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STABILITY OF INVARIANT MEASURE OF A STOCHASTIC
DIFFERENTIAL EQUATION DESCRIBING MOLECULAR ROTATION

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Summary. Stability of an invariant measure of stochastic differential equation with respect to bounded perturbations of its coefficients is investigated. The results as well as some earlier author's results on Liapunov type stability of the invariant measure are applied to a system describing molecular rotation.

Keywords: Stochastic differential equation, invariant measure, stability.

AMS Classification: 60H10.

McConell [1] studied nuclear magnetic relaxation arising from spin-rotational interactions of the molecules. He assumed the rotation of a molecule to be due to the thermal motion in a steady state and the components $\omega_1(t)$, $\omega_2(t)$, $\omega_3(t)$ of its angular velocity to obey the Euler-Langevin equations

$$(0.1) \quad \begin{aligned} I_1 \dot{\omega}_1 - (I_2 - I_3) \omega_2 \omega_3 &= -I_1 B_1 \omega_1 + I_1 \dot{W}_1 \\ I_2 \dot{\omega}_2 - (I_3 - I_1) \omega_1 \omega_3 &= -I_2 B_2 \omega_2 + I_2 \dot{W}_2 \\ I_3 \dot{\omega}_3 - (I_1 - I_2) \omega_1 \omega_2 &= -I_3 B_3 \omega_3 + I_3 \dot{W}_3, \end{aligned}$$

where I_1, I_2, I_3 are the principal moments of inertia, B_1, B_2, B_3 the frictional constants and (W_1, W_2, W_3) is a 3-dimensional Wiener process. We can write the system (0.1) in a more usual differential form

$$(0.2) \quad \begin{aligned} d\omega_1(t) &= \left(-B_1 \omega_1(t) + \frac{I_2 - I_3}{I_1} \omega_2(t) \omega_3(t) \right) dt + dW_1(t) \\ d\omega_2(t) &= \left(-B_2 \omega_2(t) + \frac{I_3 - I_1}{I_2} \omega_1(t) \omega_3(t) \right) dt + dW_2(t) \\ d\omega_3(t) &= \left(-B_3 \omega_3(t) + \frac{I_1 - I_2}{I_3} \omega_1(t) \omega_2(t) \right) dt + dW_3(t). \end{aligned}$$

In this paper we investigate the system (0.2) from the viewpoint of stability (which was suggested in MR 83m:82030). In Section 1, which is based on the previous results [4], [5], we show the existence of an invariant measure (stationary solution) of the system (0.2) and its global asymptotic Liapunov stability in the strong and the weak topology. In Section 2 we show the stability of the invariant measure with respect to bounded perturbations of coefficients of the system (0.2).

1. INVARIANT MEASURE AND ITS LIAPUNOV STABILITY

Consider an n -dimensional autonomous stochastic differential equation

$$(1.1) \quad d\zeta_t = b(\zeta_t) dt + \sigma(\zeta_t) dw_t,$$

where w_t is an l -dimensional Wiener process, b and σ are an n -dimensional vector and an $n \times l$ matrix, respectively, both b and σ defined on \mathbb{R}_n . Assume that

$$(1.2) \quad |b(x) - b(y)| + |\sigma(x) - \sigma(y)| \leq K_N |x - y|, \quad K_N > 0,$$

holds for all $N > 0$, $|x| + |y| \leq N$. Set $(a_{ij}(x)) = \sigma(x) \sigma^T(x)$ and denote by

$$L = \left(b(x), \frac{\partial}{\partial x} \right) + \frac{1}{2} \sum_{i,j} a_{ij}(x) \frac{\partial^2}{\partial x_i \partial x_j}$$

the infinitesimal operator corresponding to the equation (1.1). Assume that for some $c \in \mathbb{R}$

$$(1.3) \quad LW \leq c \beta(W)$$

holds on \mathbb{R}_n , where $W \in C_2$ satisfies

$$(1.4) \quad W_R = \inf_{|x| \geq R} W(x) \rightarrow \infty \quad \text{for } R \rightarrow \infty$$

and $\beta \in C_1(\mathbb{R}_+)$ is a nonnegative and nondecreasing function satisfying

$$\int_0^\infty \frac{du}{1 + \beta(u)} = \infty.$$

It is known (see e.g. [2], [3]) that the conditions (1.2), (1.3) guarantee the existence and uniqueness (with probability 1) of a solution of (1.1) defined on \mathbb{R}_+ . Denote by \mathcal{P} the set of probability measures defined on the σ -algebra \mathcal{B} of Borel sets of \mathbb{R}_n . Set

$$S_t: \mathcal{P} \rightarrow \mathcal{P}, \quad S_t \nu(A) = \int_{\mathbb{R}_n} P(t, x, A) \nu(dx), \quad A \in \mathcal{B}, \quad t \geq 0,$$

where $P(t, x, A)$ is the transition probability function of the solution of (1.1). Let d

stand for a metric on \mathcal{P} realizing the weak convergence of measures, and $\|\cdot\|$ for the total variation of measures. Statements in this section concern the dynamics of S_t in the spaces $(\mathcal{P}, \|\cdot\|)$ and (\mathcal{P}, d) . We consider the case of nondegenerate diffusion, i.e.

$$(1.5) \quad \sum_{i,j} a_{ij}(x) \alpha_i \alpha_j \geq m(x) |\alpha|^2$$

for all $\alpha \in \mathbb{R}_n$ and $x \in U$, where U is a region in \mathbb{R}_n and $m > 0$ is a continuous function on U .

A measure $\mu^* \in \mathcal{P}$ is called invariant if $S_t \mu^* = \mu^*$ for all $t > 0$.

Theorem 1.1. *Let (1.5) be fulfilled with $U = \mathbb{R}_n$. Then, for every $\varepsilon > 0$ and $\mu \in \mathcal{P}$, such $\delta > 0$ can be found that*

$$d(S_t \mu, S_t \nu) < \varepsilon$$

holds for all $t \geq 0$ and $\nu \in \mathcal{P}$ such that $d(\mu, \nu) < \delta$.

Theorem 1.2. *Assume that (1.5) is fulfilled with*

$$U = U_{R_0} = \{x \in \mathbb{R}_n, |x| < R_0\}$$

for some $R_0 > 0$ and let there exist a function $V \in C_2(\mathbb{R}_n)$, $V \geq 0$, satisfying

$$(1.6) \quad LV \leq -\alpha V + \beta$$

for some $\alpha > 0$, $\beta > 0$, and

$$(1.7) \quad V_{R_1} = \inf_{\mathbb{R}_n \setminus U_{R_1}} V > \frac{\beta}{\alpha}$$

for some $0 < R_1 < R_0$. Then there exists a unique invariant measure $\mu^* \in \mathcal{P}$ and

$$(1.8) \quad \|S_t \nu - \mu^*\| \rightarrow 0, \quad t \rightarrow \infty,$$

holds for all $\nu \in \mathcal{P}$.

The proof of Theorem 1.1 can be found in [4] in a more general (nonautonomous) case. Theorem 1.2 has been proved in [5] as a consequence of a more general result based on a method developed by A. Lasota [7].

We shall show that the above theorems can be applied to the equation (0.2).

Corollary 1.3. *Assume that the equation (1.1) has the form (0.2). Then the assertions of Theorems 1.1 and 1.2 are valid.*

Proof. Set

$$W(x) = \frac{1}{2}(I_1 x_1^2 + I_2 x_2^2 + I_3 x_3^2 + 1).$$

Then

$$LW(x) = -I_1 B_1 x_1^2 - I_2 B_2 x_2^2 - I_3 B_3 x_3^2 + \frac{1}{2}(I_1 + I_2 + I_3) \leq c W(x)$$

for a suitable $c > 0$ and all $x \in \mathbb{R}_3$ and hence (1.3) is fulfilled with $\beta(x) = x$. The assumptions of Theorem 1.1 are clearly satisfied. Setting $V = W$ we also see that (1.6), (1.7) are fulfilled for some $\alpha > 0$, $\beta > 0$ and $R_0 > 0$.

Remark 1.4. It is easily seen that the invariant measure μ^* is a Liapunov stable stationary point of the system S_t in the space $(\mathcal{P}, \|\cdot\|)$. Thus we have obtained the global asymptotic stability of μ^* in the space $(\mathcal{P}, \|\cdot\|)$ as well as in (\mathcal{P}, d) .

2. STABILITY WITH RESPECT TO PERTURBATIONS

Consider the equation (1.1) whose coefficients satisfy (1.2) and (1.3) with $\beta(x) = x$, i.e.

$$(2.1) \quad LW \leq cW$$

for some $c > 0$ and $W \in C_2$ satisfying (1.4). For $\eta \geq 0$ we denote by \mathcal{X}_η the set of couples $[\bar{b}, \bar{\sigma}]$ of coefficients of equations

$$(2.2) \quad d\bar{\zeta}_t = \bar{b}(\bar{\zeta}_t) dt + \bar{\sigma}(\bar{\zeta}_t) dw_t$$

satisfying (1.2) and (2.1) (with the same c and W) and such that

$$\sup_x \max_i |b_i(x) - \bar{b}_i(x)| \leq \eta$$

and

$$\sup_x \max_{i,j} |a_{ij}(x) - \bar{a}_{ij}(x)| \leq \eta,$$

where $(\bar{a}_{ij}) = \bar{\sigma}\bar{\sigma}^T$. Denote by $\mathcal{M} \subset \mathcal{P}$ and $\bar{\mathcal{M}} \subset \mathcal{P}$ the set of invariant measures with respect to the equations (1.1) and (2.2), respectively.

Theorem 2.1. *Let there exist a function $u \geq 0$, $u \in C_2$, such that*

$$(2.3) \quad \overline{\lim}_{R \rightarrow \infty} \sup_{|x|=R} \left\{ Lu(x) + \eta \left(\sum_i \left| \frac{\partial u}{\partial x_i}(x) \right| + \frac{1}{2} \sum_{i,j} \left| \frac{\partial^2 u}{\partial x_i \partial x_j}(x) \right| \right) \right\} < 0$$

for some $\eta \geq 0$. Then $\bar{\mathcal{M}} \neq \emptyset$ for all $[\bar{b}, \bar{\sigma}] \in \mathcal{X}_\eta$.

Proof. Denote by \bar{L} the infinitesimal operator corresponding to the equation (2.2). For $[\bar{b}, \bar{\sigma}] \in \mathcal{X}_\eta$ we have

$$\begin{aligned} \bar{L}u(x) &\leq Lu(x) + \max_{i,j} (|b_i(x) - \bar{b}_i(x)|, |a_{ij}(x) - \bar{a}_{ij}(x)|) \cdot \\ &\quad \cdot \left(\sum_i \left| \frac{\partial u}{\partial x_i}(x) \right| + \frac{1}{2} \sum_{i,j} \left| \frac{\partial^2 u}{\partial x_i \partial x_j}(x) \right| \right). \end{aligned}$$

By (2.3) we get

$$(2.4) \quad Lu(x) \leq -k, \quad |x| > R_0$$

for some $k > 0$, $R_0 > 0$. It can be shown by a standard argument ([8], [6]) that (2.4) implies the existence of an invariant probability measure with respect to (2.2), i.e., $\bar{\mathcal{M}} \neq \emptyset$.

The next Theorem concerns the "continuous dependence" of that invariant measures of the equation (1.1) on its coefficients.

Theorem 2.2. *Let (2.3) be strengthened to*

$$(2.5) \quad \limsup_{R \rightarrow \infty} \sup_{|x|=R} \left\{ Lu(x) + \eta \left(\sum_i \left| \frac{\partial u}{\partial x_i}(x) \right| + \frac{1}{2} \sum_{i,j} \left| \frac{\partial^2 u}{\partial x_i \partial x_j}(x) \right| \right) \right\} = -\infty.$$

Consider the metric of uniform convergence and the metric d on \mathcal{X}_η and \mathcal{P} , respectively. Then the mapping

$$\Phi: \mathcal{X}_\eta \rightarrow \exp \mathcal{P}, \quad [\bar{b}, \bar{\sigma}] \mapsto \bar{\mathcal{M}}$$

is upper semicontinuous at the point $[\bar{b}, \bar{\sigma}]$. In particular, if $\bar{\mathcal{M}} = \{\bar{\mu}\}$ contains only one point for all $[\bar{b}, \bar{\sigma}] \in \mathcal{X}_\eta$ (i.e. every equation (2.2) has a unique invariant measure), then the mapping

$$\Psi: \mathcal{X}_\eta \rightarrow (\mathcal{P}, d), \quad [\bar{b}, \bar{\sigma}] \mapsto \bar{\mu}$$

is continuous at μ^* (the invariant measure of (1.1)).

Remark 2.3. The assumption (2.5) cannot be weakened to (2.3) in Theorem 2.2. However, it can be shown that (2.3) guarantees the "continuous dependence" of invariant measures if the topology on \mathcal{P} is suitably weakened (cf. [6]).

Before proving Theorem 2.2 we give a lemma. For $f \in \mathcal{C}$, set

$$T_t f(x) = \int_{\mathbb{R}_n} P(t, x, dy) f(y), \quad t > 0,$$

and consider a sequence $[b^m, \sigma^m] \in \mathcal{X}_\eta$, $b^m \rightrightarrows b$, $\sigma^m \rightrightarrows \sigma$. Let $L^m, P^m(t, x, A), T_t^m$ and \mathcal{M}^m have the same meaning with respect to the equations

$$(2.6) \quad d_{\zeta_t^m}^m = b^m(\zeta_t^m) dt + \sigma^m(\zeta_t^m) dw_t$$

as $L, P(t, x, A), T_t$ and \mathcal{M} have with respect to (1.1).

Lemma 2.4. *Let $f: \mathbb{R}_n \rightarrow \mathbb{R}$ be a bounded Lipschitzian function. Then*

$$T_t^m f(\cdot) \rightrightarrows^{\text{loc}} T_t f(\cdot), \quad m \rightarrow \infty \quad \text{for all } t \geq 0.$$

Proof. First assume b, σ to be globally Lipschitzian. Let

$$\sup_x \max_{i,j} (|b_i(x) - b_i^m(x)|, |\sigma_{ij}(x) - \sigma_{ij}^m(x)|) < \varepsilon$$

for some $\varepsilon > 0$. It can be easily seen that

$$\mathbb{E}_x |\zeta_t - \zeta_t^m|^2 \leq K_1 \left(\varepsilon^2 + \int_0^t \mathbb{E}_x |\zeta_s - \zeta_s^m|^2 ds \right)$$

for some $K_1 > 0$ (independent of m). Gronwall's lemma yields

$$|T_t f(x) - T_t^m f(x)| \leq K_2 [\mathbb{E}_x |\zeta_t - \zeta_t^m|^2]^{1/2} \leq \varepsilon K_2 \sqrt{(e^{K_1 t} - 1)}.$$

It follows that $T_t^m f \rightrightarrows T_t f$. In the case of non-Lipschitzian b, σ we define (globally) Lipschitzian approximations $b^{0,k}, b^{m,k}, \sigma^{0,k}, \sigma^{m,k}$ such that

$$\begin{aligned} b^{0,k}(x) &= b(x), \quad b^{m,k}(x) = b^m(x) \quad \text{for } |x| \leq k, \quad k \in \mathbb{N}, \\ \sup_x \max_i |b_i^m(x) - b_i^{m,k}(x)| &\leq \sup_x \max_i |b_i(x) - b_i^{0,k}(x)| \end{aligned}$$

and similarly with $\sigma^{0,k}, \sigma^{m,k}$. Denoting by $\zeta^{m,k}$ and $\zeta^{0,k}$ solutions of the corresponding equations with the coefficients $[b^{m,k}, \sigma^{m,k}]$ and $[b^{0,k}, \sigma^{0,k}]$, respectively, we have

$$\begin{aligned} |T_t^m f(x) - T_t f(x)| &\leq |\mathbb{E}_x f(\zeta_t^m) - \mathbb{E}_x f(\zeta_t^{m,k})| + \\ &+ |\mathbb{E}_x f(\zeta_t^{m,k}) - \mathbb{E}_x f(\zeta_t^{0,k})| + |\mathbb{E}_x f(\zeta_t^{0,k}) - \mathbb{E}_x f(\zeta_t)|. \end{aligned}$$

Hence it suffices to show that

$$(2.7) \quad |\mathbb{E}_x f(\zeta_t^{m,k}) - \mathbb{E}_x f(\zeta_t^m)| + |\mathbb{E}_x f(\zeta_t^{0,k}) - \mathbb{E}_x f(\zeta_t)| \rightarrow 0, \quad k \rightarrow \infty,$$

uniformly with respect to m and locally uniformly with respect to x . Trajectories of the processes $\zeta^{m,k}$ and ζ^m ($\zeta^{0,k}$ and ζ) coincide until the exist time $\tau^{m,k}$ (τ^k) from the ball $|x| < k$. Furthermore, by (2.1) we obtain

$$P_x[\tau^{m,k} \leq t] \leq \frac{e^{ct} W(x)}{\inf_{|y| \geq k} W(y)}$$

(cf. the proof of Theorem 3.4.1 in [7]) and hence (2.7) is valid.

Proof of Theorem 2.2. Take an arbitrary sequence $\mu_m \in \mathcal{M}^m$. We need to show that $\mu_{m_i} \rightarrow \mu$ holds for some subsequence (μ_{m_i}) and a measure $\mu \in \mathcal{M}$ (\rightarrow stands for the weak convergence). First we show that the set $\mathcal{B} = \bigcup_m \mathcal{M}^m$ is relatively compact in (\mathcal{P}, d) . By (2.5) we have

$$M = \sup_{m \in \mathbb{N}} \sup_x L^m u(x) < \infty.$$

Put

$$V_R = \sup_{|x| \geq R} \sup_{[\bar{b}, \bar{\sigma}] \in \mathcal{X}_n} \bar{L}u(x).$$

The condition (2.5) yields

$$(2.8) \quad \lim_{R \rightarrow \infty} V_R = -\infty.$$

For $x \in \mathbb{R}_n$, $t > 0$, $m \in \mathbb{N}$ we obtain, by a standard application of Itô's formula and Fatou's lemma:

$$\mathbb{E}_x u(\zeta_t^m) - u(x) \leq \mathbb{E}_x \int_0^t L^m u(\zeta_s^m) ds \leq \mathbb{E}_x \int_0^t (V_R \chi_{[|\zeta_s^m| \geq R]} + M) ds.$$

Hence (we can take $V_R < 0$)

$$\mathbb{E}_x \int_0^t \chi_{[|\zeta_s^m| \geq R]} ds \leq \frac{u(x) + Mt - \mathbb{E}_x u(\zeta_t^m)}{-V_R}$$

and thus

$$(2.9) \quad \frac{1}{t} \int_0^t P^m(s, x, \mathbb{R}_n \setminus U_R) ds \leq \frac{u(x) - \mathbb{E}_x u(\zeta_t^m)}{-tV_R} + \frac{M}{-V_R}.$$

Since

$$\mu_m(\mathbb{R}_n \setminus U_R) = \int_{\mathbb{R}_n} P^m(s, x, \mathbb{R}_n \setminus U_R) \mu_m(dx) = \int_{\mathbb{R}_n} \frac{1}{t} \int_0^t P^m(s, x, \mathbb{R}_n \setminus U_R) ds \mu_m(dx)$$

for any $\mu_m \in \mathcal{M}^m$, $s > 0$, $t > 0$, by (2.9) we get

$$\mu_m(\mathbb{R}_n \setminus U_R) \leq \frac{M}{-V_R} + \int_{\mathbb{R}_n} \frac{u(x) - \mathbb{E}_x u(\zeta_t^m)}{-V_R t} \mu_m(dx).$$

The second term on the right-hand side equals zero and thus

$$\mu_m(\mathbb{R}_n \setminus U_R) \leq \frac{M}{-V_R}$$

which by (2.8) implies the weak compactness of $\bar{\mathcal{D}}$. It follows that there exist a subsequence $(\mu_{m_i}) \subset (\mu_m)$ and a measure $\mu \in \mathcal{P}$ such that $\mu_{m_i} \rightarrow \mu$. It remains to show that

$$(2.10) \quad \int_{\mathbb{R}_n} T_t f d\mu = \int_{\mathbb{R}_n} f d\mu, \quad t > 0,$$

for any bounded Lipschitzian function f , which implies $\mu \in \mathcal{M}$. To show (2.10) we write

$$\left| \int_{\mathbb{R}_n} T_t^{m_i} f d\mu_{m_i} - \int_{\mathbb{R}_n} T_t f d\mu \right| \leq \int_K |T_t^{m_i} f - T_t f| d\mu_{m_i} + 2 \sup |f| \mu_{m_i}(\mathbb{R}_n \setminus K) +$$

$$+ \left| \int_{\mathbb{R}^n} T_t f \, d\mu_{m_t} - \int_{\mathbb{R}^n} T_t f \, d\mu \right| \quad (K \subset \mathbb{R}^n \text{ compact}).$$

By Lemma 2.4 we get

$$(2.11) \quad \int T_t^{m_t} f \, d\mu_{m_t} \rightarrow \int T_t f \, d\mu.$$

On the other hand, we have

$$\int T_t^{m_t} f \, d\mu_{m_t} = \int f \, d\mu_{m_t} \rightarrow \int f \, d\mu$$

which together with (2.11) implies (2.10).

Example 2.5. For $R > 0$ set

$$M_R = \sup_{|x|=R} (b(x), Cx) + \frac{1}{2} \text{Tr}(A(x) C),$$

where $A(x) = \sigma(x) \sigma^T(x)$ and $C = (c_{ij})$ is a symmetric positive definite matrix. Assume that

$$(2.12) \quad \lim_{R \rightarrow \infty} (M_R + \varepsilon R) = -\infty$$

holds for some $\varepsilon > 0$. Then the assertions of Theorems 2.1 and 2.2 are valid with $\eta = \varepsilon/K$, where $K = n^{3/2} \max |c_{ij}| + 1$. To prove it we can use the function $u(x) = \frac{1}{2} \sum_{i,j} c_{ij} x_i x_j$. We have

$$\begin{aligned} & \lim_{R \rightarrow \infty} \sup_{|x|=R} \left\{ Lu(x) + \frac{\varepsilon}{K} \left(\sum_i \left| \sum_j c_{ij} x_j \right| + \frac{1}{2} \sum_{i,j} |c_{ij}| \right) \right\} \leq \\ & \leq \lim_{R \rightarrow \infty} \sup_{|x|=R} (Lu(x) + \varepsilon R) = \lim_{R \rightarrow \infty} (M_R + \varepsilon R) = -\infty. \end{aligned}$$

Hence (2.5) is fulfilled.

We shall apply the above results to the system (0.2).

Corollary 2.6. *Assume the equation (1.1) to have the form (0.2). Then the assertions of Theorems 2.1 and 2.2 are valid with any $\eta \geq 0$.*

Proof. We can use Example 2.5 with $c_{ij} = \delta_{ij} I_i$, $i, j = 1, 2, 3$. We have

$$\begin{aligned} & (b(x), Cx) + \frac{1}{2} \text{Tr} A(x) C = \\ & = -B_1 I_1 x_1^2 - B_2 I_2 x_2^2 - B_3 I_3 x_3^2 + \frac{1}{2} (I_1 + I_2 + I_3) \leq -\alpha |x|^2 \end{aligned}$$

for an $\alpha > 0$ and all $|x|$ sufficiently large. Hence (2.12) is fulfilled with any $\varepsilon > 0$.

Remark 2.7. By Corollary 2.6 the invariant measure of the system (0.2) is stable

with respect to bounded perturbations of the coefficients, i.e., after addition of any bounded perturbation the new equation also possesses an invariant measure which differs little from the original one if the perturbation is sufficiently small.

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Souhrn

STABILITA INVARIANTNÍ MÍRY STOCHASTICKÉ DIFERENCIÁLNÍ ROVNICE POPISUJÍCÍ MOLEKULÁRNÍ ROTACI

BOHDAN MASLOWSKI

Je vyšetřována stabilita invariantní míry stochastické diferenciální rovnice vzhledem k omezeným perturbacím jejich koeficientů. Získané výsledky a některé dřívější autorovy výsledky o stabilitě Ljapunovského typu invariantní míry jsou aplikovány na systém popisující molekulární rotaci.

Резюме

УСТОЙЧИВОСТЬ ИНВАРИАНТНОЙ МЕРЫ STOCHASTИЧЕСКОГО ДИФФЕРЕНЦИАЛЬНОГО УРАВНЕНИЯ ОПИСЫВАЮЩЕГО МОЛЕКУЛЯРНОЕ ВРАЩЕНИЕ

BOHDAN MASLOWSKI

Исследуется устойчивость инвариантной меры стохастического дифференциального уравнения при ограниченных возмущениях его коэффициентов. В качестве применения этих и некоторых прежних результатов автора, касающихся устойчивости ляпуновского типа, рассматривается система описывающая молекулярное вращение.

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