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Dyson's split action formula for transport operators

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Abstract. A proof of Dyson's formula for transport operators with fields defined on a bounded open set in $\mathbb{R}^n$ with volume is presented. Its proof stems from Lax's Equivalence Theorem for linear systems, which is the "principle of uniform boundedness" of numerical analysis.

Keywords: Dyson's formula, Lax's Equivalence Theorem, Lax-Richtmyer stability.

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1 Introduction

The linear response theory of Nonequilibrium Statistical Mechanics models transport processes, such as transport coefficients, using molecular interactions [2]. In this theory, the Mori-Zwanzig procedure extracts generalized Langevin equations from a system of evolution ordinary differential equations (o.d.e.). Dyson's split action (or decomposition) formula is used in this procedure to generate the memory and noise terms of Langevin equations. Briefly, the procedure goes as follows (see [1, 2]

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for details). Let $x'(t) = f(x(t))$ be an autonomous system of evolution o.d.e. with dynamics Φ. From the Theory of Characteristics [3], one has $f(\Phi(t,x)) = (e^{t\mathrm{L}}f)(x)$, where $e^{t\mathrm{L}}$ formally denotes the solution operator of the Liouville equation $\partial_t u(t,x) = \mathrm{L}u(t,x)$, wherein $\mathrm{L} = f(x)\cdot\nabla$ is the transport operator. As such the o.d.e. system may be written $\partial_t\Phi(t,x) = (e^{t\mathrm{L}}f)(x) = e^{t\mathrm{L}}\mathrm{L}x = e^{t\mathrm{L}}\mathrm{PL}x + e^{t\mathrm{L}}\mathrm{QL}x$, where P is a statistical projection operator and $\mathrm{Q} = \mathrm{I} - \mathrm{P}$ its orthogonal complement. Dyson's formula is then used to set $e^{t\mathrm{L}}\mathrm{QL}x = e^{t\mathrm{QL}}\mathrm{QL}x + \int_0^t e^{(t-s)\mathrm{L}}\mathrm{PL}e^{s\mathrm{QL}}\mathrm{QL}x, ds$. As such the o.d.e. system may further be written $\partial_t\Phi(t,x) = e^{t\mathrm{L}}\mathrm{PL}x + \int_0^t e^{(t-s)\mathrm{L}}\mathrm{PL}e^{s\mathrm{QL}}\mathrm{QL}x, ds + e^{t\mathrm{QL}}\mathrm{QL}x$. This is a generalized Langevin equation with Markovian term $e^{t\mathrm{L}}\mathrm{PL}x$, memory term $\int_0^t e^{(t-s)\mathrm{L}}\mathrm{PL}e^{s\mathrm{QL}}\mathrm{QL}x, ds$ and noise term $e^{t\mathrm{QL}}\mathrm{QL}x$.

An application of the Mori-Zwanzig procedure to modeling the interactions within a small set of variables extracted from a large set of interacting variables, a forerunner subject of Machine Learning, is presented in [1]. An application to data assimilation is presented in [4]. An application to the numerical stabilization of the dynamics of a cloud-resolving model (CRM) is presented in [5], where the CRM is an extension of the incompressible Navier-Stokes equations, derived from the compressible equations, toward atmospheric convective processes, such as cyclones and hurricanes, along with subgrid equations for viscous turbulence processes. This study was conducted in parabolic regime. A similar study in hyperbolic regime is under way.

Dyson's formula is the core of the dynamical stabilization method presented in [5]. A proof of Dyson's formula for transport operators with fields defined on a bounded open set in $\mathbb{R}^n$ with volume is presented in this work (for fields in $\mathbb{R}^n$ see [4], Appendix). The proof stems from Lax's Equivalence Theorem for well-posed linear initial-value problems, which states that a finite-difference scheme for such problems converges provided $\Delta t \leq \mathrm{M}\,\alpha(k)$ if, and only if, it is consistent and Lax-Richtmyer stable provided $\Delta t \leq \mathrm{M}\,\alpha(k)$, which means that for any time $t > 0$ there is $\tau > 0$ such that the set $\{|||(\mathrm{C}(\Delta x, \Delta t))^l||| : 0 < \Delta x < \tau, 0 < \Delta t \leq \mathrm{M}\,\Delta x, 0 < l\Delta t \leq t\}$ is bounded, where $\mathrm{C}(\Delta x, \Delta t)$, Δx and Δt are the scheme's matrix, grid width and time step [7, 6]. The Equivalence Theorem is the "principle of uniform boundedness" of numerical analysis.

2 Dyson's formula

Let $\mathcal{M}(k)$ be the set of real square matrices of order k.

Lemma: (Dyson's formula for matrices) If $\mathrm{A}, \mathrm{B} \in \mathcal{M}(k)$ and $x_0 \in \mathbb{R}^k$, then $e^{t(\mathrm{A}+\mathrm{B})}x_0 = e^{t\mathrm{A}}x_0 + \int_0^t e^{(t-s)(\mathrm{A}+\mathrm{B})}\mathrm{B}e^{s\mathrm{A}}x_0\, ds$.

proof: Let $x(t) = e^{t(\mathrm{A}+\mathrm{B})}x_0 - e^{t\mathrm{A}}x_0$. Taking the derivative of $x(t)$, one obtains the initial value problem

$$x'(t) = (\mathrm{A}+\mathrm{B})x(t) + \mathrm{B}e^{t\mathrm{A}}x_0, \quad t \in \mathbb{R}, \tag{2.1}$$

$$x(0) = 0 \tag{2.2}$$

Eq. 2.1 is a non-homogeneous linear ordinary differential equation with constant coefficient. Duhamel's formula for the solution of problem 2.1-2.2 is $x(t) = \int_0^t e^{(t-s)(\mathrm{A}+\mathrm{B})}\mathrm{B}e^{s\mathrm{A}}x_0\, ds$. Thus $e^{t(\mathrm{A}+\mathrm{B})}x_0 - e^{t\mathrm{A}}x_0 = \int_0^t e^{(t-s)(\mathrm{A}+\mathrm{B})}\mathrm{B}e^{s\mathrm{A}}x_0\, ds$. □

Theorem: (Dyson's formula for transport operators) Let Ω be a bounded open set in $\mathbb{R}^n$ with volume. Let $\mathrm{C}_b^0(\Omega)$ be the space of bounded continuous functions on Ω and $\mathrm{C}_b^1(\Omega)$ the space of bounded continuous functions with bounded continuous partial derivatives on Ω. If

1. $a, b : \Omega \to \mathbb{R}^n$ are $\{\mathrm{C}_b^1(\Omega)\}^n$ vector fields with flow functions defined for all $t \geq 0$;

2. $\mathrm{S}(t) : \mathrm{C}_b^1(\Omega) \to \mathrm{C}_b^1(\Omega)$, $t \geq 0$, is the solution operator of

$$\partial_t u(t,x) = a(x) \cdot \nabla u(t,x) \tag{2.3}$$

with $\mathrm{S}(0)u_0 = u_0$;

3. $\mathrm{T}(t) : \mathrm{C}_b^0(\Omega) \to \mathrm{C}_b^0(\Omega)$, $t \geq 0$, is the solution operator of

$$\partial_t w(t,x) = (a(x) + b(x)) \cdot \nabla w(t,x) \tag{2.4}$$

with $\mathrm{T}(0)w_0 = w_0$;

then

$$\mathrm{T}(t)u_0 = \mathrm{S}(t)u_0 + \int_0^t \mathrm{T}(t-s)\,\mathrm{B}\,\mathrm{S}(s)u_0\,ds,$$

for all $u_0 \in \mathrm{C}_b^1(\Omega)$, where $\mathrm{B} = b(x) \cdot \nabla : \mathrm{C}_b^1(\Omega) \to \mathrm{C}_b^0(\Omega)$.

proof: Let $\{\Omega_\alpha\}$, $0 < \alpha < 1$, be a decreasing family of uniform grids mounted inside Ω and such that $\cup\overline{\Omega}_\alpha = \Omega$, where α is the grid width of Ω_α and $\overline{\Omega}_\alpha$ is the closed region enclosed by Ω_α. Let $\mathrm{T}_k(t), \mathrm{S}_k(t) : \mathbb{R}^{p(k)} \to \mathbb{R}^{p(k)}$, $\mathrm{T}_k(t) = (\mathrm{C}_1(\alpha(k), \Delta t))^m$, $\mathrm{S}_k(t) = (\mathrm{C}_2(\alpha(k), \Delta t))^m$, denote any two sequences of finite-difference discretizations of $\mathrm{T}(t)$ and $\mathrm{S}(t)$ with constant time step Δt, mounted on a sequence of grids $\Omega_{\alpha(k)}$ with $\lim_k \alpha(k) = 0$, such that $\mathrm{T}_k(t)[w_0]$ and $\mathrm{S}_k(t)[u_0]$ converge to $\mathrm{T}(t)w_0$ and $\mathrm{S}(t)u_0$ as $k \to +\infty$ provided $\Delta t \leq \mathrm{M}\,\alpha(k)$, for some $\mathrm{M} > 0$, where $[f] \in \mathbb{R}^{p(k)}$ denotes a grid vector, $\mathrm{C}_1, \mathrm{C}_2 \in \mathcal{M}(p(k))$ are the discretization matrices of Eqs. 2.3 and 2.4, $m = m(t, \Delta t)$ is the number of time steps from time 0 to t (i.e. an integer close to $t/\Delta t$ such that $m\Delta t \to t$ as $\Delta t \to 0$) and $p(k)$ is the number of grid points in $\Omega_{\alpha(k)}$. Let $\mathrm{B}_k : \mathbb{R}^{p(k)} \to \mathbb{R}^{p(k)}$ be the discretization of B employed in $\mathrm{T}_k(t)$. Let $\mathrm{N}/\alpha(k)$, $\mathrm{N} \geq \sup_{x\in\Omega} \sum_{j=1}^n |b_j(x)|$, be a bound to the infinite operator norm of B_k, so that $|||\mathrm{B}_k\,[v]||| \leq (\mathrm{N}/\alpha(k))\,|||[v]|||$ for all $v \in \mathrm{C}_b^1(\Omega)$, where $|||[f]||| = \max_{i=1,\ldots,p(k)} |[f]_i|$ for $[f] \in \mathbb{R}^{p(k)}$ (so that $|||[f]||| \to ||f||$ as $k \to +\infty$, for any bounded $f : \Omega \to \mathbb{R}$, where $||\cdot||$ is the sup norm).

One has:

$||\mathrm{T}_k(t-s)\,\mathrm{B}_k\,\mathrm{S}_k(s)[u_0] - [\mathrm{T}(t-s)\,\mathrm{B}\,\mathrm{S}(s)u_0]||$
$= ||\mathrm{T}_k(t-s)\,\mathrm{B}_k\,\mathrm{S}_k(s)[u_0] \pm \mathrm{T}_k(t-s)\,[\mathrm{B}\,\mathrm{S}(s)u_0] \pm \mathrm{T}_k(t-s)\,\mathrm{B}_k\,[\mathrm{S}(s)u_0] - [\mathrm{T}(t-s)\,\mathrm{B}\,\mathrm{S}(s)u_0]||$
$= ||\mathrm{T}_k(t-s)\,\big(\mathrm{B}_k\,(\mathrm{S}_k(s)[u_0]-[\mathrm{S}(s)u_0]) + (\mathrm{B}_k[\mathrm{S}(s)u_0]-[\mathrm{BS}(s)u_0])\big) + \big(\mathrm{T}_k(t-s)\,[\mathrm{BS}(s)u_0] - [\mathrm{T}(t-s)\mathrm{BS}(s)u_0]\big)||$
$\leq |||\mathrm{T}_k(t-s)|||\,\big(||\mathrm{B}_k\,(\mathrm{S}_k(s)[u_0]-[\mathrm{S}(s)u_0])|| + ||\mathrm{B}_k[v_0(s)] - [\mathrm{B}v_0(s)]||\big) + ||\mathrm{T}_k(t-s)[w_0(s)] - [\mathrm{T}(t-s)w_0(s)]||,$

where $v_0(s) = \mathrm{S}(s)u_0$, $w_0(s) = \mathrm{BS}(s)u_0$ and $|||\mathrm{T}_k(t)||| = \sup\{||\mathrm{T}_k(t)[w]|| : [w] \in \mathbb{R}^{p(k)}, ||[w]|| = 1\}$.

According to Lax's Equivalence Theorem [7, 6], T_k is Lax-Richtmyer stable provided $\Delta t \leq \mathrm{M}\,\alpha(k)$ since T_k converges provided $\Delta t \leq \mathrm{M}\,\alpha(k)$. Thus for any time $t-s>0$ there is $\tau>0$ such that the set $\{|||(\mathrm{C}_1(\alpha(k),\Delta t))^l||| : 0<\alpha(k)<\tau, 0<\Delta t \leq \mathrm{M}\,\alpha(k), 0<l\Delta t \leq t-s\}$ is bounded. Hence its subset $\{|||\mathrm{T}_k(t-s)||| : 0<\alpha(k)<\tau, 0<\Delta t\leq \mathrm{M}\,\alpha(k)\}$ is bounded. In addition $||\mathrm{B}_k\,v_k(s)|| \leq (\mathrm{N}/\alpha(k))\,||v_k(s)|| \to 0$ if $||v_k(s)|| = \mathrm{O}(\alpha^2(k))$, which is the case for $v_k(s) = \mathrm{S}_k(s)[u_0]-[\mathrm{S}(s)u_0]$ if $\mathrm{S}_k(s)$ is second order accurate in space. It follows that $\mathrm{T}_k(t-s)\,\mathrm{B}_k\,\mathrm{S}_k(s)[u_0] \to \mathrm{T}(t-s)\,\mathrm{B}\,\mathrm{S}(s)u_0$ as $k\to+\infty$ provided $\Delta t \leq \mathrm{M}\,\alpha(k)$, where $(\mathrm{T}(t-s)\,\mathrm{B}\,\mathrm{S}(s)u_0)(x)$, $(s,x)\in[0,t]\times\Omega$, is integrable in s since, from the Theory of Characteristics [3], it may be written $h(s, g(t-s,x))$, where g and h are continuous functions of s.

Hence:

$\mathrm{T}_k(t)[u_0] - \mathrm{S}_k(t)[u_0] - \mathrm{R}_{km}(t)[u_0] \to \mathrm{T}(t)u_0 - \mathrm{S}(t)u_0 - \int_0^t \mathrm{T}(t-s)\,\mathrm{B}\,\mathrm{S}(s)u_0\,ds$ as $k,m\to+\infty$ provided $\Delta t\leq \mathrm{M}\,\alpha(k)$, where $\mathrm{R}_{km}(t)[u_0] = \sum_{i=0}^m (\mathrm{T}_k(t-s_i)\,\mathrm{B}_k\,\mathrm{S}_k(s_i)[u_0])\Delta t$, wherein $s_i = s_{i-1}+\Delta t$ and $s_0 = 0$.

But:

$\mathrm{T}_k(t)[u_0]-\mathrm{S}_k(t)[u_0]-\mathrm{R}_{km}(t)[u_0] \to e^{t(\mathrm{A}_k+\mathrm{B}_k)}[u_0]-e^{t\mathrm{A}_k}[u_0]-\int_0^t e^{(t-s)(\mathrm{A}_k+\mathrm{B}_k)}\mathrm{B}_k\, e^{s\mathrm{A}_k}[u_0]\,ds$ as $m \to +\infty$ upon $\Delta t \to 0$ with k held fixed, where A_k is the discretization of $a(x)\cdot\nabla$ employed in $\mathrm{S}_k(t)$ and $\mathrm{T}_k(t)$.

Since, according to the Lemma, this limit value vanishes, one has $\mathrm{T}(t)u_0 - \mathrm{S}(t)u_0 - \int_0^t \mathrm{T}(t-s)\,\mathrm{B}\,\mathrm{S}(s)u_0\,ds = \lim_k \lim_m \mathrm{T}_k(t)[u_0]-\mathrm{S}_k(t)[u_0]-\mathrm{R}_{km}(t)[u_0] = \lim_k 0 = 0$. □

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