⁰⁾ and (44) also expresses the leading terms of a variational formulation (recently submitted for publication, see also⁽¹¹⁾). The simple form (44) does not extend to higher order, in which higher derivatives are required (see Kalinay and Percus⁽⁸⁾) for the one+one dimensional version, worked out in detail, leading e.g. to Eq. (2).

In summary, we have introduced a dimensional reduction technique of very general utility. When the transient component of the dynamics—typically Markov—can be identified with a definite part of the transition operator, a corresponding series expansion for the reduced dynamics has been obtained. Application to few-body Liouville (inertial) dynamics has been studied—with its relationship to transition state theory—and will be included in a more complete

presentation now in preparation. Quantum dynamics also falls naturally into our class of applicable systems. Perhaps most interesting and promising is the corresponding theory for few-body reduction of many-body dynamics, with the thermodynamic limit imposing its own special coloration. This is now a major focus of our activity.

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