

RESEARCH STATEMENT

1 Research done

The main results of the Ph.D. thesis are the following:

1. A method of construction of a Brownian sheet with values in a compact Riemannian manifold embedded into a finite dimensional Euclidean space. This result essentially generalizes an analogous result of P. Malliavin for Lie groups.
2. An analog of Chernoff's theorem for evolutionary families of operators.
3. A method of approximation of the Uglanov surface measure by "volume" measures of properly defined surface layer subsets; proof of the surface layer theorem. The surfaces under considerations are submanifolds of codimension 1 in a locally convex space.
4. Development of a calculus of differential forms of a finite codegree on a locally convex space, proof of the Stokes formula for surfaces of codimension 1 in a locally convex space.

Post-Ph.D. research:

5. Establishing a connection between Navier-Stokes equations and forward-backward SDEs on the group of volume-preserving diffeomorphisms of a flat torus.
6. A mathematical approach to the nonequilibrium work theorem (Jarzynski's identity), mathematically rigorous formulation and proof of the identity by means of introducing probability measures on phase space paths.
7. Chernoff's theorem for evolution families generated by manifold-valued stochastic processes.
8. Uniform approximation of the heat kernel on a compact Riemannian manifold by implementation of the Smolyanov-Weizsäcker approach on approximation of surface measures on infinite dimensional manifolds.
9. Computer simulation of molecular dynamics (within a project in computational physics)

The *most interesting* results are described in more details below.

Navier-Stokes equations and forward-backward SDEs on the group of volume-preserving diffeomorphisms of a torus. To the Navier–Stokes equations we associate a certain system of forward-backward SDEs (FBSDE) on the group of volume-preserving diffeomorphisms of the n -dimensional torus. The associated system of the FBSDEs looks like this:

$$\begin{cases} dZ_s^{t,e} = Y_s^{t,e} ds + \sigma(Z_s^{t,e}) dB_s \\ dY_s^{t,e} = -\hat{V}(s, Z_s^{t,e}) ds - X_s^{t,e} dB_s, \\ Z_t^{t,e} = e; Y_T^{t,e} = \hat{h}(Z_T^{t,e}). \end{cases} \quad (1)$$

The process $Z_s^{t,e}$ takes values in the group of volume-preserving H^s -diffeomorphisms of the torus (we use the notation G_V^s for this group). The process $Y_s^{t,e}$ is an H^s -map belonging to the tangent space $T_{Z_s^{t,e}}G_V^s$. The stochastic differentials and stochastic differential equations on Hilbert manifolds are understood in the sense of Dalecky and Belopolskaya's book [4]. A solution of the associated system of FBSDEs was constructed in [2] (<http://arXiv.org/abs/0807.0421>) where existence of the solution to the Navier–Stokes equations with the initial data in the Sobolev space H^s for sufficiently large s was assumed. Conversely, if we know that the solution of the associated FBSDEs exists in some sense, we can construct the solution to the Navier–Stokes equations. The functions \hat{V} and \hat{h} are related to the gradient of the pressure and the initial condition of the Navier–Stokes equations in the following way: $\hat{V}(t, g) = \nabla p(t, \cdot) \circ g$, $\hat{h}(g) = h \circ g$ where $g \in G_V^s$.

Joint work with Prof. A. B. Cruzeiro.

Brownian sheet on a compact Riemannian manifold. Below we describe a scheme of a construction of a Brownian sheet on a compact Riemannian manifold isometrically imbedded into a Euclidean space by the Nash theorem. Let us take a partition $\mathcal{P}_1 \times \mathcal{P}_2$ of the square $[0, 1] \times [0, 1]$, where $\mathcal{P}_1 = \{0 = t_0 < \dots < t_n = 1\}$, $\mathcal{P}_2 = \{0 = s_0 < \dots < s_k = 1\}$, and a Brownian sheet on the ambient Euclidean space. We condition the Brownian sheet to take values on M at all points of the partition $\mathcal{P}_1 \times \mathcal{P}_2$. The process $\mathbf{W}_{M, \mathcal{P}_1, \mathcal{P}_2}^x$ obtained in this way can be viewed as a Brownian sheet on the ambient Euclidean space whose points (belonging to M) at times (t_i, s_j) are connected by independent Brownian bridge sheets. As the meshes $|\mathcal{P}_1|$ and $|\mathcal{P}_2|$ of partitions \mathcal{P}_1 and \mathcal{P}_2 tend to zero, the law of the process $\mathbf{W}_{M, \mathcal{P}_1, \mathcal{P}_2}^x$ converges to the law of a Brownian sheet on M . More specifically, the following theorem holds:

THEOREM 1. *For every $x \in M$, as $|\mathcal{P}_1| \rightarrow 0$ and $|\mathcal{P}_2| \rightarrow 0$, the distributions of $\mathbf{W}_{M, \mathcal{P}_1, \mathcal{P}_2}^x$ converge weakly relative to the family of bounded continuous cylinder functions to a measure \mathbb{W}_M^x . The measure \mathbb{W}_M^x has the following properties:*

- (i) *considered as the distribution of a $C([0, 1], M)$ -valued process, \mathbb{W}_M^x possesses a transition probability at time t which is the distribution of a Brownian motion on M with variance t starting at the point x ;*
- (ii) *considered as the distribution of an M -valued two-parameter stochastic process, \mathbb{W}_M^x possesses a transition probability at time (s, t) which is the heat kernel measure on M at time st , i.e., if $f \in C(M)$, then*

$$\mathbb{W}_M^x \circ \pi_{s,t}^{-1} [f] = (e^{-\frac{st}{2} \Delta_M} f)(x),$$

where $\pi_{s,t}$ is the evaluation map $C([0, 1] \times [0, 1], M) \rightarrow M$, $\omega \mapsto \omega(s, t)$, Δ_M is the Laplace–Beltrami operator on M , $e^{-\frac{\tau}{2} \Delta_M}$ is the heat semigroup.

COROLLARY 1. *Let M be a compact Lie group. Then, \mathbb{W}_M^x coincides with the distribution of the $C([0, 1], M)$ -valued Brownian motion constructed by P. Malliavin [16].*

The theorem and its corollary make it reasonable to call the two-parameter M -valued stochastic process \mathbf{W}_M^x with distribution \mathbb{W}_M^x an M -valued Brownian sheet, or a $C([0, 1], M)$ -valued Brownian motion. The method of construction of \mathbf{W}_M^x is very different to the method of [16], and generalizes the approach of [21] for two-parameter stochastic processes.

A mathematical approach to the nonequilibrium work theorem. We develop a mathematical approach to the nonequilibrium work theorem which is traditionally referred to in statistical mechanics as Jarzynski's identity. We suggest a mathematically rigorous formulation and proof of the identity.

The nonequilibrium work theorem is an equation in statistical mechanics that relates the free energy difference ΔF to the work W carried out on a system during a nonequilibrium transformation. The identity appeared in different, but as we show equivalent, formulations in [13] and [14] in 1997, and in the series of papers [5]–[8] in 1977–1981. In physics literature, the identity is usually written in the form:

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}, \tag{2}$$

where the average is taken over all possible system trajectories in the phase space, and β is the inverse temperature. The identity first appeared in this form in [13] and [14]. Traditional equilibrium thermodynamics tells us that $\langle W \rangle \geq \Delta F$ while the transformation of the system is infinitely slow. The identity (2) is a stronger statement, and in addition to this, it is valid for arbitrary transformations of the system. The identity is used effectively in computer simulations, as well as in experimental physics, to calculate the free energy difference between two states of the system by running many trajectories and taking the average value of $e^{-\beta W}$.

The paper [15] discusses the connection between two different versions of the identity, and concludes that the papers [5]–[8] use a different definition of work. The identity obtained in [5]–[8] (referred to below as Bochkov–Kuzovlev's identity) reads:

$$\langle e^{-\beta W_0} \rangle = 1,$$

where W_0 is the work (in Bochkov–Kuzovlev's sense) performed on the system, and the angle brackets have the same meaning as in (2). We prove that Jarzynski's and Bochkov–Kuzovlev's identities easily follow from each other.

Since the identities involve taking an “average over trajectories”, it is natural to interpret this average as the expectation relative to a probability measure on trajectories, while assuming that the system evolves stochastically. In terms of expectations the identities can be represented by the formulas:

$$\mathbb{E}[e^{-\beta W}] = e^{-\beta \Delta F} \quad \text{and} \quad \mathbb{E}[e^{-\beta W_0}] = 1,$$

where \mathbb{E} is the expectation relative to a probability measure on phase space paths. For this probability measure, some analytical assumptions under which the identities hold are found.

Chernoff's theorem for evolution families of operators. Let $[S, T] \subset \mathbb{R}$ be an interval, $A_t, t \in [S, T]$, be the generators of strongly continuous semigroups on a Banach space E , so that the space $F = \cap_t D(A_t)$ is dense in E . We assume that for all $x \in F$, $\|x\|_F = \|x\|_E + \sup_{[S, T]} \|A_t x\|_E < \infty$. Suppose

that the Cauchy problem

$$\begin{cases} \dot{u}(t) = -A_t u(t) \\ u(r) = x \end{cases}$$

$t \leq r$, is well-posed (backward solvable) on F , and $U(s, t)$ is the evolution family solving this Cauchy problem.

THEOREM 2. Let $Q_{t_1, t_2}, t_1, t_2 > 0$, be a two-parameter family of contractions on E , let $D \subset F$ be dense in E and such that $U(s, t)D \subset D$ for all $s < t$. Let us assume that

$$\frac{Q_{\tau, \tau + \Delta\tau} - I}{\Delta\tau} x \rightarrow A_\tau x, \tag{3}$$

as $\Delta\tau \rightarrow 0$, for all $x \in D$, for all $a > 0$, and uniformly in τ . Let $S \leq s < t \leq T$, $\{s = t_0 < t_1 < \dots < t_n = t\}$ be a partition of the interval $[s, t]$ so that $\max \Delta t_j \rightarrow 0$ as $n \rightarrow \infty$, where $\Delta t_j = t_{j+1} - t_j$. Then, for all $x \in E$,

$$Q_{t_0, t_1} \dots Q_{t_{n-1}, t_n} x \rightarrow U(s, t) x,$$

as $n \rightarrow \infty$.

Chernoff's theorem for evolution families generated by manifold-valued stochastic processes.

Let M be a C^k -smooth compact manifold, and let $A_0(t, x)$, $A_1(t, x)$, \dots , $A_d(t, x)$, $t \in [S, T]$, $x \in M$, be C^k -smooth vector fields on M . Let us consider t -dependent second order differential operators:

$$A_t = \frac{1}{2} \sum_{\alpha=1}^d A_\alpha(t, \cdot) \circ A_\alpha(t, \cdot) + A_0(t, \cdot)$$

with the common domain $C^k(M)$ independent of t . Let X_t be the unique solution to the SDE

$$\begin{aligned} dX_t &= A_\alpha(t, X_t) \circ dB_t^\alpha + A_0(t, X_t) dt \\ X_s &= x. \end{aligned}$$

We do not list here a few additional analytical assumptions.

THEOREM 3. Let Q_{t_1, t_2} , $S \leq t_1 < t_2 \leq T$, be a family of contractions on $C(M)$, and let for all $f \in C^k(M)$,

$$\lim_{\Delta\tau \rightarrow 0} \frac{Q_{\tau-\Delta\tau, \tau} - I}{\Delta\tau} f = A_\tau f$$

and the limit is uniform in τ running over closed intervals $[s, t] \subset (S, T)$. Then, for any subinterval $[s, t] \subset [S, T]$, for any sequence of partitions $\{s = t_0 < t_1 < \dots < t_n = t\}$ of $[s, t]$ such that $\max(t_{j+1} - t_j) \rightarrow 0$ as $n \rightarrow \infty$, and for all $f \in C(M)$, the following convergence holds in $C(M)$:

$$(Q_{t_0, t_1} \dots Q_{t_{n-1}, t_n} f)(\cdot) \rightarrow \mathbb{E}[f(X_t(s, \cdot))], \quad n \rightarrow \infty.$$

2 Research in progress

1. *Solving the FBSDEs by means of Picard's fixed point procedure and obtaining the Navier-Stokes solution.* One considers the FBSDEs (1) in L_2 and solves it by means of Picard's fixed point procedure. Differentiating the both SDEs with respect to $\theta \in \mathbb{T}^n$ one can prove that the iterations converge in the Sobolev space H^s as well. Thus, one gets a unique H^s -smooth solution $(Z^{t,e}, Y_s^{t,e}, X_s^{t,e})$ of the FBSDEs (1).

CONJECTURE 1. There exists a function $\nabla p(s, \cdot)$ such that the solution $(Z^{t,e}, Y_s^{t,e}, X_s^{t,e})$ to the FBSDEs (1) with $\hat{V}(s, g) = \nabla p(s, \cdot) \circ g$ possesses the following properties: There exists an H^s -smooth function $y(s, \cdot)$ such that $Y_s^{t,e} = y(s, \cdot) \circ Z_s^{t,e}$. Moreover, the pair $(y(s, \cdot), p(s, \cdot))$ verifies the Navier-Stokes equations.

2. *Finalizing of the construction of a Brownian sheet on a compact Riemannian manifold M .* We extend the distribution of the previously constructed $C([0, 1], M)$ -valued stochastic process (Brownian sheet) from the algebra of cylindric subsets of $C([0, 1] \times [0, 1], M)$ to the σ -algebra of all Borel subsets of $C([0, 1] \times [0, 1], M)$.

3 Outline of proposed research

Proposing the following below research plan I just want to demonstrate my ability to carry out an independent research. I do not mean to pursue this plan in case I'm successful for positions in other projects.

3.1 Stochastic approach to the Navier–Stokes equations.

3.1.1 Generalization to C^1 -Banach manifolds

Now we would like to associate a system of the FBSDEs to the Navier–Stokes equation without assuming that the initial data are in H^s for sufficiently large s . So let the initial data h belong to C^2 . Let us consider the space of C^1 -maps $\mathbb{T}^n \rightarrow \mathbb{T}^n$. This space has the structure of a C^∞ -smooth Banach manifold ([12]). Let us consider the subset of C^1 -diffeomorphisms $\mathbb{T}^n \rightarrow \mathbb{T}^n$ preserving the volume-measure. This subset is a topological group G_V . Unlike the H^s case, we have to deal now with Banach manifolds instead of Hilbert ones. However, the Dalecky-Belopolskaya approach to SDEs on manifolds which was effectively applied in [2] to treat SDEs on Hilbert manifolds, also works in the case of Banach manifolds. We assume that the solution to the Navier-Stokes equations $y(s, \cdot)$ exists on a small time interval, and belongs to $C^{1,2}$. Let $\hat{Y}_s(g) = y(s, \cdot) \circ g$, $g \in G_V$. We solve the associated system of the FBSDEs on the Banach manifold G_V , where $Y_s^{t,e} = \hat{Y}_s(Z_s^{t,e})$, employing the similar methods as in the H^s case. It is expected to be possible since the tangent subspace at the identity to the manifold of C^1 -maps $\mathbb{T}^n \rightarrow \mathbb{T}^n$ is a dense subspace of H^1 .

3.1.2 FBSDEs and estimation of the derivatives

Here we describe the idea of obtaining estimates for spatially periodic Navier–Stokes solution's derivatives using the associated FBSDEs. As it was shown in [2], $Y_s^{t,e} = y(s, \cdot) \circ Z_s^{t,e}$. One gets the following FBSDEs by means of differentiating the FBSDEs (1) with respect to $\theta \in \mathbb{T}^n$.

$$\begin{cases} \nabla Z_s^{t,e} = \int_t^s \nabla y(r, \cdot) \circ Z_r^{t,e} \nabla Z_r^{t,e} dr + \int_t^s \nabla \sigma(\cdot) \circ Z_r^{t,e} \nabla Z_r^{t,e} dW_r \\ \nabla y(t, \cdot) = \nabla h \circ Z_T^{t,e} \nabla Z_T^{t,e} + \int_t^T \nabla \nabla p(s, \cdot) \circ Z_r^{t,e} \nabla Z_r^{t,e} ds + \int_t^T \nabla X_s^{t,e} dW_s. \end{cases}$$

For example the first SDE implies the following estimate (for simplicity, we consider the case $\nabla \sigma(\cdot) = 0$, i.e. when $A_k = B_k = 0$, $k \in \mathbb{Z}_2^+$).

$$\|\nabla Z_s^{t,e}\|_{L_2}^2 \leq K e^{\int_t^s \|\nabla y(r, \cdot)\|_{L_2}^2 dr} \leq K e^{\|h\|_{L_2}^2}.$$

The second SDE implies that

$$\|\nabla y(t, \cdot)\|_{L_2}^2 \leq K e^{\|h\|_{L_2}^2} (\|h\|_{H^1}^2 + \int_t^T \|\nabla \nabla p(s, \cdot)\|_{L_2}^2 ds). \quad (4)$$

The Calderon-Zygmund inequality and the identity $\Delta p(s, \cdot) = -\text{tr}[\nabla y(s, \cdot)]^2$ allow one to estimate the pressure term in (4).

3.1.3 Brownian motion on the diffeomorphism group of a torus

The approach to stochastic differential equations on Banach manifolds developed by Dalecky and Belopolskaya [4] can be applied to construct an infinite dimensional Brownian motion on the diffeomorphism group of a torus. The necessary differential-geometric structures are discussed in [2].

3.2 Path-manifold-valued Brownian motions

The problem of a Brownian motion with values in paths on a manifold has been studied by many authors. In 1991, Malliavin described a construction of a Brownian motion with values on paths on a compact Lie group as a solution of an SDE [16]. Later, the Brownian motion constructed by Malliavin was studied by B. K. Driver, V. K. Srimurthy, S. Aida ([3], [11], [10]). An SDE describing a Brownian motion with values in paths on a compact Riemannian manifold has been obtained in [9]. However, for describing path-valued Brownian motions, these papers use methods of stochastic calculus. This outline offers a completely different approach to construct a Brownian motion with values in paths on a compact Riemannian manifold. This approach takes over ideas of the approach developed in the papers by O. G. Smolyanov, H. v. Weizsäcker, and their coauthors ([21], [20]) for a Brownian motion with values in a compact Riemannian manifold, and generalises the latter approach to the case of a Brownian motion on a path-manifold.

Let M be a compact Riemannian manifold without boundary isometrically embedded into \mathbb{R}^d by the Nash embedding theorem. In [1], a $C([0, 1], M)$ -valued Brownian motion was constructed by conditioning a $C([0, 1], \mathbb{R}^d)$ -valued Brownian motion to return to the manifold $C([0, 1], M)$ at the points of a given partition of $[0, 1]$. This procedure gives us some conditioned distributions on $C([0, 1], C([0, 1], \mathbb{R}^d))$. Alternatively, these distribution can be obtained by conditioning an M -valued Brownian sheet to return to the manifold M at the points of a given partition of the square $[0, 1] \times [0, 1]$. As the mesh of the partition tends to zero, the conditioned distributions converge to a distribution on the manifold $C([0, 1], C([0, 1], M))$. The latter distribution is referred to as a law of a $C([0, 1], M)$ -valued Brownian motion, or as a law of an M -valued Brownian sheet.

There are other ways to construct probability distributions on the manifold $C([0, 1], C([0, 1], M))$. For example, take the measure which is the normalized restriction of the law of a $C([0, 1], \mathbb{R}^d)$ -valued Brownian motion to the ε -neighborhood of $C([0, 1], M)$:

$$\mathbb{W}_\varepsilon = \frac{\mathbb{W}|_{C([0,1], C([0,1], M_\varepsilon))}}{\mathbb{W}_\varepsilon(C([0, 1], C([0, 1], M_\varepsilon)))}$$

In fact we obtained the law of a $C([0, 1], \mathbb{R}^d)$ -valued Brownian motion conditioned on the event that its paths do not leave $C([0, 1], C([0, 1], M_\varepsilon))$. Taking a weak limit of this distribution as ε tends to zero, we obtain a distribution on $C([0, 1], C([0, 1], M))$.

Finally, the third way of constricting a probability distribution on $C([0, 1], C([0, 1], M))$ is the following. Let us consider the process which is obtained from a $C([0, 1], \mathbb{R}^d)$ -valued Brownian motion by means of its reflection from the boundary of $C([0, 1], M_\varepsilon)$. Letting ε tend to zero, we obtain another distribution on $C([0, 1], C([0, 1], M))$.

The distributions obtained in these three ways may coincide or be absolutely continuous with respect to each other. This is the subject to study.

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