Шумы и флуктуации в джозефсоновских системах
Лекция 1

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Цель данного курса - дать студентам и аспирантам, заинтересованным в исследовании случайных процессов в нелинейных системах, средство для решения практических задач стохастической динамики. В данном курсе рассматриваются только одномерные случайные процессы диффузионного типа. Математически это соответствует случаю одномерных непрерывных марковских процессов, описываемых уравнением Фоккера-Планка-Колмогорова. В дополнение к основам теории случайных процессов, будут описаны классические методы исследования уравнения Фоккера-Планка-Колмогорова, а также новые подходы, удобные для решения прикладных задач. В заключение курса будут описаны интересные индуцированные шумом эффекты в нелинейных системах, такие как стохастический резонанс, рэтчет эффект, эффект подавления шума переключающими сигналами, а также описаны прикладные задачи джозефсоновской электроники.

I. ВВЕДЕНИЕ

Шум является общим свойством различных процессов в физике, химии и биологии. Шум возникает при описании макроскопических систем. Если система включает в себя большое число степеней свобод, она является очень сложной и обычно при еч описании следят только за несколькими наиболее важными переменными. Остальные переменные не принимаются во внимание и поэтому объявляются "шумом"или "флуктуациями".

Исследование временных масштабов (или скоростей переходов) и эволюций вероятности в различных мультистабильных системах, находящихся под воздействием шума, является крайне важным большом числе направлений физики, таких как фазовые переходы, джозефсоновская электроника, магнитные системы. Одна из пионерских работ в этом направлении была выполнена Крамерсом [1]. Он рассмотрел процесс перехода из одного состояния системы в другое как процесс броуновской диффузии и использовал уравнение Фоккера-Планка-Колмогорова для плотности вероятности броуновской частицы для нахождения нескольких приближенных формул для описания скоростей перехода. Главный подход метода Крамерса - это предположение, что поток вероятности через потенциальный барьер мал, и в силу этого постоянен. Это условие применимо только в случае, когда потенциальный барьер достаточно высокий по сравнению с интенсивностью шума. Для получения точных временных масштабов и плотностей вероятности необходимо решить нестационарное уравнение Фоккера-Планка-Колмогорова, что является основной сложностью проблемы исследования переходных процессов диффузионного типа.

Уравнение Фоккера-Планка-Колмогорова - это уравнение в частных производных. В подавляющем большинстве случаев его аналитическое решение не известно. Также, в многомерном случае даже нахождение стационарного решения удачтся не всегда. Поэтому, при анализе динамики переходных процессов диффузионного типа, наиболее простым подходом является приближенное нахождение временных характеристик. Следует отметить, что нестационарное уравнение Фоккера-Планка-Колмогорова простой заменой переменных и заменой действительного времени на мнимое сводится к нестационарному уравнению Шредингера, так что при решении этих уравнений исследователь сталкивается с одними и теми же проблемами. Таким образом, теория случайных процессов в классических системах, и теория квантовых систем имеют много общего.

Рассматривая процесс одномерной броуновской диффузии (т.е. броуновское движение в пре-

деле большой вязкости), следует отметить, что для еч описания используются различные временные характеристики, описываемые различным образом (см. обзоры [2], [?] и книги [4],[5]), например время жизни метастабильного состояния, или время релаксации к стационарному состоянию. Часто используемый метод разложения решения в ряд по собственным функциям, когда характерный временной масштаб (время релаксации) предполагается равным обратному минимальному ненулевому собственному числу, неприменим для случая больших интенсивностей шума, поскольку тогда высшие собственные числа должны приниматься во внимание. В случае одномерного уравнения Фоккера-Планка-Колмогорова, моменты времени первого достижения (ВПД) поглощающей границы могут быть вычислены точно, по крайней мере могут быть выражены в квадратурах [6]. Но при методе ВПД предполагается наличие в системе поглощающих границ. Однако, в большом числе прикладных физических задач системы описываются гладкими потенциальными профилями, не имеющими поглощающих границ, и моменты ВПД могут дать некорректный результат для исследуемых временных масштабов.

Данный курс, в добавление к классическим методам, представит новые аналитические подходы для получения точных временных характеристик диффузионных процессов, позволяющие также в ряде случаев описать эволюцию вероятностей случайных процессов.

II. ДЕЛЬТА-ФУНКЦИЯ И ЕЕ ОСНОВНЫЕ СВОЙСТВА

Необходимым аппаратом для описания случайных процессов является аппарат обобщенных функций. Прежде всего, для представления дальнейшего материала нам потребуется обсудить свойства дельта-функции $\delta(x-a)$. Дельта-функция $\delta(x-a)$ равна нулю везде кроме точки $x=a$, в которой она принимает бесконечное значение. Дельта-функция может быть представлена как предельный случай гауссовского распределения:

$$\delta(x-a)=\lim_{D\to 0}\frac{1}{\sqrt{2\pi D}}e^{-\frac{(x-a)^2}{2D}}.$$

Дельта-функция $\delta(x-a)$ имеет следующие свойства:
1. Первое интегральное свойство.

$$\int\limits_{-\infty}^{+\infty}\delta(x-a)dx=1. \tag{1}$$

Следует отметить, что достаточно рассмотреть этот интеграл только в окрестности точки $x=a$:

$$\int\limits_{a-\epsilon}^{a+\epsilon}\delta(x-a)dx=1.$$

2. Функция единичного скачка обычно вводится в следующем виде:

$$1(x-a)\equiv\int\limits_{-\infty}^{x}\delta(y-a)dy=\begin{cases}1, & x>a\\ 1/2, & x=a\\ 0, & x<a\end{cases} \tag{2}$$

3. Дельта-функция является четной по отношению к точке a:

$$\int\limits_{-\infty}^{a}\delta(x-a)dx=\int\limits_{a}^{+\infty}\delta(x-a)dx=1/2. \tag{3}$$

4. Второе интегральное свойство:

$$\delta(x-a)f(x) = \delta(x-a)f(a),$$

$$\int\limits_{-\infty}^{+\infty} \delta(x-a)f(x)dx = f(a), \tag{4}$$

$$\int\limits_{-\infty}^{a} \delta(x-a)f(x)dx = \int\limits_{a}^{+\infty} \delta(x-a)dx = \frac{1}{2}f(a).$$

5. Если C - константа, то:

$$\delta[C(x-a)] = \frac{1}{|C|}\delta(x-a). \tag{5}$$

6. Если $\alpha(x)$ плавная функция и x_k - корни уравнения $\alpha(x) = 0$, расположенные в интервале (a, b) тогда (третье интегральное свойство):

$$\begin{gathered} \delta[\alpha(x)] = \sum_k \frac{\delta(x-x_k)}{|\alpha'_x(x)|_{x=x_k}}, \\ \int\limits_a^b f(x)\delta[\alpha(x)]dx = \sum_k \frac{f(x_k)}{|\alpha'_x(x)|_{x=x_k}}. \end{gathered} \tag{6}$$

7. Как выглядит производная дельта-функции? Можно легко взять производную нужного порядка от гауссовского распределения и устремить дисперсию D к нулю:

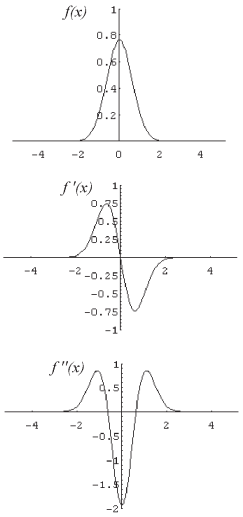

Рис. 1: Гауссовское распределение и его производные.

Четвертое интегральное свойство:

$$\begin{gathered} \int\limits_{-\infty}^{+\infty} \delta^{(n)}(x-y)g(x)dx = (-1)^n g^{(n)}(y), \\ \int\limits_{-\infty}^{+\infty} \delta^{(n)}(y-x)g(x)dx = g^{(n)}(y). \end{gathered} \tag{7}$$

III. СЛУЧАЙНАЯ ВЕЛИЧИНА И ОДНОМЕРНАЯ ПЛОТНОСТЬ ВЕРОЯТНОСТИ

We call ξ a random variable if the number ξ can not be predicted (for instance because of lack of initial conditions or of some other unknown factors). By repeating the experiment N times (N realizations) we obtain N numbers:

$$\xi_1, \xi_2, \ldots, \xi_N.$$

These numbers ξ_i may take either integer or continuous numbers.

Instead of repeating the experiment with one system N times we may also think that we have an ensemble of N identical systems and make one experiment for every system.

Whereas the numbers $\xi_1, \xi_2, \ldots, \xi_N$ can not be predicted, some averages for $N \to \infty$ may be predicted and should give the same value for identical systems. The simpleast average value is the mean value

$$< \xi >= \lim_{N\to\infty} \frac{1}{N}(\xi_1 + \xi_2 + \ldots + \xi_N).$$

A general average value is

$$< f(\xi) >= \lim_{N\to\infty} \frac{1}{N}(f(\xi_1) + f(\xi_2) + \ldots + f(\xi_N)). \tag{8}$$

where $f(\xi)$ is some arbitrary function.

Probability Density

If we choose the function in (8) the shifted step function

$$f(\xi) = 1(x - \xi) \tag{9}$$

we obtain

$$P(\xi < x) + (1/2)P(\xi = x) =< 1(x-\xi) >= \lim_{N\to\infty}[< 1(x-\xi_1) + \ldots + < 1(x-\xi_N)] = \lim_{N\to\infty} M/N. \tag{10}$$

The definition (10) differs from the usual one by a different weight of the probability at $\xi = x$. This is done because our definition of the step function (2). If we would have used $1(x) = 1$ for $x \geq 0$ and $1(x) = 0$ for $x < 0$ then the left hand side should be replaced by $P(\xi \leq x)$. For continuous processes (only such we will consider in the present course), where the probability to find the discrete value x is usually zero, both definitions agree.

In (10) M is the number of experiments (realizations) where $\xi \leq x$. Thus M/N is the relative frequency where the random variable is equal to or less than x. In the limit $N \to \infty$ this relative frequency is called the probability $P(\xi \leq x)$ that the random variable is equal to or less than x. It follows from (10) that $P(\xi \leq x)$ must be a nondecreasing function of x with $P(\xi \leq \infty) = 1$. The probability density function $W_\xi(x)$ of the random variable ξ is the derivative of P with respect to x

$$W_\xi(x) = \frac{d}{dx}P(\xi \leq x) = \frac{d}{dx} < 1(x - \xi) >=< \frac{d}{dx}1(x - \xi) >=< \delta(x - \xi) >, \tag{11}$$

where $\delta(x - \xi)$ is the Dirac delta function. The probability dP to find the continuous stochastic variable in the interval $x \leq \xi \leq x + dx$ is given by (assumong that P is differentiable):

$$P(\xi \leq x + dx) - P(\xi \leq x) = \frac{d}{dx}P(\xi \leq x)dx = W_\xi(x)dx.$$

The probability density (11) is usually a smooth function for continuous random variables.

The one-dimensional statistical properties of the random variable ξ are completely determined by by the probability density, because any average can be obtained from $W_\xi(x)$ by integration. This is seen as follows: because of the property (4) we get by taking averages

$$< f(\xi) >=< \int f(x)\delta(x-\xi)dx >= \int f(x) < \delta(x-\xi)dx >= \int f(x)W_\xi(x)dx. \tag{12}$$

- The stochastic variable was denoted as ξ, where as the variable in the distribution function was denoted as x. Further for simplicity we will omit the index ξ of the probabilities and the probability densities.

IV. TRANSFORMATION OF A RANDOM VARIABLE

If we use the random variable

$$\eta = g(\xi)$$

instead of the random variable ξ, the probability density $W_\eta(y)$ of the random variable η is, according to (11),(8), given by

$$W_\eta(y) =< \delta(y-\eta) >=< \delta(y-g(\xi)) >= \int \delta(y-g(\xi))W_\xi(x)dx. \tag{13}$$

The last integral is easily evaluated. If $g_n(y)$ is the n-th simple root of $g(x)-y=0$, then, following property (6) of the delta function one can get

$$W_\eta(y) = \sum_n \frac{W_{xi}(g_n(y))}{|g'_x(x)|_{x=x_n=g_n(y)}}. \tag{14}$$

Home exercise.

Please, calculate from the one-dimensional Maxwell distribution

$$W(v) = \sqrt{\frac{m}{2\pi kT}} \exp\left(-\frac{mv^2}{2kT}\right)$$

the probability density of the energy $E = \frac{1}{2}mv^2 = g(v)$.

V. RANDOM PROCESS AND ITS n-DIMENSIONAL PROBABILITY DENSITY

Definition: If for each instant of time t $\xi = \xi(t)$ represents a random variable then $\xi(t)$ is called as random (stochastic) process. Random variable is completely defined by setting its values and probability to take these values.

The one-dimensional (one-moment) probability density $W(x,t)$ of a random process is a single-parameter set of random values:

$$W(x,t)dx = P\{x \le \xi(t) \le x+dx\}, \quad \int_{-\infty}^{+\infty} W(x,t)dx = 1.$$

If one knows one-dimensional probability density, he can easily find averages:

$$< f[\xi(t)] >= \int_{-\infty}^{+\infty} f(x)W(x,t)dx.$$

Now let us consider the random process $\xi(t)$ at two different instants of time: $\xi(t_1)$ and $\xi(t_2)$. Then their ensemble is described by two-dimensional probability density $W(x_1, t_1; x_2, t_2)$. The probability

$$W(x_1, t_1; x_2, t_2)dx_1dx_2 = P\left\{ \begin{array}{l} x_1 \leq \xi \leq x_1 + dx_1) \\ x_2 \leq \xi \leq x_2 + dx_2) \end{array} \right\} \tag{15}$$

is the probability for realization of a random process to be at the time t_1 within the interval $(x_1, x_1 + dx_1)$ and at t_2 within $(x_2, x_2 + dx_2)$.

Further by inductance may be introduced n-dimensional probability density $W(x_1, t_1; \ldots; x_n, t_n)$. For $n \to \infty$ we get complete description of a random process. It is necessary to mention that from the point of view of rigorous mathematics we should know the functional of the probability density $W[x(t)]$.

Definition

Random processes having equal n-dimensional probability densities are called as equivalent.

Main properties of the probability density

1. Nonnegativity: $W(x_1, t_1; \ldots; x_n, t_n) \geq 0$.
2. Normalization: $\int\limits_{-\infty}^{+\infty} \ldots \int\limits_{-\infty}^{+\infty} W(x_1, t_1; \ldots; x_n, t_n)dx_1 \ldots dx_n = 1$.
3. Simmetricity: $W(x_1, t_1; x_2, t_2) \equiv W(x_2, t_2; x_1, t_1)$.
4. Consistency:

$$\int\limits_{-\infty}^{+\infty} \ldots \int\limits_{-\infty}^{+\infty} W(x_1, t_1; \ldots; x_n, t_n)dx_{m+1} \ldots dx_n = W(x_1, t_1; \ldots; x_m, t_m),$$

supernumerary parameters are automatically deleted.

VI. CONDITIONAL PROBABILITY DENSITIES OF RANDOM PROCESS

You probably remember one of the basic theorems of the probability theory about conditional probability. The same property takes place for n-dimensional (n-moment) probability densities. Let we have two-dimensional probability density $W(x_1, t_1; x_2, t_2)$. This probability density may be expressed as the product of one-dimensional probability density $W(x_1, t_1)$ and conditional one $W(x_2, t_2|x_1, t_1)$:

$$W(x_1, t_1; x_2, t_2) = W(x_1, t_1) \cdot W(x_2, t_2|x_1, t_1).$$

Thus, we introduce the conditional probability density as:

$$W(x_2, t_2|x_1, t_1) = \frac{W(x_1, t_1; x_2, t_2)}{W(x_1, t_1)}. \tag{16}$$

Here x_2 is real argument and t_2,t_1, x_1 are parameters of the conditional probability density. If we multiply $W(x_2, t_2|x_1, t_1)$ by dx_2, it is possible to say that this is the probability of a random process to be within the interval $(x_2, x_2 + dx_2)$ at the time t_2 if at the time t_1 it was at the point x_1:

$$W(x_2, t_2|x_1, t_1)dx_2 = P\left\{x_2 \leq \xi(t_2) \leq x_2 + dx_2|\xi(t_1) = x_1\right\}. \tag{17}$$

Main properties of the conditional probability density

1. Nonnegativity: $W(x_2, t_2|x_1, t_1) \geq 0$.
2. Normalization: $\int\limits_{-\infty}^{+\infty} W(x_2, t_2|x_1, t_1)dx_2 = 1$.

3. *Remark.* One can introduce

$$W(x_1,t_1|x_2,t_2)=\frac{W(x_1,t_1;x_2,t_2)}{W(x_2,t_2)},\quad t_2>t_1, \tag{18}$$

but this property is fulfilled for time-reversible processes only.

Using conditional probability density one can find conditional averages.

Some remarks about dependence of $W(x_2,t_2|x_1,t_1)$ *on time difference* t_2-t_1.

Values of a random process are independent if $W(x_1,t_1;x_2,t_2)=W(x_1,t_1)\cdot W(x_2,t_2)$, or, equivalently, if $W(x_2,t_2|x_1,t_1)=W(x_2,t_2)$.

For real processes having finite memory $W(x_2,t_2|x_1,t_1)\to W(x_2,t_2)$ for $t_2-t_1\to\infty$.

For real processes having continuous trajectories $W(x_2,t_2|x_1,t_1)\to\delta(x_2-x_1)$ for $t_2-t_1\to 0$.

Analogically to the conditional probability density $W(x_2,t_2|x_1,t_1)$ n-dimensional conditional probability densities may be introduced:

$$W(x_n,t_n|x_1,t_1;\ldots;x_{n-1},t_{n-1})=\frac{W(x_1,t_1;\ldots;x_n,t_n)}{W(x_1,t_1;\ldots;x_{n-1},t_{n-1})}. \tag{19}$$

Thus, we can write n-dimensional probability density $W(x_1,t_1;\ldots;x_n,t_n)$ as product of one-dimensional probability density and conditional probability densities:

$$W(x_1,t_1;\ldots;x_n,t_n)=$$
$$=W(x_1,t_1)\cdot W(x_2,t_2|x_1,t_1)\cdot W(x_3,t_3|x_1,t_1;x_2,t_2)\cdot\ldots\cdot W(x_n,t_n|x_1,t_1;\ldots;x_{n-1},t_{n-1}). \tag{20}$$

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[1] H. Kramers, Physica **7**, 284 (1940).

[2] P. Hanggi, P. Talkner and M. Borkovec, Rev. Mod. Phys., **62**, 251 (1990).

[3] A.N. Malakhov, A.L. Pankratov, Adv. Chem. Phys. **121**, 357 (2002).

[4] H. Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).

[5] C.W. Gardiner, Textbook of Stochastic methods (Springer-Verlag, 1985).

[6] L.A. Pontryagin, A.A. Andronov and A.A. Vitt, Zh. Eksp. Teor. Fiz. **3**, 165 (1933) [translated by J.B. Barbour and reproduced in "Noise in Nonlinear Dynamics 1989, edited by F. Moss and P.V.E. McClintock (Cambridge University Press, Cambridge) Vol. 1, p.329].

Stochastic processes and applications
Lecture 2

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I. FEW MODELS OF RANDOM PROCESSES

Random processes may be distinguished by conditional probability densities.

Absolutely random process.

Definition. Absolutely random process is a process whose values in different moments of time are absolutely statistically independent:

$$W(x_1, t_1; \ldots; x_n, t_n) = \prod_{i=1}^{n} W(x_i, t_i), \tag{1}$$

i.e. for complete description of absolutely random process it is enough to know only one-dimensional probability density. White noise is an example of absolutely random process.

If the time of inertion of the system τ_{sys} is much larger than the characteristic time of the process τ_p ($\tau_{sys} \gg \tau_p$) then the process may be treated as absolutely random process. One more name of absolutely random process is "process without memory":

$$W(x_n, t_n | x_1, t_1; \ldots; x_{n-1}, t_{n-1}) = W(x_n, t_n). \tag{2}$$

Further by inductance let us introduce more complicated processes.

Markov (Markovian) process.

Definition. The process $\xi(t)$ is Markov process if for any ordered n moments of time $t_1 < \ldots < t < \ldots < t_n$ n-dimensional conditional probability density depends only on the last fixed value:

$$W(x_n, t_n | x_1, t_1; \ldots; x_{n-1}, t_{n-1}) = W(x_n, t_n | x_{n-1}, t_{n-1}). \tag{3}$$

Markov processes are processes without aftereffect:

$$W(x_1, t_1; \ldots; x_n, t_n) = W(x_1, t_1) \prod_{i=2}^{n} W(x_i, t_i | x_{i-1}, t_{i-1}), \tag{4}$$

In detail Markov processes will be considered in further lectures.

General random processes.

Next one may consider processes where the conditional probability density depends only on the values of the random variable at the two latest times. In this case the complete information about the process is contained in $W(x_1, t_1; x_2, t_2; x_3, t_3)$. Hence we may continue, i.e. we may have process where the complete information is contained in $W(x_1, t_1; x_2, t_2; x_3, t_3; x_4, t_4)$ and so on. Due to Wang and Uhlenbeck [1], however, this further classification is not suitable to describe non-Markovian processes, i.e. processes where the complete information is not contained in W_2. For non-Markovian processes one may take into account besides $\xi(t) = \xi_1(t)$ more random variables $\xi_2(t)$, ..., $\xi_n(t)$. By a proper choice of these additional variables one may then have a Markov process for n random variables. Another possibility is the following. As you will see in the next lecture, the equation of motion of the probability density for continuous Markov process is the Fokker-Planck-Kolmogorov

equation. For non-Markovian processes one may then use generalized Fokker-Planck equations [2] which contain a memory function.

Quasi-deterministic random processes.

What is the deterministic process from the point of view of probabilistic description?

Let we have deterministic function $\xi(t) = s(t)$. For example, $s(t) = A_0 \cos(\omega_0 t + \varphi_0)$. In this case the one-dimensional probability density looks like: $W(x_1, t_1) = \delta(x_1 - s(t_1))$. Two-dimensional: $W(x_1, t_1; x_2, t_2) = \delta(x_1 - s(t_1))\delta(x_2 - s(t_2))$. And n-dimensional: $W(x_1, t_1; \ldots; x_2, t_2) = \prod_{i=1}^{n} \delta(x_i - s(t_i))$. Certainly, nobody describes deterministic processes by this way, but this approach gives an opportunity to describe quasi-deterministic random processes.

Definition. Quasi-deterministic random process is a process whose realization is described by the function of known form, containing one or some random parameters: $\xi(t) = s(t, \lambda)$; λ is random value described by the probability density $W_\lambda(\lambda)$.

How to find the n-dimensional probability density $W(x_1, t_1; \ldots; x_n, t_n)$? The conditional probability density for known λ is:

$$W(x_1, t_1; \ldots; x_n, t_n|\lambda) = \prod_{i=1}^{n} \delta(x_i - s(t_i, \lambda)).$$

First let us write $n + 1$-dimensional probability density:

$$W(x_1, t_1; \ldots; x_n, t_n; \lambda) = W_\lambda(\lambda) \cdot W(x_1, t_1; \ldots; x_n, t_n|\lambda).$$

The required n-dimensional probability density of quasideterministic process may be obtained by integration of $n + 1$-dimensional probability density:

$$W(x_1, t_1; \ldots; x_n) = \int_{-\infty}^{+\infty} W(x_1, t_1; \ldots; x_n, t_n; \lambda) d\lambda = \int_{-\infty}^{+\infty} W_\lambda(\lambda) \prod_{i=1}^{n} \delta(x_i - s(t_i, \lambda)).$$

Example. Consider process $\xi(t) = A_0 \cos(\omega_0 t + \varphi)$, where φ is random phase:

$$W_\varphi(\varphi) = \begin{cases} \frac{1}{2\pi}, & \varphi \in [0, 2\pi], \\ 0, & \varphi \ni [0, 2\pi]. \end{cases} \tag{5}$$

Its one-dimensional probability density is

$$W(x, t) = \int_{-\infty}^{+\infty} W_\varphi(\varphi) \delta[x - A_0 \cos(\omega_0 t + \varphi)] d\varphi.$$

II. CHARACTERISTIC FUNCTION OF A RANDOM PROCESS

The characteristic function is Fourier transformation of the probability density. One-dimensional characteristic function looks like:

$$\Theta(u, t) \equiv \int_{-\infty}^{+\infty} W(x, t) e^{jux} dx, \tag{6}$$

where $j = \sqrt{-1}$.

In n-dimensional case the characteristic function has the following form:

$$\Theta(u_1,t_1;\ldots;u_n,t_n)\equiv\int\limits_{-\infty}^{+\infty}\ldots\int\limits_{-\infty}^{+\infty}W(x_1,t_1;\ldots;x_n,t_n)e^{j(u_1x_1+\ldots+u_nx_n)}dx_1\ldots dx_n\equiv\left\langle e^{j\sum\limits_{i=1}^{n}u_ix_i}\right\rangle. \quad (7)$$

If the characteristic function is known, one can get the n-dimensional probability density:

$$W(x_1,t_1;\ldots;x_n,t_n)\equiv\frac{1}{(2\pi)^n}\int\limits_{-\infty}^{+\infty}\ldots\int\limits_{-\infty}^{+\infty}\Theta(u_1,t_1;\ldots;u_n,t_n)e^{-j(u_1x_1+\ldots+u_nx_n)}du_1\ldots du_n. \quad (8)$$

Main properties of characteristic function.

1. $\Theta(0,t_1;\ldots;0,t_n)=1$.
2. $|\Theta(u_1,t_1;\ldots;u_n,t_n)|\le|\Theta(0,t_1;\ldots;0,t_n)|=1$.
3. $\Theta(-u_1,t_1;\ldots;-u_n,t_n)=\Theta^*(u_1,t_1;\ldots;u_n,t_n)$.
4. $\Theta(u_1,t_1;\ldots;u_m,t_m)=\Theta(u_1,t_1;\ldots;u_m,t_m;0,t_{m+1};\ldots;0,t_n)$, $n>m$.
5. $\int\limits_{-\infty}^{\infty}\Theta(u_1,t_1;\ldots;u_n,t_n)e^{-j(u_1x_1+\ldots+u_nx_n)}du_1\ldots du_n\ge0$, for any x - the characteristic function is positively defined.

For absolutely random processes: $\Theta(u_1,t_1;\ldots;u_n,t_n)=\prod\limits_{i=1}^{n}\Theta(u_i,t_i)$.

III. MOMENT FUNCTIONS OF A RANDOM PROCESS

The simplest moment function is the mean value:

$$\alpha_1(t)\equiv<\xi(t)>\equiv\int\limits_{-\infty}^{+\infty}xW(x,t)dx.$$

The second moment function is the correlation function:

$$\alpha_2(t_1,t_2)\equiv K_\xi[t_1,t_2]\equiv<\xi(t_1)\xi(t_2)>\equiv\int\limits_{-\infty}^{+\infty}x_1x_2W(x_1,t_1;x_2,t_2)dx_1dx_2. \quad (9)$$

And so on, in general, the n-th moment function is:

$$\alpha_n(t_1,t_2,\ldots,t_n)\equiv<\xi(t_1)\xi(t_2)\ldots\xi(t_n)>.$$

The n-dimensional probability density should be known to find the n-th moment function.

Connection between the characteristic function and moment functions.

Let us expand the characteristic function $\Theta(u_1,t_1;\ldots;u_n,t_n)$ into Maclauren series:

$$\begin{aligned}\Theta(u_1,t_1;\ldots;u_n,t_n)=\Theta(0,t_1;\ldots;0,t_n)+\sum_{k=1}^{n}\left.\frac{\partial\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_k}\right|_{u_1,\ldots,u_n=0}u_k+\\+\frac{1}{2!}\sum_{k_1=1}^{n}\sum_{k_2=1}^{n}\left.\frac{\partial^2\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_{k_1}\partial u_{k_2}}\right|_{u_1,\ldots,u_n=0}u_{k_1}u_{k_2}+\ldots+\\+\frac{1}{s!}\sum_{k_1,\ldots,k_s=1}^{n}\left.\frac{\partial^s\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_{k_1}\ldots\partial u_{k_s}}\right|_{u_1,\ldots,u_n=0}u_{k_1}u_{k_2}\ldots u_{k_s}+\ldots\end{aligned} \quad (10)$$

The derivative of the characteristic function is directly connected to the corresponding moment function:

$$\left.\frac{\partial\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_k}\right|_{u_1,\ldots,u_n=0} =$$

$$\int\ldots\int W(x_1,t_1;\ldots;x_n,t_n)\cdot jx_k e^{j[(u_1x_1+\ldots+u_nx_n]}dx_1\ldots dx_n\Big|_{u_1,\ldots,u_n=0} = j<\xi(t_k)>. \qquad (11)$$

$$\left.\frac{\partial^s\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_{k_1}\ldots\partial u_{k_s}}\right|_{u_1,\ldots,u_n=0} = j^s<\xi(t_{k_1})\ldots\xi(t_{k_s})>=j^s\alpha_s(t_{k_1},\ldots,t_{k_s}). \qquad (12)$$

Thus, the characteristic function may be represented as an infinite moment expansion:

$$\Theta(u_1,t_1;\ldots;u_n,t_n) = 1+\sum_{s=1}^{\infty}\frac{j^s}{s!}\sum_{k_1,\ldots,k_s=1}^{n}\alpha_s(t_{k_1},\ldots,t_{k_s})u_{k_1}\ldots u_{k_s}. \qquad (13)$$

In this formula we used the first property of the characteristic function. For obtaining the characteristic function it is necessary to know n-dimensional moment functions of any order.

Central moment functions.

For simplicity, and because central moments are not widely used, we present here only one-dimensional central moment functions.

Central moments are defined as:

$$\mu_n(t) \equiv <(\xi(t)-<\xi(t)>)^n>,$$

$<\xi(t)>=\alpha_1(t)=m(t)$ is the mean value.

If $\alpha_1(t)=0$, then $\mu_n(t)=\alpha_n(t)$.

$$\mu_1(t) \equiv <(\xi(t)-<\xi(t)>)>=0,$$

$$\mu_2(t) \equiv <(\xi(t)-<\xi(t)>)^2> \equiv <\xi(t)^2-2\xi(t)<\xi(t)>+<\xi(t)>^2> \equiv$$
$$\equiv <\xi(t)^2>-<\xi(t)>^2=\alpha_2(t)-\alpha_1(t)^2=D(t),$$

i.e. the second central moment is variance.

Main characteristics of a random process are its mean $m(t)$ and variance $D(t)$. For normally distributed random values the mean and the variance completely define its one-dimensional probability density. If $W(x,t)$ is Gaussian (normal) distribution, then:

$$W(x,t)=\frac{1}{\sqrt{2\pi D(t)}}e^{-\frac{(x-m(t))^2}{2D(t)}}.$$

Thus, from previous two sections one can conclude that if all moments are known, then they can be summarized into the characteristic function and inverse Fourier transformed into the probability density. This is generally true, but not applicable in practice. Why? The answer is the following:

One example. Consider deterministic process. Its probability density is $W(x,t)=\delta(x-m(t))$. One can easily get all moments: $\alpha_1(t)=m(t)$, $\alpha_2(t)=m^2(t)$, ..., $\alpha_k(t)=m^k(t)$; $\mu_1(t)=\mu_2(t)=\ldots=\mu_k(t)=0$. Even in this simplest case all moments should be taken into account to obtain the required characteristic function (probability density). We can not stop summation of the infinite set

in formula (13) and I do not know examples of process which are described by finite set of moments. But in real tasks the result of summation of the set (13) is unknown.

Home exercise. In difference from real tasks the infinite set of moments in the above-mentioned example can be summarized. Please, obtain probability density of deterministic process using one more property of Dirac delta function that was not presented in the first lecture.

The representation of characteristic function via cumulants (semiinvariants) [3] (see also [2]) allows to avoid problems of summation of an infinite set, because there exists at least one class of processes that may be completely described by only two cumulants (Gaussian processes) and in many practical cases higher cumulants may be neglected and an infinite set may be approximately substituted by finite one.

IV. CUMULANT FUNCTIONS OF A RANDOM PROCESS

Cumulant functions are introduced as follows:

$$\ln\Theta(u_1,t_1;\ldots;u_n,t_n)\equiv\ln\Theta(0,t_1;\ldots;0,t_n)+\sum_{s=1}^{\infty}\frac{j^s}{s!}\sum_{k_1,\ldots,k_s=1}^{n}æ_s(t_{k_1},\ldots,t_{k_s})u_{k_1}\ldots u_{k_s},\qquad(14)$$

where $æ_s(t_{k_1},\ldots,t_{k_s})$ are cumulant functions of the s-th order (let us mention that the first term $\ln\Theta(0,t_1;\ldots;0,t_n)$ in (14) is obviously zero).

$$\left.\frac{\partial^s\ln\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_{k_1}\ldots\partial u_{k_s}}\right|_{u_1,\ldots,u_n=0}=j^s æ_s(t_{k_1},\ldots,t_{k_s}).$$

The characteristic function may be expressed as the set of cumulants in the following form:

$$\Theta(u_1,t_1;\ldots;u_n,t_n)\equiv\exp\left\{\sum_{s=1}^{\infty}\frac{j^s}{s!}\sum_{k_1,\ldots,k_s=1}^{n}æ_s(t_{k_1},\ldots,t_{k_s})u_{k_1}\ldots u_{k_s}\right\}.\qquad(15)$$

This representation is more useful than the analogous representation via moments.

Connection between cumulant and moment functions

$$æ_1(t_k)=\frac{1}{j}\left.\frac{\partial\ln\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_k}\right|_{u_1,\ldots,u_n=0}=\frac{1}{j}\left\{\frac{1}{\Theta(\ldots)}\frac{\partial\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_k}\right\}_{u_1,\ldots,u_n=0}=\alpha_1(t_k),$$

i.e. the first cumulant function is equal to the first moment function $æ_1(t_k)=\alpha_1(t_k)$, because $\Theta(\ldots)=1$ when its arguments equal zero $u_1=\ldots=u_n=0$.

$$æ_2(t_{k_1},t_{k_2})=\frac{1}{j^2}\left.\frac{\partial^2\ln\Theta(u_1,t_1;\ldots;u_n,t_n)}{\partial u_{k_1}u_{k_2}}\right|_{u_1,\ldots,u_n=0}=$$

$$=\frac{1}{j^2}\left\{-\frac{1}{\Theta^2(\ldots)}\frac{\partial\Theta(\ldots)}{\partial u_{k_1}}\frac{\partial\Theta(\ldots)}{\partial u_{k_2}}+\frac{1}{\Theta(\ldots)}\frac{\partial^2\Theta(\ldots)}{\partial u_{k_1}\partial u_{k_2}}\right\}_{u_1,\ldots,u_n=0}=\alpha_2(t_{k_1},t_{k_2})-\alpha_1(t_{k_1})\alpha_1(t_{k_2}).$$

The second cumulant function

$$æ_2(t_{k_1},t_{k_2})=\alpha_2(t_{k_1},t_{k_2})-\alpha_1(t_{k_1})\alpha_1(t_{k_2})\equiv B_\xi[t_{k_1},t_{k_2}]\qquad(16)$$

is known as covariation function. The covariation function in coinciding moments of time is variance: $B_\xi[t,t] = <\xi^2(t)> - <\xi(t)>^2 \equiv D(t) \equiv \sigma_\xi^2(t)$, where $\sigma_\xi(t)$ is the mean square deviation.

If $B_\xi[t_1,t_2] = 0$ for any moments of time, then such process is called as uncorrelated. In this case the correlation function (9) is equal to: $K_\xi[t_1,t_2] = <\xi(t_1)><\xi(t_2)>$.

There is often used normalized covariation function:

$$R_\xi[t_1,t_2] \equiv \frac{B_\xi[t_1,t_2]}{\sigma_\xi(t_1)\sigma_\xi(t_2)} \equiv \frac{B_\xi[t_1,t_2]}{\sqrt{B_\xi[t_1,t_1]B_\xi[t_2,t_2]}}.$$

Below (for simplicity in one-dimensional case) you may see relations between cumulants and moments of up to the sixth order.

Representation of the first six cumulants via moments looks like:

$$æ_1 = \alpha_1 = m,$$

$$æ_2 = \alpha_2 - \alpha_1^2 = D,$$

$$æ_3 = \alpha_3 - 3\alpha_1\alpha_2 + 2\alpha_1^3,$$

$$æ_4 = \alpha_4 - 3\alpha_2^2 - 4\alpha_1\alpha_3 + 12\alpha_1^2\alpha_2 - 6\alpha_1^4,$$

$$æ_5 = \alpha_5 - 5\alpha_1\alpha_4 - 10\alpha_2\alpha_3 + 20\alpha_1^2\alpha_3 + 30\alpha_1\alpha_2^2 - 60\alpha_1^3\alpha_2 + 24\alpha_1^5,$$

$$æ_6 = \alpha_6 - 6\alpha_1\alpha_5 - 15\alpha_2\alpha_4 + 30\alpha_1^2\alpha_4 - 10\alpha_3^2 + 120\alpha_1\alpha_2\alpha_3 - 120\alpha_1^3\alpha_3 + 30\alpha_2^3 - 270\alpha_1^2\alpha_2^2 + 360\alpha_1^4\alpha_2 - 120\alpha_1^6.$$

On the other hand, the representation of the first six moments via cumulants looks like:

$$\alpha_1 = æ_1,$$

$$\alpha_2 = æ_2 + æ_1^2,$$

$$\alpha_3 = æ_3 + 3æ_1æ_2 + æ_1^3,$$

$$\alpha_4 = æ_4 + 3æ_2^2 + 4æ_1æ_3 + 6æ_1^2æ_2 + æ_1^4,$$

$$\alpha_5 = æ_5 + 5æ_1æ_4 + 10æ_2æ_3 + 10æ_1^2æ_3 + 10æ_1^3æ_2 + 15æ_1æ_2^2 + æ_1^5,$$

$$\alpha_6 = æ_6 + 6æ_1æ_5 + 15æ_2æ_4 + 15æ_1^2æ_4 + 10æ_3^2 + 60æ_1æ_2æ_3 + 20æ_1^3æ_3 + 15æ_2^3 + 45æ_1^2æ_2^2 + 15æ_1^4æ_2 + æ_1^6.$$

From the above presented material we can conclude that first two cumulants (one-dimensional cumulant functions) have clear sense: the first one is the mean and the second one is the variance. For Gaussian distributions higher cumulants equal zero.

Not only two first cumulants have clear sense. Clear interpretation may be also given for the third and the fourth cumulants. The third cumulant $æ_3$ is called as "asymmetry" of distribution. Asymmetry is distinct from zero only for probability densities asymmetric relatively mean $æ_1$. The fourth cumulant $æ_4$ is called as excess. Excess of distribution is often describes deviation of the distribution from Gaussian one to sharper ($æ_4 > 0$) or more flat ($æ_4 < 0$) shape, however this is not always true (see [3]).

Quasimoments and Edgeworth series.

It is important to mention that cumulants æ$_3$, æ$_4$, æ$_5$,... describe the extent of deviation of the probability distribution from the Gaussian one. This gives an opportunity to quantitatively estimate this deviation and write arbitrary distribution as the set of Gaussian one and its derivatives.

Let us consider an arbitrary distribution $W(x)$, having in general all cumulants. Its characteristic function (15) may be presented in the following form:

$$\Theta(u) = \exp\left(jmu - \frac{D}{2}u^2\right)\left[1 + \sum_{k=3}^{\infty}\frac{(ju)^k}{k!}\beta_k\right]. \qquad (17)$$

where

$$\left[1 + \sum_{k=3}^{\infty}\frac{(ju)^k}{k!}\beta_k\right] \equiv \exp\left[\sum_{k=3}^{\infty}\frac{(ju)^k}{k!}æ_k\right].$$

Comparing this equality with the representation of characteristic function via moments (13) and via cumulants (15) (supposing one-dimensional case) it is easy to see that coefficients β_k represents nothing else as moments α_k calculated with the condition æ$_1$ = æ$_2$ = 0. Thus we get:

$$\beta_3 = æ_3,\ \beta_4 = æ_4,\ \beta_5 = æ_5,\ \beta_6 = æ_6 + 10æ_3^2, \ldots$$

and so on.

These coefficients are called as "quasimoments" of distribution. They are different from zero for non-Gaussian distributions only.

Performing Fourier transformation of formula (17) we get:

$$W(x) = W_G(x) + \sum_{k=3}^{\infty}(-1)^k\frac{\beta_k}{k!}W_G^{(k)}(x),$$

where $W_G^{(k)}(x)$ is the derivative of the Gaussian distribution of the k-th order. The obtained expansion is called as Edgeworth series. It gives an expansion of arbitrary probability density by derivatives of Gaussian distribution. In the case when higher cumulants are relatively small, only first four terms of expansion may be considered:

$$W(x) = W_G(x) - \frac{æ_3}{3!}W_G^{(3)}(x) + \frac{æ_4}{4!}W_G^{(4)}(x) - \frac{æ_5}{5!}W_G^{(5)}(x) + \frac{æ_6 + æ_3^2}{6!}W_G^{(6)}(x).$$

From this formula especial worth of cumulants æ$_3$, æ$_4$, æ$_5$, æ$_6$ is seen for estimation of deviation of the probability density from Gaussian one.

- It is necessary to mention that the Edgeworth series gives correct results for distributions close to Gaussian one and in some cases non-suitable use of the Edgeworth series may give probability densities significantly far from real one and even negative probability density.

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[1] M.C.Wang and G.E.Uhlenbeck, Rev. Mod. Phys., v. 17, p.323 (1945).

[2] H.Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).

[3] A.N.Malakhov, Cumulant analysis of random Non-Gaussian processes and its transformations (Sovetskoe Radio, Moscow, 1978, in Russian).

Stochastic processes and applications
Lecture 3

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I. CONTINUOUS MARKOV PROCESSES

If we will consider arbitrary random process, then for this process the conditional probability density $W(x_n, t_n|x_1, t_1; \ldots; x_{n-1}, t_{n-1})$ depends on x_1, x_2, ... x_{n-1}. This lead to definite "temporal connexity" of the process, to existence of strong aftereffect, and, finally, to more precise reflection of peculiarities of real smooth processes. However, mathematical analysis of such processes becomes significantly sophisticated, up to complete impossibility of their deep and detailed analysis. Because of this reason, some "tradeoff" models of random processes are of interest, which are simple in analysis and in the same time are correctly and satisfactory describe real processes. Namely such processes, having wide dissemination and recognition, are Markov processes.

Consider continuous Markov processes. Continuous process is characterized by the fact that during any small period of time Δt some small (of the order of $\sqrt{\Delta t}$) variation of state takes place.

Let us define continuous Markov process $x(t)$. Let us take in consecutive moments of time $t_1 < t_2 < \ldots < t_n$ values of random process $x_1 = x(t_1)$, $x_2 = x(t_2)$, ..., $x_n = x(t_n)$.

Definition. The process $x(t)$ is Markov process if for any ordered n moments of time $t_1 < \ldots < t < \ldots < t_n$ n-dimensional conditional probability density depends only on the last fixed value:

$$W(x_n, t_n|x_1, t_1; \ldots; x_{n-1}, t_{n-1}) = W(x_n, t_n|x_{n-1}, t_{n-1}). \tag{1}$$

Markov processes are processes without aftereffect. Thus, formula (20) of the first lecture may be written as:

$$W(x_1, t_1; \ldots; x_n, t_n) = W(x_1, t_1) \prod_{i=2}^{n} W(x_i, t_i|x_{i-1}, t_{i-1}). \tag{2}$$

Formula (2) contains only one-dimensional probability density $W(x_1, t_1)$ and the conditional probability density.

The term "transition probability" is closely connected with Markov processes. This term was introduced in physics without any connection to mathematical theory of random processes. The "transition probability" is related to such physical system, which state at the current moment completely defines its further evolution. "Transition probability" treates the probability of transition of the system from the state x_1 existing at the moment of time t_1 to the state x_2 at the next moment of time t_2. However, not for each system, subjected by random transitions, it was possible to introduce the term "transition probability". Here the independence of the probability of the next transition from history of states of the system was important. Thus, the term "transition probability" exists only for systems, the present state of which comprehensively determines the probabilities of next transitions.

Because for Markov processes formula (1) is fulfilled, then it is clear, that the probability density in the right hand side is nothing else as transition probability density from the state x_{n-1} to the state x_n during the time period between t_{n-1} and t_n.

Characteristic property of Markov process is that the initial one-dimensional probability density and the transition probability density completely determine Markov random process.

The transition probability density satisfy the following conditions:

1. The transition probability density is non-negative and normalized quantity:

$$W(x,t|x_0,t_0) \geq 0, \quad \int\limits_{-\infty}^{+\infty} W(x,t|x_0,t_0)dx = 1.$$

2. The transition probability density becomes Dirac delta function for coinciding moments of time (physically this means small variation of the state during small period of time):

$$\lim_{t \to t_0} W(x,t|x_0,t_0) = \delta(x - x_0).$$

3. The transition probability density fulfill Smoluchowski equation:

   Let we have at the moment t_0: $x(t_0) = x_0$. We are looking for probability to find random process at t_1 in the interval $(x_1, x_1 + dx_1)$ and at t_2 in the interval $(x_2, x_2 + dx_2)$. Let us remind that $P\{x_2 < x(t_2) < x_2 + dx_2 | x(t_0) = x_0\} = W(x_2,t_2|x_0,t_0)dx_2$. Following the condition that the process $x(t)$ is Markov process we have that $W(x_1,t_1|x_0,t_0)dx_1$ and $W(x_2,t_2|x_1,t_1)dx_2$ are statistically independent. For transition probability density the Smoluchowski equation takes place (in western literature Chapman-Kolmogorov equation):

$$W(x_2,t_2|x_0,t_0) = \int\limits_{-\infty}^{+\infty} W(x_2,t_2|x_1,t_1)W(x_1,t_1|x_0,t_0)dx_1. \tag{3}$$

   One can easily see the correctness of this equation. On the basis of (2) we can write:

$$\int\limits_{-\infty}^{+\infty} W_3(x_2,t_2;x_1,t_1;x_0,t_0)dx_1 = W(x_0,t_0) \int\limits_{-\infty}^{+\infty} W(x_2,t_2|x_1,t_1)W(x_1,t_1|x_0,t_0)dx_1.$$

   Because of condition of consistency of the probability density (see lecture 1) the left integral is equal to two-dimensional probability density, which may be expressed from the transition probability density as:

$$W_2(x_2,t_2;x_0,t_0) = W(x_0,t_0)W(x_2,t_2|x_0,t_0).$$

   Equating right parts of these equalities we get Smoluchowski equation (3).

If initial probability density $W(x_0,t_0)$ is known and the transition probability density $W(x,t|x_0,t_0)$ has been obtained then one can easily get one-dimensional probability density in arbitrary instant of time:

$$W(x,t) = \int\limits_{-\infty}^{\infty} W(x_0,t_0)W(x,t|x_0,t_0)dx_0. \tag{4}$$

Which equation can describe Markov process? We now know all properties of Markov process and can guess that Markov process should be described by a first order differential equation, because only a first order differential equation is uniquely determined by its initial value. Markov process is a random process, thus equation, describing this process should contain a noise source. But which characteristics should the noise source have? This can be only absolutely random (δ-correlated) process, because only for such process at former moments of time the conditional probability density at later moments of time will not be changed.

II. BROWNIAN MOTION IN A FIELD OF FORCE AND LANGEVIN EQUATION

In the most general case Brownian motion in a field of force is described by simple dynamic equation with noise source:

$$\frac{m}{h}\frac{d^2x(t)}{dt^2} + \frac{dx(t)}{dt} = -\frac{d\Phi(x)}{hdx} + \xi(t). \tag{5}$$

where $\xi(t)$ may be treated as white Gaussian noise (Langevin force), $<\xi(t)>=0$, $<\xi(t)\xi(t+\tau)>= D(x,t)\delta(\tau)$, $\Phi(x)$ is a potential profile, m is a mass of Brownian particle and h is viscosity. But this is second order equation which describes not Markov process itself, but a set of two Markov processes: $x(t)$ and $dx(t)/dt$. Restricting present course by consideration of only Markov processes we will call as Langevin equation the limiting case of the above-mentioned equation (for $m/h \to 0$), that in physical interpretation corresponds to overdamped Brownian motion:

$$\frac{dx(t)}{dt} = -\frac{d\Phi(x)}{hdx} + \xi(t), \tag{6}$$

Often, instead of potential, one can speak about drift coefficient $a(x) = -\frac{d\Phi(x)}{hdx}$. If the diffusion coefficient $D(x,t)$ does not depend on x, then eq. (6) is called a Langevin equation with an additive noise source. For $D(x,t)$ depending on x one speaks of a Langevin equation with multiplicative noise source. This distinction between additive and multiplicative noise may not be considered very significant because for the one-variable case (6), for time-independent drift and diffusion coefficients and for $D(x,t) \neq 0$, the multiplicative noise always becomes an additive noise by a simple transformation of variables [2].

Equation (6) is stochastic differential equation. Some required characteristics of stochastic process may be obtained even from this equation either by cumulant analysis technique or by other methods, presented in detail in [1].

But the most powerful methods of obtaining the required characteristics of stochastic processes are associated with the use of the Fokker-Planck-Kolmogorov equation for the transition probability density.

III. THE FOKKER-PLANCK-KOLMOGOROV EQUATION

The transition probability density of continuous Markov process satisfy to the following partial differential equations:

$$\frac{\partial W(x,t|x_0,t_0)}{\partial t} = \left\{\frac{\partial}{\partial x}\left[-a(x,t)W(x,t|x_0,t_0)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[D(x,t)W(x,t|x_0,t_0)\right]\right\} \tag{7}$$

$$\frac{-\partial W(x,t|x_0,t_0)}{\partial t_0} = \left\{a(x_0,t_0)\frac{\partial}{\partial x_0}W(x,t|x_0,t_0) + \frac{1}{2}D(x_0,t_0)\frac{\partial^2}{\partial x_0^2}W(x,t|x_0,t_0)\right\} \tag{8}$$

Equation (7) is called as the Fokker-Planck-Kolmogorov equation (FPKE) or forward Kolmogorov equation, because it contains time derivative of final moment of time $t > t_0$. In western literature this equation is also known as Smoluchowski equation. The second equation (8) is called as backward Kolmogorov equation, because it contains time derivative of initial moment of time $t_0 < t$. These names are associated with the fact that the first equation used Fokker (1914) and Planck (1917)

for description of Brownian motion, but Kolmogorov was first who gave rigorous mathematical argumentation for eq. (7) and he was first who obtained eq. (8).

Let us obtain equations (7) and (8), supposing that all operations that we will use (existing of limits, derivation, integration and so on) are valid.

For obtaining forward Kolmogorov equation (7) we should in the Smoluchowski equation (3) take the medium instant of time t' close to the final instant t and for obtaining of backward Kolmogorov equation (8) - close to initial instant t_0. Because all mathematical calculations are identical in both cases, we consider only how to get forward Kolmogorov equation.

Let us write Smoluchowski equation (3) in the following form:

$$W(x,t+\Delta t|x_0,t_0)=\int\limits_{-\infty}^{+\infty}W(x,t+\Delta t|x',t)W(x',t|x_0,t_0)dx', \quad t+\Delta t>t>t_0, \tag{9}$$

where the time interval Δt is supposed to be small.

Let us introduce into consideration the conditional characteristic function $\Theta(\Omega,t+\Delta t|x',t)$ of random increment $(x-x')$ during small period Δt with the condition that x' is fixed. By the definition of the characteristic function we have:

$$\Theta(\Omega,t+\Delta t|x',t)=<\exp\{j\Omega(x-x')\}|x',t>=\int\limits_{-\infty}^{+\infty}\exp\{j\Omega(x-x')\}W(x,t+\Delta t|x',t)dx.$$

According to inverse Fourier transformation we can write:

$$W(x,t+\Delta t|x',t)=\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}\exp\{-j\Omega(x-x')\}\Theta(\Omega,t+\Delta t|x',t)d\Omega. \tag{10}$$

Decomposing the conditional characteristic function into Taylor expansion we get:

$$\Theta(\Omega,t+\Delta t|x',t)=\sum_{n=0}^{\infty}\frac{m_n(x',t)}{n!}(j\Omega)^n, \tag{11}$$

where $m_n(x',t)=<\{x(t+\Delta t)-x'(t)\}^n|x'(t)>$ are conditional moments of increment $x-x'$ during the time Δt

$$m_n(x',t)=\int\limits_{-\infty}^{+\infty}(x-x')^nW(x,t+\Delta t|x',t)dx.$$

If we substitute formula (11) in formula (10) and make some transformations, then we get:

$$W(x,t+\Delta t|x',t)=\sum_{n=0}^{\infty}(-1)^n\frac{m_n(x',t)}{n!}\frac{\partial^n}{\partial x^n}\delta(x'-x). \tag{12}$$

Substituting this expression into Smoluchowski equation (3) and performing integration with delta function we get:

$$W(x,t+\Delta t|x_0,t_0)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}(m_n(x,t)W(x,t|x_0,t_0)). \tag{13}$$

or

$$W(x,t+\Delta t|x_0,t_0)-W(x,t|x_0,t_0)=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}(m_n(x,t)W(x,t|x_0,t_0)). \tag{14}$$

Dividing both parts of this differential equation by Δt and transiting to the limit for $\Delta t\to 0$, we get:

$$\frac{\partial}{\partial t}W(x,t|x_0,t_0)=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}(K_n(x,t)W(x,t|x_0,t_0)), \tag{15}$$

where

$$K_n(x,t)=\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int(x(t+\Delta t)-x(t))^nW(x,t+\Delta t|x,t))dx. \tag{16}$$

It is necessary to point that equation (15), which was obtained only using the formula of total probability, is valid for arbitrary random processes, for which coefficients $K_n(x,t)$ exist.

Consider now one particular, but important case of the obtained equation (15), when first two coefficients are not zero, but further coefficients $K_n(x,t)$ for $n\geq 3$ are equal to zero:

$$K_n(x,t)\neq 0,\quad n=1,2;\qquad K_n(x,t)=0,\quad n\geq 3. \tag{17}$$

Markov processes, satisfying these conditions are called as diffusive processes.

As it follows from (16), the condition (17) characterizes the speed of decrease of the probability with decrease of Δt. There are possible fast enough variations of the process $x(t)$ but in opposite directions. That is why the average increment of the process during small interval Δt is of the order of $\sqrt{\Delta t}$. Thus, the fulfillment of the condition (17) is enough for continuous random process $x(t)$ to be Markov diffusive process.

Thus, for diffusive Markov processes equation (15) is simplifying and transit to the Fokker-Planck-Kolmogorov equation. Consequently, drift and diffusion coefficients are: $a(x,t)=K_1(x,t)$, $D(x,t)=K_2(x,t)$.

Both partial differential equations (7) and (8) are linear and of the parabolic type. The solution of these equations should be nonnegative and normalized to unity. Besides, this solution should satisfy to the initial condition:

$$W(x,t|x_0,t_0)=\delta(x-x_0). \tag{18}$$

Let us focus at the time on equation (7) as much widely used than (8) and discuss boundary conditions and methods of solution of this equation.

The solution of equation (7) for infinite interval and delta-shaped initial distribution is called as fundamental solution of Cauchy problem. If initial value of Markov process is not fixed, but distributed with the probability density $W_0(x)$, then as initial condition should be indicated this probability density:

$$W(x,t_0)=W_0(x). \tag{19}$$

In this case the one-dimnesional probability density $W(x,t)$ may be obtained by two different ways.

1. The first way is obtaining the transition probability density by the solution of equation (7) with delta-shaped initial distribution and after that averaging it over initial distribution $W_0(x)$, see formula (4).

2. The second way is obtaining the solution of equation (7) for one-dimensional probability density with the initial distribution (19). Indeed, multiplying (7) by $W(x_0,t_0)$ and integrating by x_0 taking into account (4) we get the same Fokker-Planck-Kolmogorov equation (7).

Thus, one-dimensional probability density of Markov process fulfill the Fokker-Planck-Kolmogorov equation and for delta-shaped initial distribution coincide with the transition probability density. Later we sometimes instead of transition probability density will speak about one-dimensional probability density with initial delta-shaped distribution.

For solution of real tasks, depending on concrete set up of the task, may be used either forward or backward Kolmogorov equation. If the one-dimensional probability density with known initial distribution deserves interest, then it is naturally to use the forward Kolmogorov equation. Contrariwise, if it is necessary to calculate distribution of the Mean First Passage Time as function of initial state x_0 then one should use the backward Kolmogorov equation.

Boundary conditions.

For obtaining the solution of the Fokker-Planck-Kolmogorov equation, besides initial condition one should know boundary conditions. Boundary conditions may be quite diverse and determined by essence of the task. Enough complete representation of boundary conditions the reader may find in [1].

Let us discuss four main types of boundary conditions: reflecting, absorbing, periodic, and the so called natural boundary conditions as much wider used than others, especially for computer simulations.

First of all we should mention that the Fokker-Planck-Kolmogorov equation may be represented as continuity equation:

$$\frac{\partial W(x,t)}{\partial t} + \frac{\partial G(x,t)}{\partial x} = 0. \tag{20}$$

Here $G(x,t)$ is the probability current:

$$G(x,t) = a(x,t)W(x,t) - \frac{1}{2}\frac{\partial}{\partial x}\left[D(x,t)W(x,t)\right]. \tag{21}$$

Reflecting boundary. Reflecting boundary may be represented as infinitely high potential wall. Use of the reflecting boundary assume that there is no probability current behind the boundary. Mathematically reflecting boundary condition is written as:

$$G(d,t) = 0, \tag{22}$$

where d is the boundary point. Any trajectory of random process is reflected when it contacts the boundary.

Let us consider example of Markov process evolution under the influence of the force $a(x,t) = -c$ (linear potential). If we will locate the reflecting boundary at the point $x = 0$, the time evolution of the transition probability density will be as presented in Fig. 1. For this particular example one can see the effect, called as transition bi-modality. In spite that we have the potential with only one minimum at the point $x = 0$, which will lead to uni-modal steady-state probability distribution and initial distribution was also uni-modal (delta-shaped), we can see bi-modal distribution of transition probability density for some moments of time. This is due to the backward effect of the reflecting boundary on the probability density.

Absorbing boundary. Absorbing boundary may be represented as infinitely deep potential well just behind the boundary. Mathematically absorbing boundary condition is written as:

$$W(d,t) = 0, \tag{23}$$

where d is the boundary point. Any trajectory of random process is captured by the absorbing boundary when it crosses the boundary and is not considered in the preboundary interval. If you have, say, one reflecting and one absorbing boundaries then eventually the whole probability will be captured by the absorbing boundary and if you consider the probability density only in the interval between two boundaries then you can guess that the normalization condition is not fulfilled (see Fig. 2). If, however, you will think that the absorbing boundary is nothing else as an infinitely deep potential well, and will take it into account, then total probability density (in pre-boundary region and behind it) will be normalized.

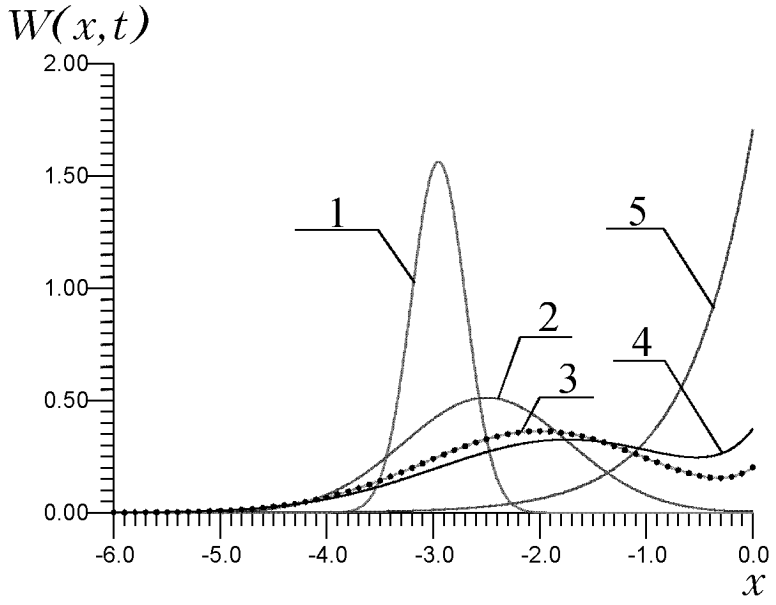

FIG. 1. Probability distribution in linear potential with reflecting boundary. Time evolution from 1 to 5.

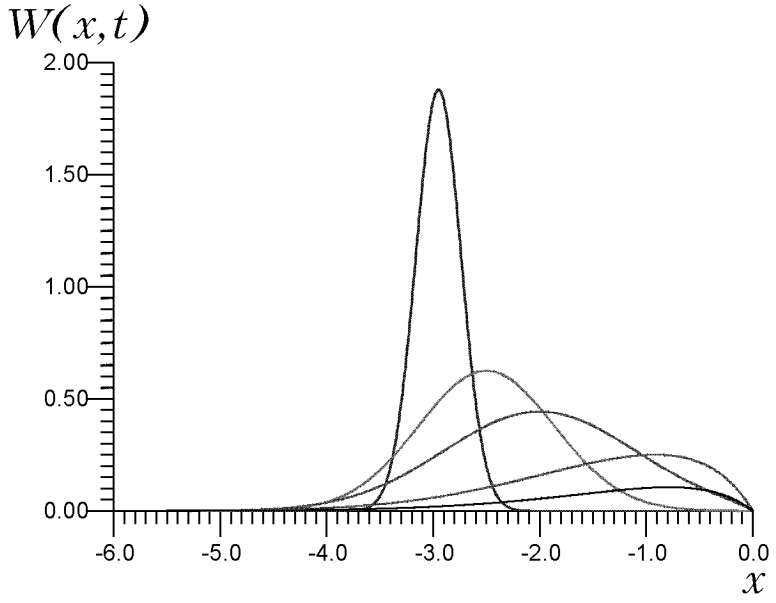

FIG. 2. Probability distribution in linear potential with absorbing boundary.

Periodic boundary condition.

If you consider Markov process in periodic potential, then the condition of periodicity of the probability density may be treated as boundary condition:

$$W(x,t) = W(x+2\pi,t). \tag{24}$$

The use of this boundary condition is especially comfortable for computer simulations.

Natural boundary conditions. If you consider Markov process in infinite interval, then boundary conditions at $\pm\infty$ are called as natural. There are two possible situations. If the considered potential at $+\infty$ or $-\infty$ tends to $-\infty$ (infinitely deep potential well) then the absorbing boundary should be supposed at $+\infty$ or $-\infty$, respectively. If, however, the considered potential at $+\infty$ or $-\infty$ tends to $+\infty$ then it is naturally to suppose the reflecting boundary at $+\infty$ or $-\infty$, respectively.

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[1] C.W.Gardiner, Handbook of Stochastic methods (Springer-Verlag, 1985).
[2] H.Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).
[3] R.L.Stratonovich, Topics of the Theory of Random Noise (Gordon and Breach, New York, 1963).

Stochastic processes and applications
Lecture 4

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I. METHODS OF SOLUTION OF THE FOKKER-PLANCK-KOLMOGOROV EQUATION

In the present lecture we consider methods of solution of nonstationary and stationary Fokker-Planck-Kolmogorov equation (1) with constant in time drift and diffusion coefficients, i.e. methods of obtaining of temporal dynamics of the probability density $W(x,t)$ and its steady-state distribution. We will not consider singular diffusion Markov processes, for which the diffusion coefficient vanishes near a boundary of the considered interval.

1. Stationary solution of the Fokker-Planck-Kolmogorov equation.

For one-dimensional Markov processes one can easily find in many cases the steady-state probability density. If we consider the case when the drift and the diffusion coefficients are constant in time, then for steady-state the transition probability density $W(x,t|x_0,t_0)$ depends only on the difference of considered moments of time. One dimensional steady-state probability density $W_{st}(x) = \lim\limits_{t\to\infty} W(x,t)$, if it is exist, is absolutely independent of time and initial distribution $W_0(x)$. That is why for a steady-state $\partial W_{st}(x)/\partial t = 0$ and, thus, $G(x) = G = const$.

The steady-state probability distribution may be easily obtained as a solution of the Fokker-Planck-Kolmogorov equation

$$\frac{\partial W(x,t)}{\partial t} = \left\{ \frac{\partial}{\partial x}\left[-a(x)W(x,t)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[D(x)W(x,t)\right] \right\} \tag{1}$$

with the condition that $\partial W(x,t)/\partial t = 0$. Indeed, then we get linear ordinary differential equation of the second order:

$$\left\{ \frac{\partial}{\partial x}\left[-a(x)W_{st}(x)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[D(x)W_{st}(x)\right] \right\} = 0. \tag{2}$$

For example, if we consider the case of zero probability current $G = 0$ at boundaries, integrating this equation twice we get:

$$W_{st}(x) = \frac{C}{D(x)} \exp\left[2\int\limits_{x'}^{x} \frac{a(x)}{D(x)} dx \right], \tag{3}$$

where C is determined from normalization condition. For a constant diffusion coefficient $D(x) = D = const$ we get even more simple formula:

$$W_{st}(x) = \frac{C}{D} \exp\left[-\frac{2\Phi(x)}{hD} \right]. \tag{4}$$

where we have substituted the drift coefficient by the derivative of potential $a(x) = -\frac{d\Phi(x)}{hdx}$, here h is damping (viscosity).

Thus, if we can determine from the equation, describing the behavior of the system, the drift and diffusion coefficients, then in some cases it is possible to immediately write the expression for one-dimensional steady-state probability density. This demonstrates the effectiveness of the use of the Fokker-Planck-Kolmogorov equation.

2. **Method of eigenfunction and eigenvalue analysis.**

The method of eigenfunction and eigenvalue analysis is the most widely used method is western literature. This method is comfortable to use in cases when both drift and diffusion coefficients do not depend on time. In this case the Fokker-Planck-Kolmogorov equation takes the form (1).

We will search for a solution in the form:

$$W(x,t) = X(x) \cdot T(t), \tag{5}$$

where X and T are functions of coordinate and time, respectively. Dividing both parts of equation (1) by (5) we get:

$$\frac{1}{T(t)}\frac{\partial T(t)}{\partial t} = \left\{-\frac{\partial}{\partial x}\left[a(x)X(x)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[D(x)X(x)\right]\right\} X^{-1}(x). \tag{6}$$

The left part of (6) depends only on t, while the right one depends only on x. Therefore both parts are equal to the same constant which we define as $-\gamma$, $\gamma \geq 0$. Thus, from equation (6) we get two ordinary differential equations:

$$\frac{1}{T(t)}\frac{\partial T(t)}{\partial t} = -\gamma, \tag{7}$$

$$\left\{\frac{\partial}{\partial x}\left[-a(x)X(x)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[D(x)X(x)\right]\right\} = -\gamma X(x). \tag{8}$$

Simple equation of the first order (7) has the solution

$$T(t) = e^{-\gamma t}, \tag{9}$$

and the solution of linear second order equation (8) may be found by known methods of solution of ordinary differential equations with variable coefficients. This solution $X(x, A, B, \gamma)$ depends on two arbitrary constants A and B. Since equation (1) is linear, the general solution has the form:

$$W(x,t) = \sum_{n=0}^{\infty} X(x, A_n, B_n, \gamma_n) e^{-\gamma_n t}, \tag{10}$$

where constants A_n, B_n. and γ_n are defined by initial and boundary conditions.

It can be demonstrated (see [1]) that if difference of currents $G(x,t)$ through boundaries is equal to zero, then the solution (10) can be represented in the form:

$$W(x,t) = T_0 W_{st}(x) + \sum_{n=1}^{\infty} X_n(x) T_n e^{-\gamma_n (t-t_0)}, \tag{11}$$

where $X_n(x)$ are eigenfunctions of equation (8) corresponding to eigenvalues γ_n, T_n are constant coefficients. Functions $X_n(x)$ are orthonormalized with the weight $\dfrac{1}{W_{st}(x)}$:

$$\int \frac{X_m(x) X_n(x) dx}{W_{st}(x)} = \delta_{mn} = \begin{cases} 1, & m = n, \\ 0, & m \neq n. \end{cases}$$

If the initial probability density is known, $W(x,t_0) = W_0(x)$, then coefficients T_n are defined by the following expression:

$$T_n = \int \frac{W_0(x) X_n(x)}{W_{st}(x)} dx.$$

If initial probability density is Dirac delta function, $W_0(x) = \delta(x - x_0)$, then the solution (10) has the form:

$$W(x,t) = W(x,t|x_0,t_0) = \sum_{n=0}^{\infty} \frac{X_n(x) X_n(x_0)}{W_{st}(x_0)} e^{-\gamma_n (t-t_0)},$$

where $X_0(x) = W_{st}(x)$ and $\gamma_0 = 0$.

3. **Method of Laplace transformation.**

The sense of application of Laplace transformation to the FPKE is eliminating of time variable t that allows to reduce partial differential equation to ordinary differential equation. The Laplace transformation method is usually used when drift and diffusion coefficients of the FPKE are constant in time.

Let us denote the Laplace transformation of the function $W(x,t)$ as:

$$Y(x,s) = \int_0^{\infty} W(x,t) e^{-st} dt.$$

Applying rules of Laplace transformation (see, e.g., [4] or its translations) to equation (1) we get:

$$sY(x,s) - W_0(x) = \left\{ -\frac{d}{dx} \left[a(x) Y(x,s) \right] + \frac{1}{2} \frac{d^2}{dx^2} \left[D(x) Y(x,s) \right] \right\}. \tag{12}$$

Here $W_0(x)$ is initial probability distribution.

Equation (12) is heterogeneous ordinary differential equation of the second order. The initial condition is inserted into equation (12). Boundary conditions for function $W(x,t)$ transform into boundary conditions for the function $Y(x,s)$ and should be taken into account when solving equation (12).

When the solution of eq. (12) is found, the probability density $W(x,t)$ may be obtained using inverse Laplace transformation.

Let us mention, that namely on the basis of Laplace transformation method recently were elaborated new powerful approaches, that will be presented in further lectures. But solution of equation (12) itself is very complicated task. Say, if you will consider process of Brownian diffusion in piecewise parabolic potentials, then the solution of equation (12) will be expressed via special functions - Weber (parabolic cylinder) functions [5]. For more complicated potentials the special functions are unknown (but may be obtained, I did it for potentials of the fourth order). Thus, there is no hope at the present time that one can get exact probability density using inverse Laplace transformation from the solution of eq. (12) (except few simplest cases of purely parabolic or linear potentials).

4. **Method of characteristic function.**

Sometimes it is possible to get simplification by the transition in equation (1) from probability density $W(x,t)$ to characteristic function:

$$\Theta(u,t) = \int\limits_{-\infty}^{+\infty} W(x,t)e^{jux}dx. \tag{13}$$

Usually this may be performed using the following procedure. After substitution of concrete drift $a(x,t)$ and diffusion $D(x,t)$ coefficients, both sides of equation (1) first are multiplied by e^{jux} and integrated over x (or one can directly use rules of Fourier transformation if possible). The initial condition may be found by substitution of initial probability density $W_0(x)$ into (13). Namely this approach is called as method of characteristic function.

5. **Method of exchange of independent variables.**

There also may be used the method of exchange of independent variables for solution of the FPKE. The aim of this method is to reduce the FPKE to the diffusion equation (see example below), describing dynamics of the so-called Wiener process. But there is exist the theorem by Cherkasov, proving that necessary transformation of variables may be done only for restricted class of drift and diffusion coefficients, for example for such that: $a(x,t) = b(t)x + f(t)$, $D(x,t) = F(t)$.

6. **Explicit difference scheme.**

At the present time, when we have strong computers, the FPKE may be easily solved numerically. There are many different methods of numeric solution of the FPKE, e.g., explicit difference scheme, implicit difference scheme, method of matrix continued fractions. We consider the most simple method - explicit difference scheme. This scheme is the most slow, but may be easily understood and, besides, it is not a serious problem to correctly write boundary conditions for this scheme.

Let we need to get a solution of the FPKE with initial condition $W(x,t_0) = W_0(x)$. Consider the net of nodes, located in points of crosses of two families of parallel lines:

$$x = c + ih, \quad (i = 0,1,...,N; \quad N = (d-c)/h, \quad t = jl, \quad (j = 0,1,...).$$

Nodes, located at the lines $x = c$, $x = d$, $t = 0$ we will call boundary nodes, all other nodes are internal. For each internal node (i,j) let us write difference scheme, approximating with some precision the FPKE. Previously, let us note, that the FPKE may be presented in the form:

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{2}D(x,t)\frac{\partial^2}{\partial x^2}W(x,t) + \left[\frac{\partial}{\partial x}D(x,t) - a(x,t)\right]\frac{\partial}{\partial x}W(x,t) + \\ + \left[\frac{1}{2}\frac{\partial^2}{\partial x^2}D(x,t) - \frac{\partial}{\partial x}a(x,t)\right]W(x,t). \tag{14}$$

In equation (14) we can approximately substitute derivatives by differences in the following form:

$$\frac{\partial W(x,t)}{\partial x} \approx \frac{W_{i+1,j} - W_{i-1,j}}{2h}, \tag{15}$$

$$\frac{\partial^2 W(x,t)}{\partial x^2} \approx \frac{W_{i+1,j} - 2W_{i,j} + W_{i-1,j}}{h^2}, \tag{16}$$

where $W_{i,j} = W(c + ih, jl)$. The time derivative we substitute by difference forward relation:

$$\frac{\partial W(x,t)}{\partial t} \approx \frac{W_{i,j+1} - W_{i,j}}{l}. \tag{17}$$

Substituting (15), (16), (17) into (14), we get:

$$W_{i,j+1} = \alpha_{i,j}W_{i+1,j} + \beta_{i,j}W_{i,j} + \gamma_{i,j}W_{i-1,j} \quad (j \geq 0), \tag{18}$$

where

$$\begin{aligned} \alpha(x,t) &= \frac{l}{2h^2}D(x,t) + \frac{l}{2h}\left[\frac{1}{2}\frac{\partial^2}{\partial x^2}D(x,t) - a(x,t)\right], \\ \beta(x,t) &= 1 - \frac{l}{h^2}D(x,t) + l\left[\frac{1}{2}\frac{\partial^2}{\partial x^2}D(x,t) - \frac{\partial}{\partial x}a(x,t)\right], \\ \gamma(x,t) &= \frac{l}{2h^2}D(x,t) - \frac{l}{2h}\left[\frac{\partial}{\partial x}D(x,t) - a(x,t)\right]. \end{aligned} \tag{19}$$

Difference scheme (19) contains values of solution in four nodes, one at the current moment of time and three at the previous one. This scheme approximates FPKE equation (14) with the precision $O(l + h^2)$.

In the first iteration of the program you should record initial values of the probability distribution, corresponding to $x = c+ih$. Boundary conditions may be either absorbing $W_{0,j} = W_{N,j} = 0$ or reflecting:

$$\begin{aligned} W_{0,j} &= -\frac{2h}{D(x,t)}\left[2a(x,t) - \frac{\partial D(x,t)}{\partial x}\right]W_{1,j} + W_{2,j}, \\ W_{N,j} &= \frac{2h}{D(x,t)}\left[2a(x,t) - \frac{\partial D(x,t)}{\partial x}\right]W_{N-1,j} + W_{N-2,j}, \end{aligned}$$

Thus, the formula (18) gives explicit expression of the solution in the layer $j + 1$ via previously obtained solution in the layer j.

For the use of explicit difference scheme, the conditions of stability of algorithm should be fulfilled. It can be demonstrated that the explicit difference scheme is stable, if in the considered interval the following inequalities are fulfilled:

$$D(x,t) \geq 0, \quad l/h^2 < 1/D(x,t).$$

It follows from the second inequality, that explicit difference scheme require very small time step.

II. SOME EXAMPLES OF PROCESSES, WHICH TRANSITION PROBABILITY DENSITIES KNOWN ANALYTICALLY

Wiener process.

A process which is described by the FPKE (1) with vanishing drift coefficient $a(x) = 0$ and constant diffusion coefficient is called a Wiener process. The equation for the transition probability density is then the diffusion equation:

$$\frac{\partial W(x,t|x_0,t_0)}{\partial t} = \frac{D}{2}\frac{\partial^2}{\partial x^2} W(x,t|x_0,t_0). \tag{20}$$

with the delta-shaped initial distribution $W(x,t_0|x_0,t_0) = \delta(x-x_0)$. The solution of this equation reads:

$$W(x,t|x_0,t_0) = \frac{1}{\sqrt{2\pi D(t-t_0)}} \exp\left(-\frac{(x-x_0)^2}{2D(t-t_0)}\right). \tag{21}$$

Ornstein-Uhlenbeck process.

A process which is described by the FPKE (1) with a linear drift coefficient $a(x) = -bx$ and constant diffusion coefficient is called the Ornstein-Uhlenbeck process. The equation for the transition probability density is then:

$$\frac{\partial W(x,t|x_0,t_0)}{\partial t} = \left\{ \frac{\partial}{\partial x}\left[bxW(x,t|x_0,t_0)\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[D(x)W(x,t|x_0,t_0)\right] \right\}. \tag{22}$$

The solution of this equation is also Gaussian distribution:

$$W(x,t|x_0,0) = \frac{1}{\sqrt{2\pi \mathcal{D}(t)}} \exp\left(-\frac{(x-x_0e^{-bt})^2}{2\mathcal{D}(t)}\right). \tag{23}$$

where $\mathcal{D}(t) = D(1-e^{-2bt})/2b$ is variance.

The probability distribution (23) may be obtained from equation (22) using the method of eigenfunction analysis. The required probability density may be represented as an infinite Hermite series and summarized into the probability density (23). But the same probability distribution may be obtained by much more easy way using cumulant analysis technique [6].

If you know that your system is linear and the noise is Gaussian, then the steady-state probability distribution always will be Gaussian. In the case of delta-shaped initial distribution the one-dimensional probability density (the transition probability density) will be Gaussian for any moment of time. If you have some arbitrary initial probability distribution then you may get the one-dimensional probability density by simple averaging of transition probability density over

initial probability distribution. But your system is linear for the case of linear drift coefficient $a(x,t) = -bx + f(t)$ where $f(t)$ is an arbitrary function of time.

In this case you may use the cumulant analysis technique, get linear differential equations of the first order for the mean $m(t)$ and the variance $\mathcal{D}(t)$:

$$\frac{dm(t)}{dt} = -bm(t) + f(t),$$

$$\frac{d\mathcal{D}(t)}{dt} = -2b\mathcal{D}(t) + D,$$

and easily solve them. The obtained mean and variance you should substitute in the Gaussian distribution of the general form:

$$W(x,t|x_0,0) = \frac{1}{\sqrt{2\pi\mathcal{D}(t)}} \exp\left(-\frac{(x-m(t))^2}{2\mathcal{D}(t)}\right) \tag{24}$$

and then you get the required transition probability density.

However, I know only one real superconductive device which has small nonlinearity and may be approximately treated as linear: this is a microwave nonhysteretic SQUID.

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[1] R.L.Stratonovich, Topics of the Theory of Random Noise (Gordon and Breach, New York, 1963).

[2] V.I.Tikhonov and M.A.Mironov, Markovian processes (Sovetskoe Radio, Moscow, 1978, in Russian).

[3] H.Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).

[4] G.Doetsch, Anleitung zum Praktischen Gebrauch der Laplace-Transformation (R.Oldenbourg, Munchen, 1961).

[5] A.N.Malakhov and A.L.Pankratov, Exact solution of the Kramers' problem for piece-wise parabolic potential profiles, Physica A, 229, No. 1 (1996) pp. 109-126.

[6] A.N.Malakhov, Cumulant analysis of random Non-Gaussian processes and its transformations (Sovetskoe Radio, Moscow, 1978, in Russian).

Stochastic processes and applications
Lecture 5

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I. TIME SCALES OF BROWNIAN DIFFUSION. INTRODUCTION

The Fokker-Planck equation is a partial differential equation. In most cases, its time dependent solution is not known analytically. Also, if it has more than one state variable, exact stationary solutions are very rare. That is why the most simple thing is to obtain approximate time characteristics when analyzing the dynamics of diffusion transition processes.

The first paper devoted to escape problem to appear in western literature, was paper by Kramers [1] published in 1940, and presented approximate, but complete analytic results. Some years before, in 1933, Pontryagin, Andronov and Vitt [2] published a paper, where were presented exact analytic results on the same subject, but this paper remained unknown outside the USSR for a long time.

The original work of Kramers stimulated research devoted to calculation of escape rates in different systems driven by noise. Now the problem of calculating escape rates is known as Kramers' problem.

II. TIME SCALES OF BROWNIAN DIFFUSION. KRAMERS' APPROACH

Let us consider the potential $\Phi(x)$, describing a metastable state, depicted in Fig.1.

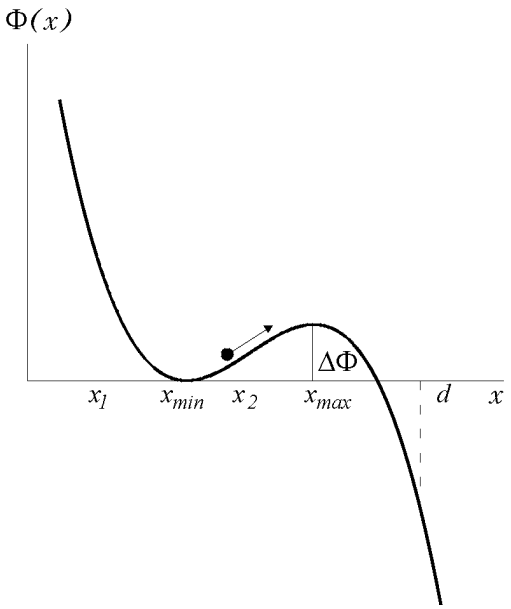

FIG. 1. Potential, describing metastable state.

Initially, an overdamped Brownian particle is located in the potential minimum, say somewhere between x_1, x_2. Subjected to noise perturbations, the Brownian particle will after some time escape over the potential barrier of the height $\Delta\Phi$. It is necessary to obtain the mean life time of metastable state (inverse of the mean life time (escape time) is called the escape rate).

To calculate the mean escape time over a potential barrier, let us apply the Fokker-Planck-Kolmogorov equation, which may be also presented in the form:

$$\frac{\partial W(x,t)}{\partial t} = \frac{\partial}{\partial x}\left\{\frac{kT}{h}e^{-\Phi(x)/kT}\frac{\partial}{\partial x}\left[e^{\Phi(x)/kT}W(x,t)\right]\right\}, \tag{1}$$

where we substituted $a(x) = -\frac{d\Phi(x)}{hdx}$. Here h is viscosity, $D = 2kT/h$.

Let us consider the case when the diffusion coefficient is small, or, more precisely when the barrier height $\Delta\Phi$ is much larger than the diffusion coefficient D. As it turns out, one can get analytic expressions for the mean escape time in this limiting case. Further more, we restrict ourselves to a constant diffusion coefficient D. Then the probability current G over the barrier top near x_{max} is very small, so the probability density $W(x,t)$ almost does not vary in time, representing quasi-stationary distribution. For this quasi-stationary state the small probability current G must be approximately independent of coordinate x and can be presented in the form:

$$G = -\left\{\frac{kT}{h}e^{-\Phi(x)/kT}\frac{\partial}{\partial x}\left[e^{\Phi(x)/kT}W(x,t)\right]\right\}. \tag{2}$$

Integrating (2) between x_{min} and d we obtain:

$$G\int\limits_{x_{min}}^{d} e^{\Phi(x)/kT}dx = \frac{kT}{h}\left[e^{\Phi(x_{min})/kT}W(x_{min},t) - e^{\Phi(d)/kT}W(d,t)\right]; \tag{3}$$

or if we assume that at $x = d$ the probability density is nearly zero (particles may for instance be taken away that corresponds to absorbing boundary) we can express the probability current by the probability density at $x = x_{min}$, i.e.

$$G = \frac{kT}{h}e^{\Phi(x_{min})/kT}W(x_{min},t)/\int\limits_{x_{min}}^{d} e^{\Phi(x)/kT}dx. \tag{4}$$

If the barrier is high, the probability density near x_{min} will be given approximately by the stationary distribution:

$$W(x,t) \approx W(x_{min},t)e^{-[\Phi(x)-\Phi(x_{min})]/kT}. \tag{5}$$

The probability P to find the particle near x_{min} is:

$$P = \int\limits_{x_1}^{x_2} W(x,t)dx \approx W(x_{min},t)e^{\Phi(x_{min})/kT}\int\limits_{x_1}^{x_2} e^{-\Phi(x)/kT}dx. \tag{6}$$

If kT is small, the probability density becomes very small for x values appreciably different from x_{min}, which means that the x_1, x_2 values need not be specified in detail.

The escape time is introduced as the probability P devided by the probability current G. Then, using (4) and (6), we can get the following expression for the escape time:

$$\tau = \frac{h}{kT}\int\limits_{x_1}^{x_2} e^{-\Phi(x)/kT}dx\int\limits_{x_{min}}^{d} e^{\Phi(x)/kT}dx. \tag{7}$$

Whereas the main contribution to the first integral stems from the region around x_{min}, the main contribution to the second integral stems from the region around x_{max}. We therefore expand $\Phi(x)$ for the first and second integrals according to:

$$\Phi(x) \approx \Phi(x_{min}) + \frac{1}{2}\Phi''(x_{min})(x - x_{min})^2, \tag{8}$$

$$\Phi(x) \approx \Phi(x_{max}) - \frac{1}{2}|\Phi''(x_{max})|(x - x_{max})^2. \tag{9}$$

We may then extend the integration boundaries in both integrals to $\pm\infty$ and thus obtain the well-known Kramers' escape time:

$$\tau = \frac{2\pi h}{\sqrt{\Phi''(x_{min})|\Phi''(x_{max})|}} e^{\Delta\Phi/kT}, \tag{10}$$

where $\Delta\Phi = \Phi(x_{max}) - \Phi(x_{min})$. As shown by Edholm and Leimar [6], one can improve (10) by calculating the integrals (7) more accurately, e.g. by using the expansion of the potential in (8) and (9) up to the fourth term.

One can ask the question: What if the considered potential is such that either $\Phi''(x_{max}) = 0$ or $\Phi''(x_{min}) = 0$? You may see that Kramers' formula (10) does not work in this case. This is a pity, but because you know how Kramers' formula has been obtained, you may substitute the required potential into integrals in (7) and derive another formula, similar to Kramers' one:

$$\tau = \tau_0(kT) e^{\Delta\Phi/kT}, \tag{11}$$

where the prefactor $\tau_0(kT)$ is a function of temperature and reflects particular shape of your potential. For example you may easily get this formula for a piecewise potential of the fourth order. Formula (11) for $\tau_0(kT) = const$ is also known as Arrhenius law.

Influence of the shape of potential well and barrier on escape times was studied in detail in paper by Adudov and Malakhov [7] and some of their results will be discussed here.

In the table 1, the temperature dependencies of prefactor $\tau_0(kT)$ for potential barriers and wells of different shape are shown in the limiting case of small temperature. For the considered functions $\Phi_b(x)$ and $\Phi_t(x)$ the dependence $\tau_0(kT)$ vary from $\tau_0 \sim (kT)^3$ to $\tau_0 \sim (kT)^{-1}$. The functions $\Phi_b(x)$ and $\Phi_t(x)$ are, respectively, potentials at the bottom of the well and the top of the barrier. As it follows from table 1, the Arrhenius law (11), i.e. $\tau_0(kT) = const$, occur only for such forms of potential barrier and well that $1/p + 1/q = 1$. This will be the case for a parabolic well and barrier ($p = 2$, $q = 2$), and also for a flat well ($p = \infty$) and triangle barrier ($q = 1$), and, vice versa, for a triangle well ($p = 1$) and flat barrier ($q = \infty$).

$\tau_0(kT) \sim$		$\Phi_t(x) \sim$					
		$\lvert x\rvert^{\frac{1}{2}}$	$\lvert x\rvert^{\frac{2}{3}}$	$\lvert x\rvert$	x^2	x^4	x^∞, $\lvert x\rvert \le L/2$
$\Phi_b(x) \sim$	$\lvert x\rvert^{\frac{1}{2}}$	$(kT)^3$	$(kT)^{\frac{5}{2}}$	$(kT)^2$	$(kT)^{\frac{3}{2}}$	$(kT)^{\frac{5}{4}}$	$(kT)^1$
	$\lvert x\rvert^{\frac{2}{3}}$	$(kT)^{\frac{5}{2}}$	$(kT)^2$	$(kT)^{\frac{3}{2}}$	$(kT)^1$	$(kT)^{\frac{3}{4}}$	$(kT)^{\frac{1}{2}}$
	$\lvert x\rvert$	$(kT)^2$	$(kT)^{\frac{3}{2}}$	$(kT)^1$	$(kT)^{\frac{1}{2}}$	$(kT)^{\frac{1}{4}}$	$(kT)^0$
	x^2	$(kT)^{\frac{3}{2}}$	$(kT)^1$	$(kT)^{\frac{1}{2}}$	$(kT)^0$	$(kT)^{-\frac{1}{4}}$	$(kT)^{-\frac{1}{2}}$
	x^4	$(kT)^{\frac{5}{4}}$	$(kT)^{\frac{3}{4}}$	$(kT)^{\frac{1}{4}}$	$(kT)^{-\frac{1}{4}}$	$(kT)^{-\frac{1}{2}}$	$(kT)^{-\frac{3}{4}}$
	$\lvert x\rvert^\infty$, $\lvert x\rvert \le L/2$	$(kT)^1$	$(kT)^{\frac{1}{2}}$	$(kT)^0$	$(kT)^{-\frac{1}{2}}$	$(kT)^{-\frac{3}{4}}$	$(kT)^{-1}$

Table 1

III. TIME SCALES OF BROWNIAN DIFFUSION. EIGENFUNCTION AND EIGENVALUE ANALYSIS

Let us now consider symmetric bistable potential.

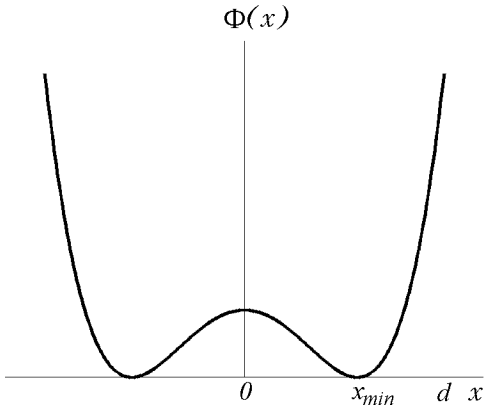

FIG. 2. Bistable potential.

Let us calculate the decay time of particles in the well which agrees with inverse of the lowest nonvanishing eigenvalue γ_1 (see previous lecture). Using the method of eigenfunction analysis as presented in lecture 4 we search for the solution of the Fokker-Planck-Kolmogorov equation in the form

$$W(x,t) = X(x) \cdot T(t), \tag{12}$$

where $X(x)$ and $T(t)$ are functions of coordinate and time, and get the system of two equations for functions $X(x)$ and $T(t)$:

$$\frac{1}{T(t)} \frac{\partial T(t)}{\partial t} = -\gamma, \tag{13}$$

$$\left\{ \frac{\partial}{\partial x} \left[-a(x) X(x) \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[D(x) X(x) \right] \right\} = -\gamma X(x). \tag{14}$$

Using the boundary conditions and a delta-shaped initial distribution, we can write the solution of the Fokker-Planck-Kolmogorov equation in the form:

$$W(x,t) = \sum_{n=0}^{\infty} \frac{X_n(x) X_n(x_0)}{W_{st}(x_0)} e^{-\gamma_n (t - t_0)}, \tag{15}$$

where $X_0(x) = W_{st}(x)$ and $\gamma_0 = 0$. Here we consider only the case where the steady-state probability distribution does exist: $W_{st}(x) \neq 0$, and thus we should suppose reflecting boundary conditions $G(\pm d) = 0$. Analyzing expression (15) and taking into account that the eigenvalues γ_n represent a set such that $\gamma_1 < \gamma_2 < ... < \gamma_n$, we can see that the exponent with minimal eigenvalue will decay slower than others, and will thus reflect the largest time scale of decay which equals the inversed minimal nonzero eigenvalue.

So, equation (14) with boundary conditions is the equation for eigenfunction $X_n(x)$ of the $n-th$ order. For $X_0(x)$ the equation (14) will be an equation for stationary probability distribution with zero eigenvalue $\gamma_0 = 0$ and for $X_1(x)$ the equation will have the following form:

$$\frac{\partial}{\partial x} \left\{ \frac{kT}{h} e^{-\Phi(x)/kT} \frac{\partial}{\partial x} \left[e^{\Phi(x)/kT} X_1(x) \right] \right\} = -\gamma_1 X_1(x). \tag{16}$$

Integrating equation (16) with account of reflecting boundary conditions (probability current is equal to zero at the points $\pm d$) we get:

$$\frac{kT}{h} \frac{\partial}{\partial x} e^{\Phi(x)/kT} X_1(x) = -\gamma_1 e^{\Phi(x)/kT} \int_y^d X_1(z) dz. \tag{17}$$

Integrating this equation once again, the following integral equation for eigenfunction $X_1(x)$ may be obtained:

$$X_1(x) = e^{-\Phi(x)/kT} \left[e^{\Phi(d)/kT} X_1(d) - \frac{h\gamma_1}{kT} \int_x^d e^{\Phi(y)/kT} dy \int_y^d X_1(z) dz \right]. \tag{18}$$

The eigenfunction $X_1(x)$ belonging to the lowest nonvanishing eigenvalue must be an odd function for the bistable potential, i.e. $X_1(0) = 0$. The integral equation (18) together with reflecting

boundary conditions determine the eigenfunction $X_1(x)$ and the eigenvalue γ_1. We may apply an iteration procedure which is based on the assumption that the noise intensity is small compared to the barrier height (this iteration procedure is described in the book by Risken [4]) and get the following expression for the required eigenvalue in the first order approximation:

$$\gamma_1 = (kT/h) / \int_0^d e^{\Phi(y)/kT} dy \int_y^d e^{-\Phi(z)/kT} dz. \tag{19}$$

For a small noise intensity, the double integral may be evaluated analytically and finally we get the following expression for the escape time (inverse of the eigenvalue γ_1) of the considered bistable potential:

$$\tau_b = \frac{\pi h}{\sqrt{\Phi''(x_{min})|\Phi''(0)|}} e^{\Delta\Phi/kT}. \tag{20}$$

The obtained escape time τ_b for the bistable potential is two times smaller than the Kramers' time, because we considered transition over the barrier top $x = 0$, that is why we have got only a half.

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[1] H.Kramers, Physica **7**, 284 (1940).

[2] L.A.Pontryagin, A.A.Andronov and A.A.Vitt, Zh. Eksp. Teor. Fiz. **3**, 165 (1933) [translated by J.B.Barbour and reproduced in "Noise in Nonlinear Dynamics", 1989, edited by F.Moss and P.V.E. McClintock (Cambridge University Press, Cambridge) Vol. 1, p.329].

[3] C.W.Gardiner, Textbook of Stochastic methods (Springer-Verlag, 1985).

[4] H.Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).

[5] P.Hanggi, P.Talkner and M.Borkovec, Rev.Mod.Phys., **62**, 251 (1990).

[6] O.Edholm, O.Leimar, Physica A, **98**, 313 (1979).

[7] N.V.Agudov and A.N.Malakhov, Applied nonlinear dynamics, **3**, N3, 75 (1995) (in Russian).

[8] A.N.Malakhov and A.L.Pankratov, Physica A, **229**, 109 (1996).

Stochastic processes and applications
Lecture 6

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I. THE FIRST PASSAGE TIME APPROACH

The first approach to get exact time characteristics of Markov processes with nonlinear drift coefficients was proposed in 1933 by Pontryagin, Andronov and Vitt [1]. This approach allows to obtain exact values of moments of the First Passage Time for arbitrary potentials and arbitrary noise intensity, and moreover, the noise intensity (diffusion coefficient) may be nonlinear function of coordinate. The only disadvantage of this method is that it requires an artificial introducing of absorbing boundaries, which changes the process of diffusion in real smooth potentials.

Probability to reach a boundary by one-dimensional Markov processes

Let continuous one-dimensional Markov process $x(t)$ at initial instant of time $t = 0$ has a fixed value $x(0) = x_0$ within the interval (c, d), i.e. the initial probability density is the delta function:

$$W(x, 0) = \delta(x - x_0), \quad x_0 \in (c, d).$$

It is necessary to find the probability $Q(x_0, t)$ that a random precess, having initial value x_0 will reach during the time $t > 0$ the boundaries of the interval (c, d), i.e. will reach either boundary c or d: $Q(x_0, t) = \int\limits_{-\infty}^{c} W(x, t)dx + \int\limits_{d}^{+\infty} W(x, t)dx$.

Instead of the probability to reach boundaries, one can be interested in the probability

$$P(x_0, t) = 1 - Q(x_0, t)$$

of nonreaching of boundaries c and d by Markov process, having initial value x_0. By other words

$$P(x_0, t) = P\{c < x(t) < d, \quad 0 < t < T\}, \quad x_0 \in (c, d),$$

where $T = T(c, x_0, d)$ is a random instant of the First Passage Time of boundaries c or d.

We will not present here how to obtain the first Pontryagin's equation for the probability $Q(x_0, t)$ or $P(x_0, t)$. The intersted reader can see it in [1] or in [2] and [3]. We only mention, that the first Pontryagin's equation either may be obtained via transformation of the backward Kolmogorov equation or by simple decomposition of the probability $P(x_0, t)$ into Teylor expansion in the vicinity of x_0 at different moments τ and $t + \tau$, some transformations and limiting transition to $\tau \to 0$ [4].

The first Pontryagin's equation looks like:

$$\frac{\partial Q(x_0, t)}{\partial t} = a(x_0)\frac{\partial Q(x_0, t)}{\partial x_0} + \frac{D(x_0)}{2}\frac{\partial^2 Q(x_0, t)}{\partial {x_0}^2}. \tag{1}$$

Let us point out the initial and boundary conditions of equation (1). It is obvious that for all $x_0 \in (c, d)$ the probability to reach boundary at $t = 0$ is equal to zero:

$$Q(x_0, 0) = 0, \quad c < x_0 < d. \tag{2}$$

At the boundaries of the interval, i.e. for $x_0 = c$ and $x_0 = d$ the probability to reach boundaries for any instant of time t is equal to unity:

$$Q(c,t) = Q(d,t) = 1. \tag{3}$$

This means that for $x_0 = c$, $x_0 = d$ the boundary will be surely reached already at $t = 0$. Besides these conditions usually one more condition must be fulfilled:

$$\lim_{t\to\infty} Q(x_0,t) = 1, \quad c \le x_0 \le d,$$

expressing the fact that the probability to pass boundaries somewhen for a long enough time is equal to unity.

The compulsory fulfilment of conditions (2), (3) physically follows from the fact that one-dimensional Markov process is nondifferentiable, i.e. the derivative of Markov process has an infinite variance (instantaneous speed is an infinitely high). However the particle with the probability equals unity drifts for the finite time to the finite distance. That is why the particle velocity changes its sign during the time and the motion occur in an opposite directions. If the particle is located at some finite distance from the boundary, it can not reach the boundary in a trice - the condition (2). On the contrary, if the particle is located near a boundary then it necessarily cross the boundary - the condition (3).

Let us mention that analogically may be solved the tasks about the probability to cross either only left boundary c or the right one d or about the probability to do not leave the considered interval $[c,d]$. In this case equation (1) is valid, and only boundary conditions should be changed.

Also, one can be intersted in the probability to reach the boundary by Markov process, having random initial distribution. In this case one should first solve the task with the fixed initial value x_0 and after that the averaging for all possible values of x_0 should be performed. If initial value x_0 is distributed in the interval $(c_1,d_1) \in (c,d)$ with the probability $W_0(x_0)$ then, following the theorem about the sum of probabilities, the complete probability to reach boundaries c and d is defined by the expression:

$$Q(t) = \int_c^d Q(x_0,t)W_0(x_0)dx_0 + P\{c_1 < x_0 < c, t = 0\} + P\{d < x_0 < d_1, t = 0\}. \tag{4}$$

Moments of the First Passage Time

One can get analytic (exact) solution of the first Pontryagin's equation only in a few simplest cases. That is why in practice one restricts by calculation of moments of the First Passage Time of absorbing boundaries, and, in particular, by the mean and the variance of the First Passage Time.

If the probability density $w_T(x_0,t)$ of the First Passage Time of boundaries c and d exists, then by the definition [4]:

$$w_T(x_0,t) = \frac{d}{dt}Q(x_0,t) = -\frac{d}{dt}P(x_0,t). \tag{5}$$

Taking derivative from equation (1) we get that $w_T(x_0,t)$ fulfils the following equation:

$$\frac{\partial w_T(x_0,t)}{\partial t} = a(x_0)\frac{\partial w_T(x_0,t)}{\partial x_0} + \frac{D(x_0)}{2}\frac{\partial^2 w_T(x_0,t)}{\partial {x_0}^2}. \tag{6}$$

with initial and boundary conditions:

$$w_T(x_0,0) = 0, \quad c < x_0 < d,$$

$$w_T(c,t) = w_T(d,t) = \delta(t), \tag{7}$$

for the case of both absorbing boundaries and

$$w_T(d,t) = \delta(t), \quad \left.\frac{\partial w_T(x_0,t)}{\partial x_0}\right|_{x_0=c} = 0, \tag{8}$$

for the case of one absorbing and one reflecting boundary.

The task to get the solution of equation (6) with the above mentioned initial and boundary conditions is mathematically quite difficult even for simplest potentials $\varphi(x_0)$.

Moments of the First Passage Time may be expressed from the probability density $w_T(x_0,t)$ as:

$$T_n = T_n(c,x_0,d) = \int_0^\infty t^n w_T(x_0,t)dt, \quad (n = 1,2,3,\ldots). \tag{9}$$

Multiplying both sides of equation (6) by $e^{i\Omega t}$ and integrating it for t going from 0 to ∞ we get the following differential equation for the characteristic function $\Theta(x_0,i\Omega)$:

$$-i\Omega\Theta(x_0,i\Omega) = a(x_0)\frac{\partial\Theta(x_0,i\Omega)}{\partial x_0} + \frac{D(x_0)}{2}\frac{\partial^2\Theta(x_0,i\Omega)}{\partial {x_0}^2}. \tag{10}$$

where $\Theta(x_0,i\Omega) = \int_0^\infty e^{i\Omega t} w_T(x_0,t)dt$.

Equation (10) allows to find one-dimensional moments of the First Passage Time. For this purpose let us use well-known representation of the characteristic function as the set of moments:

$$\Theta(x_0,i\Omega) = 1 + \sum_{n=1}^{\infty}\frac{(i\Omega)^n}{n!}T_n(c,x_0,d). \tag{11}$$

Substituting (11) and its derivatives in (10) and equating terms of the same order of $i\Omega$ we get the chain of linear differential equations of the second order with variable coefficients:

$$\frac{D(x_0)}{2}\frac{d^2T_n(c,x_0,d)}{d{x_0}^2} + a(x_0)\frac{dT_n(c,x_0,d)}{dx_0} = -n\cdot T_{n-1}(c,x_0,d). \tag{12}$$

Equations (12) allow to sequentially find moments of the First Passage Time for $n = 1,2,3,\ldots$ ($T_0 = 1$). These equations should be solved at the corresponding boundary conditions and by physical implication all moments $T_n(c,x_0,d)$ must be nonnegative values, $T_n(c,x_0,d) \geq 0$.

Boundary conditions for equations (12) may be obtained from the corresponding boundary conditions (7), (8) of equations (1) and (6). If boundaries c and d are absorbing, we get from (7):

$$T(c,c,d) = T(c,d,d) = 0. \tag{13}$$

If one boundary, say c, is reflecting, then one can get from (8):

$$T(c,d,d) = 0, \quad \left.\frac{\partial T(c,x_0,d)}{\partial x_0}\right|_{x_0=c} = 0. \tag{14}$$

If we will start solving the equation (12) from $n = 1$, then further moments $T_n(c,x_0,d)$ will be expressed from previous moments $T_m(c,x_0,d)$. In particular, for $n = 1,2$ we get:

$$\frac{D(x_0)}{2}\frac{d^2T_1(c,x_0,d)}{d{x_0}^2} + a(x_0)\frac{dT_1(c,x_0,d)}{dx_0} + 1 = 0. \tag{15}$$

$$\frac{D(x_0)}{2}\frac{d^2T_2(c,x_0,d)}{dx_0{}^2}+a(x_0)\frac{dT_2(c,x_0,d)}{dx_0}+2T_1(c,x_0,d)=0. \tag{16}$$

Equation (15) was first obtained by Pontryagin and is called as the second Pontryagin equation.

System of equations (12) may be easily solved. Indeed, making substitution $Z=dT_n(c,x_0,d)/dx_0$ each equation may be transformed in the first order differential equation:

$$\frac{D(x_0)}{2}\frac{dZ}{dx_0}+a(x_0)Z=-n\cdot T_{n-1}(c,x_0,d). \tag{17}$$

The solution of (17) may be written by quadratures:

$$Z(x_0)=\frac{dT_n(c,x_0,d)}{dx_0}=e^{\varphi(x_0)}\left[A-\int\limits_c^{x_0}\frac{2nT_{n-1}(c,y,d)}{D(y)}e^{-\varphi(y)}dy\right], \tag{18}$$

where $\varphi(y)=-\int\frac{2a(y)}{D(y)}dy$, A is an arbitrary constant, determined from boundary conditions.

When one boundary is reflecting (e.g. c), and another one is absorbing (e.g. d), then from (18) and bondary conditions (14) we get:

$$T_n(c,x_0,d)=2n\int\limits_{x_0}^{d}e^{\varphi(x)}\int\limits_c^x\frac{T_{n-1}(c,y,d)}{D(y)}e^{-\varphi(y)}dydx. \tag{19}$$

Because $dT_n(c,x_0,d)/dx_0<0$ for any $c<x_0<d$ and $dT_n(c,x_0,d)/dx_0=0$ for $x_0=c$, and, as follows from (12), $d^2T_n(c,x_0,d)/dx_0^2<0$ for $x_0=c$, the maximal value of the function $T_n(c,x_0,d)$ is reached at $x_0=c$.

For the case when both boundaries are absorbing, the required moments of the First Passage Time has more complicated form.

When the initial probability distribution is not delta function, but some arbitrary function $W_0(x_0)$, where $x_0\in(c,d)$, then it is possible to calculate moments of the First Passage Time, averaged over initial probability distribution:

$$T_n(c,d)=\int\limits_c^d T_n(c,x_0,d)W_0(x_0)dx_0. \tag{20}$$

II. GENERALIZED MOMENT EXPANSION FOR RELAXATION PROCESSES

As we discussed in previous section, the Mean First Passage Time approach requires artificial introducing the absorbing boundaries and, therefore, the steady-state probability distribution in such systems does not exist, because eventually all particles will be absorbed by boundaries. But in the large number of real systems the steady-state distributions do exist, and namely such systems are considered in accordance with tasks of Josephson electronics (e.g. SQUIDs, memory cells, and so on).

Moreover, in experiments are usually measured stationary processes, and, thus, different steady-state characteristics, such as correlation functions, spectra, different averages.

First paper, devoted to obtaining characteristic time scales of different observables in systems having steady states was paper by Nadler and Schulten [6]. Their approach is bazed on the generalized moment expansion of observables and, thus, called as "generalized moment approximation" (GMA).

The observables considered are of the type:

$$M(t) = \int_c^d \int_c^d f(x) W(x,t|x_0) g(x_0) dx_0 dx, \tag{21}$$

where $W(x,t|x_0)$ is the transition probability density governed by the Fokker-Planck-Kolmogorov equation

$$\frac{\partial W(x,t)}{\partial t} = \left\{ \frac{\partial}{\partial x} \left[-\frac{a(x)}{kT} W(x,t) \right] + \frac{\partial^2}{\partial x^2} \left[D(x) W(x,t) \right] \right\}, \tag{22}$$

$g(x_0)$ is initial probability distribution and $f(x)$ is some test function that monitors the distribution at the time t. The reflecting boundary conditions at points c and d are supposed, which leads to the existance of steady-state probability distribution $W_{st}(x)$ (see lecture 4):

$$W_{st}(x) = \frac{C}{D(x)} \exp \left[2 \int_{x'}^{x} \frac{a(x)}{D(x)} dx \right], \tag{23}$$

where C is normalization constant.

The observable has initial value $M(0) =< f(x) g_0(x) >$ and relaxes asymptotically to $M(\infty) =< f(x) >< g_0(x) >$. Here $<>$ is ensemble average and $g_0(x) = g(x)/W_0(x)$,

$$W_0(x) = \exp \left[\int_{x'}^{x} \frac{a(x)}{kT} dx \right], \tag{24}$$

Since the time development of $M(t)$ is solely due to the relaxation process, one needs to consider only $\Delta M(t) = M(t) - M(\infty)$.

Starting point of the generalized moment approximation (GMA) is the Laplace transformation of observable

$$\Delta M(\omega) = \int_0^\infty \Delta M(t) e^{-\omega t} dt. \tag{25}$$

$\Delta M(\omega)$ may be expanded for low and high frequencies

$$\Delta M(\omega) \sim_{\omega \to 0} \sum_{n=0}^{\infty} \mu_{-(n+1)} (-\omega)^n, \tag{26}$$

$$\Delta M(\omega) \sim_{\omega \to \infty} \sum_{n=0}^{\infty} \mu_n (-1/\omega)^n, \tag{27}$$

where the expansion coefficients μ_n, the "generalized moments", are given by

$$\mu_n = (-1)^n \int_c^d g(x) \left\{ (L^+(x))^n \right\}_b f(x) dx, \tag{28}$$

where $\{\}_b$ denotes operation in a space of functions which obey the adjoint reflecting boundary conditions, $L^+(x)$ is the adjoint Fokker-Planck operator:

$$L^+(x) = -\left\{ \frac{a(x)}{kT} \frac{\partial}{\partial x} + D(x) \frac{\partial^2}{\partial x^2} \right\}. \tag{29}$$

In veiw of expansions (26) and (27) we will refer to μ_n, $n \geq 0$ as the high-frequency moments and to μ_n, $n < 0$ as the low-frequency moments.

The moment μ_0 is identical to the initial value $\Delta M(t)$ and assumes the simple form:

$$\mu_0 = < f(x) g_0(x) > - < f(x) >< g_0(x) > . \tag{30}$$

For negative n (see [6]), the following recurrent expressions for the moments μ_{-n} may be obtained:

$$\mu_{-n} = \int_c^d \frac{dx}{D(x) W_0(x)} \int_c^x W_0(x) \mu_{-(n-1)}(y) dy \int_c^x W_0(z) (g_0(z) - < g_0(z) >) dz, \tag{31}$$

where

$$\mu_{-n}(x) = C - \int_c^x \frac{dy}{D(y) W_0(y)} \int_c^y W_0(z) \mu_{-(n-1)}(z) dz, \tag{32}$$

where C is an integration constant, chosen to satisfy the orthogonality property. For $n = 1$ holds

$$\mu_{-1} = \int_c^d \frac{dx}{D(x) W_0(x)} \int_c^x W_0(x) (f(y) - < f(y) >) dy \int_c^x W_0(z) (g_0(z) - < g_0(z) >) dz. \tag{33}$$

Moments with negative index, which account for the low-frequency behaviour of observables in relaxation processes, can be evaluated by means of simple quadratures. Let us consider now, how the moments μ_n may be employed to approximate the observable $\Delta M(t)$.

We want to approximate $\Delta M(\omega)$ by a Pade approximant $\Delta m(\omega)$. The functional form of $\Delta m(\omega)$ should be such, that the corresponding time-dependent function $\Delta m(t)$ is a series of N exponentials describing the relation of $\Delta M(t)$ to $\Delta M(\infty) = 0$. This implies that $\Delta m(\omega)$ is an $[N-1, N]$-Pade approximant which can be written in the form:

$$\Delta m(\omega) = \sum_{n=1}^{N} a_n / (\lambda_n + \omega) \tag{34}$$

or, correspondingly,

$$\Delta m(t) = \sum_{n=1}^{N} a_n \exp(-\lambda_n t). \tag{35}$$

The function $\Delta m(\omega)$ should describe the low- and high-frequency behaviour of $\Delta M(\omega)$ to a desired degree. We require that $\Delta m(\omega)$ reproduces N_h high- and N_l low-frequency moments. Since $\Delta m(\omega)$ is determined by an even number of constants a_n and λ_n one needs to choose $N_h + N_l = 2N$. We refer to the resulting description as the (N_h, N_l)-generalized-moment approximation (GMA). The description represents a two-sided Pade approximation. The moments determine the parameters a_n and λ_n through the relations

$$\sum_{n=1}^{N} a_n \lambda_n^m = \mu_m, \tag{36}$$

where $m = -N_l, -N_l + 1, ..., N_h - 1$).

Algebraic solution of equation (36) is feasible only for $N = 1, 2$. For $N > 2$ the numerical soluiton of (36) is possible by means of an equivalent eigenvalue problem, for references see [6].

Let us mention in conclusion, that approach by Nadler and Schulten allows to obtain characteristic time scales of different observables. Moreover, for one particular example of rectangular barrierless potential well, the authors demonstrated that even one-exponential approximation describes the required observable with a good precision.

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[1] L.A.Pontryagin, A.A.Andronov and A.A.Vitt, Zh. Eksp. Teor. Fiz. **3**, 165 (1933) [translated by J.B.Barbour and reproduced in "Noise in Nonlinear Dynamics", 1989, edited by F.Moss and P.V.E. McClintock (Cambridge University Press, Cambridge) Vol. 1, p.329].

[2] C.W.Gardiner, Textbook of Stochastic methods (Springer-Verlag, 1985).

[3] P.Hanggi, P.Talkner and M.Borkovec, Rev.Mod.Phys., **62**, 251 (1990).

[4] V.I.Tikhonov and M.A.Mironov, Markovian processes (Sovetskoe Radio, Moscow, 1978, in Russian).

[5] H.Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).

[6] W.Nadler and K.Schulten, Journ. Chem. Phys., **82**, 151 (1985).

[7] A.Szabo, K.Schulten and Z.Schulten, Journ. Chem. Phys., **72**, 4350 (1980).

Stochastic processes and applications
Lecture 7

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I. INTRODUCTION

When the noise-induced transition occurs over a potential barrier high enough in comparison with noise intensity, the probability of transition is a simple exponent $\sim \exp(-t/\tau)$ [1], where τ is the mean transition time. In this case the mean transition time gives complete information about the probability evolution. The boundaries of validity of exponential approximation of the probability were previously studied in [2], [3]. In [2] authors extended the Mean First Passage Time to the case of "radiation" boundary condition and for two barrierless examples demonstrated good coincidence between exponential approximation and numerically obtained probability. In a more general case the exponential behavior of observables was demonstrated in [3] for relaxation processes in systems having steady states. Using the approach of "generalized moment approximation" the authors of [3] obtained the exact mean relaxation time to steady state and for particular example of a rectangular potential well demonstrated good coincidence of exponential approximation with numerically obtained observables (including probability). The considered in [3] example of the rectangular well does not have a potential barrier, and the authors of that paper supposed that their approach (and the corresponding formulas) should also give good approximation in tasks with diffusive barrier crossing for a wide range of noise intensity.

In the frame of this lecture, let us consider a different case than in [2], [3]: let us analyse temporal dynamics of the nondecay probability of a metastable state (see [4] and also [5] where a bistable system was considered). We treat the decay as a transition of a Brownian particle outside the region of a metastable state. Using the approach proposed by Malakhov [6], [7], that requires only knowledge of the behavior of a potential at $\pm\infty$, the required nondecay probability may be decomposed into a set of moments (cumulants), obtained recurrent formulas for these moments and approximately summarized them into the required probability. We will see, that the obtained nondecay probability demonstrates exponential behavior with a good precision even in the case of a small potential barrier in comparison with noise intensity.

II. MAIN EQUATIONS AND SET UP OF THE PROBLEM

Consider a process of Brownian diffusion in a potential profile $\Phi(x)$. Let a coordinate $x(t)$ of the Brownian particle described by the probability density $W(x,t)$ at initial instant of time has a fixed value $x(0) = x_0$ within the interval (c,d), i.e. the initial probability density is the delta function: $W(x,0) = \delta(x - x_0)$, $x_0 \in (c,d)$.

In this case the one-dimensional probability density $W(x,t)$ is the transition probability density from the point x_0 to the point x: $W(x,t) = W(x,t;x_0,0)$. It is known that the probability density $W(x,t)$ of the Brownian particle in the overdamped limit satisfies to the Fokker–Planck equation (FPE):

$$\frac{\partial W(x,t)}{\partial t} = -\frac{\partial G(x,t)}{\partial x} = \frac{1}{B}\left\{\frac{\partial}{\partial x}\left[\frac{d\varphi(x)}{dx}W(x,t)\right] + \frac{\partial^2 W(x,t)}{\partial x^2}\right\}. \qquad (1)$$

with the delta-shaped initial distribution. Here $B = h/kT$, $G(x,t)$ is the probability current, h is the viscosity (in computer simulations we put $h = 1$), T is the temperature, k is the Boltzmann constant and $\varphi(x) = \Phi(x)/kT$ is the dimensionless potential profile. In this paper we restrict ourselves by the case of metastable potentials, i.e. we consider an overdamped Brownian motion in a potential field $\varphi(x)$ in systems, having metastable states, such that $\varphi(-\infty) = +\infty$ and $\varphi(+\infty) = -\infty$. This leads to the following boundary conditions: $G(-\infty,t) = W(+\infty,t) = 0$. Note, that the results obtained may be generalized for potentials of arbitrary types, e.g. for such that $\varphi(\pm\infty) = \infty$.

It is necessary to find the probability $P(x_0,t)$ of a Brownian particle, located at the point x_0 $(t = 0)$ within the interval (c,d) to be at the time $t > 0$ inside of the considered interval: $P(x_0,t) = \int_c^d W(x,t)dx$. Further we for simplicity will call the probability $P(x_0,t)$ as nondecay probability. We suppose, that c and d are arbitrary chosen points of an arbitrary potential profile $\varphi(x)$ and boundary conditions at these points may be arbitrary: $W(c,t) \geq 0$, $W(d,t) \geq 0$. In this case there is the possibility for a Brownian particle to come back in the interval (c,d) after crossing boundary points.

III. MOMENTS OF DECAY TIME

Consider the nondecay probability $P(x_0,t)$. We can decompose this probability to the set of moments. On the other hand, if we know all moments, we can in some cases construct a probability as the set of moments. Thus, analogically to moments of the First Passage Time [8]- [10] we can introduce moments of decay time $\tau_n(c,x_0,d)$ (or, generally, moments of transition time, see [11], where it was performed for the probability $Q(x_0,t) = 1 - P(x_0,t)$):

$$\tau_n(c,x_0,d) = < t^n > = \frac{\int_0^\infty t^n \frac{\partial P(x_0,t)}{\partial t} dt}{P(x_0,\infty) - P(x_0,0)}. \tag{2}$$

Here we can formally denote the derivative of the probability divided by the normalization factor as $w(x_0,t)$ and thus introduce the probability density of decay time $w(x_0,t)$ in the following way [11]:

$$w(x_0,t) = \frac{\partial P(x_0,t)}{\partial t} \frac{1}{[P(x_0,\infty) - P(x_0,0)]}. \tag{3}$$

It is important to mention that the moments of decay (transition) time (2) is a generalization of the well-known moments of the First Passage Time for the case of arbitrary boundary conditions (see discussion in [11]). For example, in the considered case of the potential $\varphi(x)$ (such that $\varphi(-\infty) = +\infty$ and $\varphi(+\infty) = -\infty$) the moments of decay time coincide with the corresponding moments of the First Passage Time, if a reflecting boundary at the point c and an absorbing boundary at the point d are introduced. On the other hand, if we consider the decay of metastable state as transition over a barrier top, and compare mean decay time obtained via approach discussed in the present paper (case of a smooth potential without absorbing boundary) and the mean First Passage Time of the absorbing boundary located at the barrier top, we get two times difference between these time characteristics even in the case of a high potential barrier in comparison with the noise intensity. This difference may be significantly larger for a small barrier height, moments of the First Passage Time may both underestimate and overestimate the moments of decay time, depending on the concrete shape of the potential profile.

The cumulants of decay time æ$_n$ [12], [10] are much more useful for our purpose to construct the probability $P(x_0,t)$, that is the integral transformation of the just introduced probability density of decay time $w(x_0,t)$. Unlike the representation via moments, the Fourier transformation of the probability density (3) - the characteristic function - decomposed into the set of cumulants may be inversely transformed into the probability density.

The required moments of decay time may be obtained via the approach proposed by Malakhov [6], [7]. This approach is based on the Laplace transformation method of the FPE (1). Following this approach, one can introduce the function $H(x,s) \equiv s\hat{G}(x,s)$, where $\hat{G}(x,s) = \int\limits_0^\infty G(x,t)e^{-st}dt$ is the Laplace transformation of the probability current, and expand it in the power series in s:

$$H(x,s) \equiv s\hat{G}(x,s) = H_0(x) + sH_1(x) + s^2H_2(x) + \dots \tag{4}$$

It is possible to find the differential equations for $H_n(x)$ (see [6], [7]; $dH_0(x)/dx = 0$):

$$\begin{aligned} &\frac{dH_1(x)}{dx} = \delta(x - x_0), \\ &\frac{d^2H_n(x)}{dx^2} + \frac{d\varphi(x)}{dx}\frac{dH_n(x)}{dx} = BH_{n-1}(x), \quad n = 2,3,4,\dots \end{aligned} \tag{5}$$

Using the boundary conditions $W(+\infty,t) = 0$ and $G(-\infty,t) = 0$, one can obtain from (5) $H_1(x) = 1(x - x_0)$ and

$$\begin{aligned} H_2(x) &= -B\int\limits_{-\infty}^{x} e^{-\varphi(v)}\int\limits_{v}^{\infty} e^{\varphi(y)}1(y - x_0)dydv, \\ H_n(x) &= -B\int\limits_{-\infty}^{x} e^{-\varphi(v)}\int\limits_{v}^{\infty} e^{\varphi(y)}H_{n-1}(y)dydv, \quad n = 3,4,5,\dots \end{aligned} \tag{6}$$

Why did we calculate this recurrent formula for the functions $H_n(x)$? The matter is, that from formula (2) (taking the integral by parts and Laplace transforming it using the property $P(x_0,0) - s\hat{P}(x_0,s) = \hat{G}(d,s) - \hat{G}(c,s)$ together with the expansion (4)) one can get the following expressions for moments of decay time:

$$\begin{aligned} &\tau_1(c,x_0,d) = -(H_2(d) - H_2(c)), \\ &\tau_2(c,x_0,d) = 2(H_3(d) - H_3(c)), \\ &\tau_3(c,x_0,d) = -2\cdot 3(H_4(d) - H_4(c)), \dots \\ &\tau_n(c,x_0,d) = (-1)^n n!(H_{n+1}(d) - H_{n+1}(c)). \end{aligned} \tag{7}$$

One can represent the n-th moment in the following form:

$$\tau_n(c,x_0,d) = n!\tau_1^n(c,x_0,d) + r_n(c,x_0,d), \tag{8}$$

where the remainder $r_n(c,x_0,d)$ is much smaller than $n!\tau_1^n(c,x_0,d)$ for $\Delta\varphi \gg 1$ ($\Delta\varphi = \Delta\Phi/kT$ is the dimensionless barrier height). For $\Delta\varphi \leq 1$ the remainder becomes of importance and should be taken into account. Using the properties of cumulants [12], similar representation can be obtained for æ$_n$:

$$æ_n(c,x_0,d) = (n-1)!æ_1^n(c,x_0,d) + R_n(c,x_0,d). \tag{9}$$

It is known that the characteristic function $\Theta(x_0,\omega) = \int\limits_0^\infty w(x_0,t)e^{j\omega t}dt$ ($j = \sqrt{-1}$) can be represented as the set of cumulants ($w(x_0,t) = 0$ for $t < 0$):

$$\Theta(x_0,\omega) = \exp\left[\sum_{n=1}^{\infty}\frac{æ_n(c,x_0,d)}{n!}(j\omega)^n\right].$$

Unfortunately, nobody knows how to summarize this set exactly. If we will neglected by the remainders $R_n(c, x_0, d)$ in (9) then the required set may be summarized and inverse Fourier transformed, so we get:

$$w(x_0, t) = \frac{e^{-t/\tau}}{\tau}, \tag{10}$$

where τ is the mean decay time [6], [7] ($\tau(c, x_0, d) \equiv \tau_1 \equiv æ_1$):

$$\tau(c, x_0, d) = B \left\{ \int_{x_0}^{d} e^{\varphi(x)} \int_{c}^{x} e^{-\varphi(v)} dv dx + \int_{d}^{\infty} e^{\varphi(x)} dx \int_{c}^{d} e^{-\varphi(v)} dv \right\}. \tag{11}$$

Probably, similar procedure was previously used (see [9] and references therein and also [13]) for summation of the set of moments of the First Passage Time, when exponential distribution of the First Passage Time probability density was demonstrated for the case of a high potential barrier in comparison with noise intensity.

IV. NONDECAY PROBABILITY EVOLUTION

Integrating probability density (10), taking into account definition (3), we get the following expression for the nondecay probability $P(x_0, t)$ ($P(x_0, 0) = 1$, $P(x_0, \infty) = 0$):

$$P(x_0, t) = \exp(-t/\tau), \tag{12}$$

where mean decay time τ is expressed by (11). Where is the boundary of validity of formula (12) (and formulas (8)-(10))? To answer this question let us consider three examples of potentials having metastable states and compare numerically obtained nondecay probability with its exponential approximation (12). We can use the usual explicit difference scheme to solve the FPE (2), supposing the reflecting boundary condition $G(c_b, t) = 0$ far above the potential minimum and the absorbing one $W(d_b, t) = 0$ far below the potential maximum, instead of boundary conditions at $\pm\infty$, such that the influence of boundaries at c_b and d_b on the process of diffusion was negligible.

The first considered system is described by the potential $\Phi(x) = ax^2 - bx^3$ (see Fig. 1). For example, the following particular parameters may be taken: $a = 2$, $b = 1$ that leads to the barrier height $\Delta\Phi \approx 1.2$, $c = -2$, $d = 2a/3b$, and $kT = 0.5; 1; 3$. The corresponding curves of the numerically simulated probability and its exponential approximation are presented in Fig.2. In the worse case when $kT = 1$ the maximal difference between the corresponding curves is 3.2%.

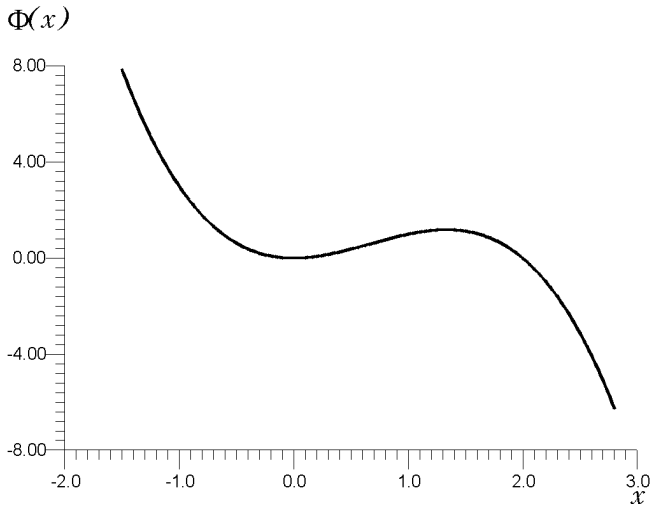

FIG. 1. Potential profile $\Phi(x) = ax^2 - bx^3$.

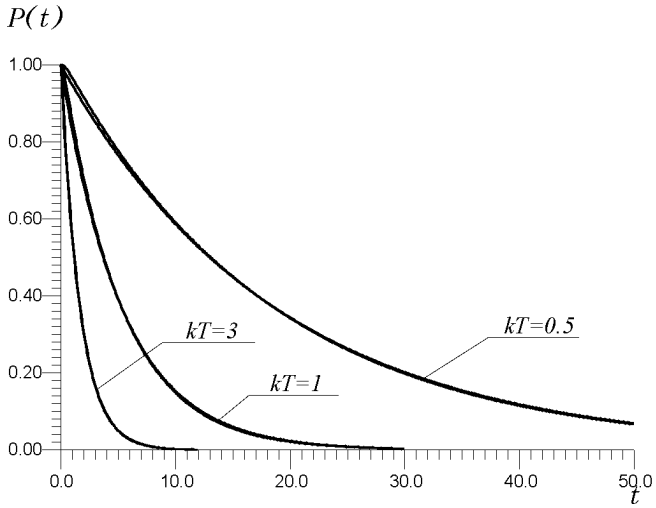

FIG. 2. Probability evolution in the potential $\Phi(x) = ax^2 - bx^3$.

The second considered system is described by the potential $\Phi(x) = ax^4 - bx^5$ (see Fig. 3). We can take the following particular parameters: $a = 1$, $b = 0.5$ that leads to the barrier height $\Delta\Phi \approx 1.3$, $c = -1.5$, $d = 4a/5b$, and $kT = 0.5; 1; 3$. The corresponding curves of the numerically simulated probability and its exponential approximation are presented in Fig.4. In the worse case ($kT = 1$) the maximal difference between the corresponding curves is 3.4%.

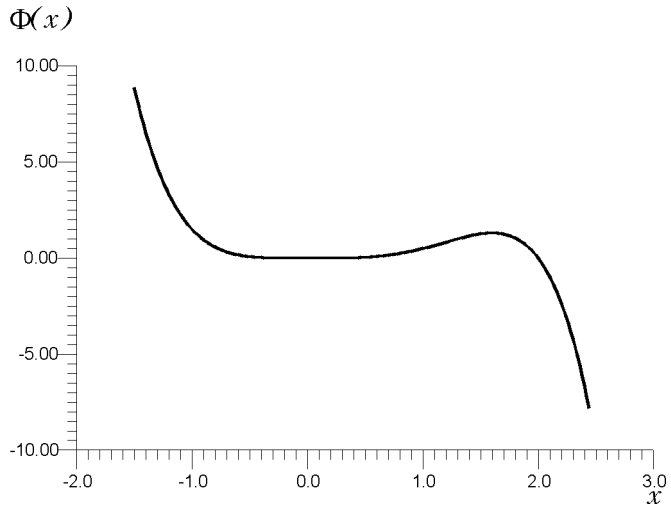

FIG. 3. Potential profile $\Phi(x) = ax^4 - bx^5$.

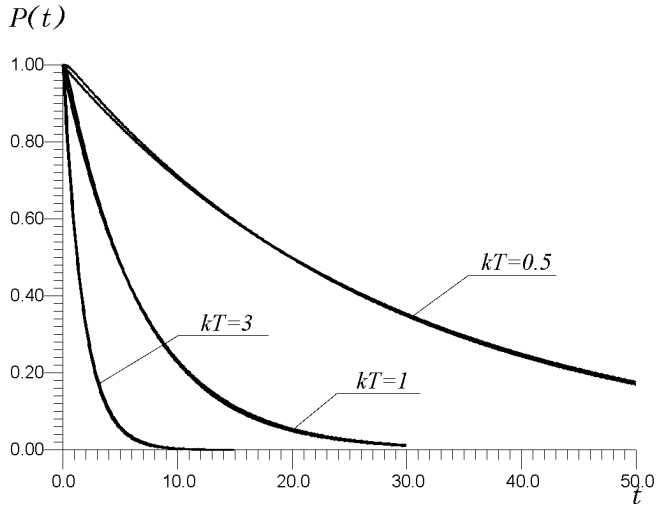

FIG. 4. Probability evolution in the potential $\Phi(x) = ax^4 - bx^5$.

The third considered system is described by the potential $\Phi(x) = 1 - \cos(x) - ax$ (see Fig. 5). This potential is multistable. Let us considere it in the interval $[-10, 10]$, taking into account three neighboring minima. Let, we take $a = 0.85$ that leads to the barrier height $\Delta\Phi \approx 0.1$, $c = -\pi - \arcsin(a)$, $d = \pi - \arcsin(a)$, $x_0 = \arcsin(a)$, and $kT = 0.1; 0.3; 1$. The corresponding curves of the numerically simulated probability and its exponential approximation are presented in Fig.6. In difference with two previous examples, this potential was considered in essentially longer interval and with smaller barrier. Thus, the difference between curves of the numerically simulated probability and its exponential approximation is significantly larger. Nevertheless, the qualitative coincidence is good enough.

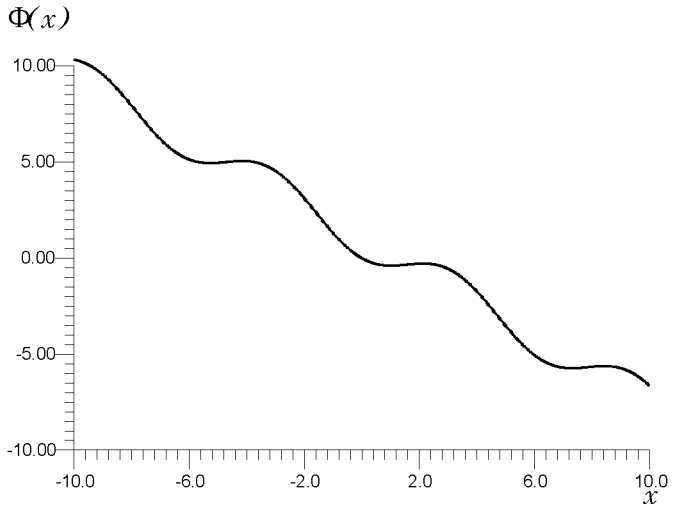

FIG. 5. Potential profile $\Phi(x) = 1 - \cos(x) - ax$.

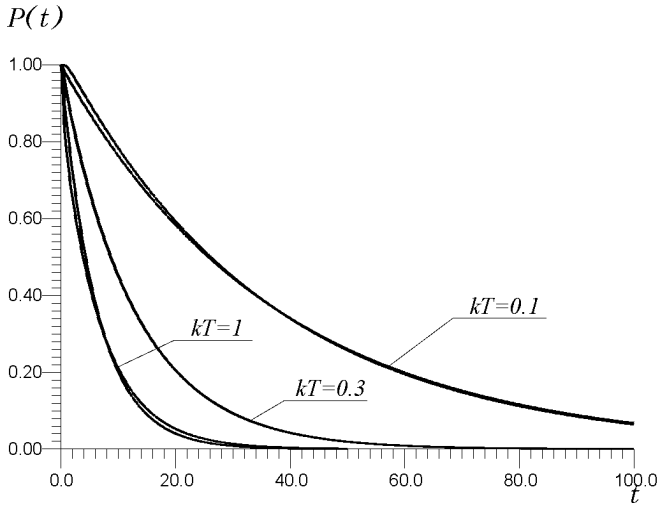

FIG. 6. Probability evolution in the potential $\Phi(x) = 1 - \cos(x) - ax$.

V. CONCLUSION

For all investigated examples, the exponential approximation gives an adequate behavior of the probability, if proper time scale is substituted into the factor of exponent. This approximation may be used in a wide range of parameters, enough for solution of many practical tasks, but it is necessary to remark, that the exponential approximation will lead to a significant error in the case of extremely large noise intensity, and in the case when the noise intensity is small, the potential is tilted, and the barrier is absent (purely dynamical motion slightly modulated by noise perturbations).

[1] C.W.Gardiner, Handbook of Stochastic methods (Springer-Verlag, 1985).
[2] A.Szabo, K.Schulten and Z.Schulten, Journ. Chem. Phys., **72**, 4350 (1980).

[3] W.Nadler and K.Schulten, Journ. Chem. Phys., **82**, 151 (1985).
[4] S.P.Nikitenkova and A.L.Pankratov, Preprint N adap-org/9807001 at http://xxx.lanl.gov.
[5] S.P.Nikitenkova and A.L.Pankratov, Physical Review E, **58**, 6964 (1998).
[6] A.N.Malakhov and A.L.Pankratov, Physica C **269**, 46 (1996).
[7] A.N.Malakhov, CHAOS **7**, 488 (1997).
[8] L.A.Pontryagin, A.A.Andronov and A.A.Vitt, Zh. Eksp. Teor. Fiz. **3**, 165 (1933) [translated by J.B.Barbour and reproduced in "Noise in Nonlinear Dynamics", 1989, edited by F.Moss and P.V.E. McClintock (Cambridge University Press, Cambridge) Vol. 1, p.329].
[9] P.Hanggi, P.Talkner and M.Borkovec, Rev.Mod.Phys., **62**, 251 (1990).
[10] H.Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).
[11] A.L.Pankratov, Physics Letters A **234**, 329 (1997).
[12] A.N.Malakhov, Cumulant analysis of random Non-Gaussian processes and its transformations (Sovetskoe Radio, Moscow, 1978, in Russian).
[13] K.Lindenberg and B.West, J. Stat. Phys., **42**, 201 (1986).

Stochastic processes and applications
Lecture 8

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I. INTRODUCTION

The investigation of nonlinear properties of Josephson junctions (JJs) is very important owing to their broad applications in logic devices. In past ten years, a lot of attention was payed to Josephson logic devices with high damping [1]- [4] because of their high-speed switching in comparison with underdamped devices. Papers [3], [4] present a description and analysis of the entire system of logic elements (single flux quantum logic devices). The processes going on in such devices are based on a reproduction of quantum pulses due to spasmodic changing by 2π of the phase difference of overdamped JJs.

It is well known that the use of HTS overdamped Josephson junctions as logic devices and memory cells is quite perspective because of low cooling costs and high operating frequencies (see, e.g., [5], [6], and also proceedings of the last ASC, ISEC, and EUCAS conferences). However, higher operation temperatures lead to higher noise levels and an increase in thermally-induced switching errors [7]. One of the problems arising in the design of HTS Josephson devices is the absence of a complete theory of noise-induced transitions in nonlinear systems, valid for arbitrary noise intensity. Moreover, the difference between the theoretically predicted (on the basis of approximate approaches [8]) and the experimentally observed switching probability of a Josephson balanced comparator has been recently demonstrated for temperatures above 25 K [6].

The aim of the present lecture is detailed analysis of noise properties of two simple overdamped Josephson elements forming the basis of many different types of logic devices: single Josephson junction and bistable memory cell on the basis of single junction SQUID.

II. SINGLE OVERDAMPED JOSEPHSON JUNCTION: THE MODEL AND MAIN EQUATIONS

It is known, that processes going on in a single JJ of a small size under a current I with fluctuations taken into account are well described by the Langevin equation. Let us restrict our consideration by JJs with high damping $\beta \ll 1$, which are widely used in logic elements with high-speed switching. Here $\beta = \dfrac{2e}{\hbar} I_c R_N^2 C$ is the McCamber–Stewart parameter, I_c is the critical current, $R_N^{-1} = G_N$ is the normal conductivity of a JJ, C is the capacitance, e is the electron charge and $\hbar$ is the Planck constant. In this case the Langevin equation takes the following form:

$$\omega_c^{-1} \frac{d\varphi(t)}{dt} = -\frac{du(\varphi)}{d\varphi} - i_F(t), \tag{1}$$

where

$$u(\varphi) = 1 - \cos\varphi - i\varphi \tag{2}$$

is the dimensionless potential profile (see Fig. 1.), φ is the difference in the phases of the order parameter on opposite sides of the junction, $i = \dfrac{I}{I_c}$, $i_F(t) = \dfrac{I_F}{I_c}$, I_F is the random component of the current, $\omega_c = \dfrac{2eR_N I_c}{\hbar}$ is the characteristic frequency of the JJ.

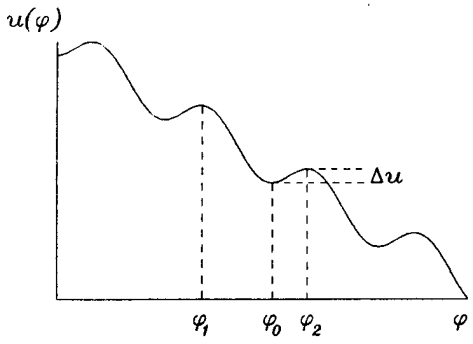

FIG. 1. Potential profile, describing single Josephson junction.

In the case when only thermal fluctuations are taken into account [9], the random current may be represented by the white Gaussian noise:

$$< i_F(t) >= 0, \quad < i_F(t) i_F(t+\tau) >= \frac{2\gamma}{\omega_c}\delta(\tau),$$

where $\gamma = \dfrac{2ekT}{\hbar I_c} = \dfrac{I_T}{I_c}$ is the dimensionless intensity of fluctuations, T is the temperature and k is the Boltzmann constant.

If fluctuations are small enough, we can neglect it and Eq. (1) transforms to the dynamic equation:

$$\omega_c^{-1}\frac{d\varphi(t)}{dt} = -\frac{du(\varphi)}{d\varphi}. \tag{3}$$

Let us consider a single JJ, biased by a constant current I_0 [3]. If the current going on across the junction is not so large, $I_0 < I_c$, then Eq. (3) has the set of the steady-state solutions:

$$\varphi_n = \arcsin(I_0/I_c) + 2\pi n, \qquad (n = 0, \pm 1, \pm 2, ...).$$

Any such a solution describes a "superconductive" or a "steady-state" S-state of the JJ: if $I_0 < I_c$ a voltage across the junction is equal to zero. It is obviously, that if there are no fluctuations in the system, the phase difference will be infinitely long time located in the potential minimum number n and without any restrictions we can assume that $n_{initial} = 0$. However, if the fluctuations intensity is not equal to zero, there is a finite probability of the phase difference jump across a barrier towards a neighbour potential minimum. The mean time between two sequential jumps is called the life time of the S-state.

If a current across the JJ is larger than the critical current, $I > I_c$, there are no steady-state solutions of Eq. (3) and such a state is known as the resistive state (R-state).

If the current $I > I_c$ is applied, the JJ switches to the R-state. However, an output pulse will be born not at the same moment, but at the later time. Such a time is called the turn-on delay time between input and output (reproduced) pulses [3], [10]. Thus, the input pulse at the time $t = 0$ changes the current across the junction from the value $I_0 < I_c$ to the value $I > I_c$, turns-on the system from the superconductive state to the resistive one and the phase difference begins to slide down in the potential profile, causes the process of Josephson generation.

If the duration of the pulse front is much smaller than the turn-on delay (a rectangular pulse) then at initial instant of time the phase difference will be still located at the point, where it was in the

S-state and no generation would be observed. In this case the time of the turn-on delay like the life time of the S-state may be defined as the transition time of the phase difference from the point φ_0 (a minimum of an initial potential well) to some point φ over a barrier. Such an identity of these time definitions is connected with the fact that at the presence of fluctuations the distinction between terms the S-state and the R-state has no sense, because Josephson generation becomes possible at $I < I_c$ [11]. That is why it has significance to introduce a unite term of the life time of metastable state τ, implying the life time of the S-state at $I < I_c$ and the turn-on delay time at $I > I_c$. In the paper [10] τ was defined as a reach time from the point $\pi/2$ to the point $\pi/2 + 1/2$. We following this procedure, for unification change $\pi/2 + 1/2$ to π and then τ, obtained analytically in the paper [10] without any fluctuations, takes the form ($i > 1$):

$$\tau_d = \frac{1}{\omega_c}\left(\frac{1}{\sqrt{i^2-1}}\left[\pi - 2\arctan\left(\frac{i-1}{\sqrt{i^2-1}}\right)\right]\right). \tag{4}$$

The use of high-T_c superconductors are connected with increasing of fluctuations intensity, because the parameter $I_T = \dfrac{2ekT}{\hbar}$ increases with increasing of temperature T. In the case when γ increases, ignoring of the fluctuations becomes incorrect and it is necessary to operate directly with Eq. (1), so the phase difference becomes a random value described by the probability density $W(\varphi, t)$.

It is well known that the Fokker-Planck equation (FPE) for the probability density $W(\varphi, t)$ corresponding to Eq. (1) has the form:

$$\frac{\partial W(\varphi,t)}{\partial t} = -\frac{\partial G(\varphi,t)}{\partial \varphi} = \omega_c \frac{\partial}{\partial \varphi}\left\{\frac{du(\varphi)}{d\varphi}W(\varphi,t) + \gamma\frac{\partial W(\varphi,t)}{\partial \varphi}\right\}. \tag{5}$$

The initial and boundary conditions on the probability density and the probability current for the potential profile (2) are as follows:

$$W(\varphi,0) = \delta(\varphi - \varphi_0),\ W(+\infty,t) = 0,\ G(-\infty,t) = 0.$$

The presence of fluctuations not only causes the finiteness of the life time of S-state [11], but also in determined manner influences on the turn-on delay time. And we will analyze now influence of fluctuations on these time characteristics, but first let us consider how fluctuations affect the current-voltage characteristic of an overdamped single Josephson junction.

III. CURRENT-VOLTAGE CHARACTERISTIC OF SINGLE OVERDAMPED JOSEPHSON JUNCTION

As you remember, the voltage $V(t)$ of a Josephson junction is connected with the phase $\varphi(t)$ by the relation:

$$V(t) = \frac{\hbar}{2e}\frac{d\varphi(t)}{dt}. \tag{6}$$

This means, that if we know time evolution of the phase as function of bias current - we know the voltage. But we have a phase subjected to noise perturbations and wish to get averaged phase $<\varphi(t)>$ which will give us averaged voltage $<V(t)>$.

Let us return again to the Langevin equation (1). This equation expresses the time derivative of random phase. If we now perform averaging of the Langevin equation, taking into account that mean value of noise is zero and substituting the concrete function for derivative of the potential (2) we get:

$$\omega_c^{-1}\frac{d<\varphi(t)>}{dt} = i - <\sin(\varphi)> . \qquad (7)$$

Thus, if we know $<\sin(\varphi)>$, then we know the required voltage. Moreover, we have to know only stationary function $<\varphi(t)>$ and, thus, stationary function $<\sin(\varphi(t))>$ to get the current-voltage characteristic which significantly simplifies our task.

How can we get the function $<\sin(\varphi)>$? The most natural way is to obtain the probability density of the phase $W(\varphi,t)$ and get the required $<\sin(\varphi)>$ as: $<\sin(\varphi)> = \int\limits_{-\infty}^{\infty} \sin(x)W(x,t)dx$. But as you can guess, the stationary probability density is equal to zero in the considered case, described by the potential (2) with the mentioned boundary conditions at $\pm\infty$.

Here one old trick can help us, I even do not remember who first used it, but it was known long time before the original paper by Ambegaokar and Halperin [11], who first applied it to get the current-voltage characteristic of overdamped single JJ with noise taken into account.

Because of periodicity of the required function $\sin(\varphi)$ one can introduce periodic boundary conditions $W(\pi,t) = W(-\pi,t)$ and consider the process of diffusion within the reduced interval $(-\pi,\pi)$ due to the fact that: $\int\limits_{-\infty}^{\infty} \sin(x)W(x,t)dx = \sum\limits_{n=-\infty}^{\infty} \int\limits_{-\pi}^{\pi} \sin(x+2\pi n)W(x+2\pi n,t)dx = \int\limits_{-\pi}^{\pi} \sin(x)W_r(x,t)dx$, where $W_r(x,t)$ is the reduced probability density. This reduced probability density will already reach nonzero steady-state distribution for $t \to \infty$. The steady-state reduced probability density $W_r(\varphi,\infty) = W_{rst}(\varphi)$ may be obtained from equation (5), supposing that the time derivative is equal to zero, and integrating the reminder twice. Two arbitrary constants are determined from the periodic boundary condition and from normalization condition $\int\limits_{-\pi}^{\pi} W_{rst}(x)dx = 1$. The reduced steady-state probability density $W_{rst}(\varphi)$ has the form:

$$W_{rst}(\varphi) = \frac{e^{-u(\varphi)/\gamma} \int\limits_{x}^{x+2\pi} e^{u(y)/\gamma}dy}{\int\limits_{-\pi}^{\pi} e^{-u(x)/\gamma} \int\limits_{x}^{x+2\pi} e^{u(y)/\gamma}dydx}, \qquad (8)$$

where the potential $u(\varphi)$ is expressed by formula (2), γ is the dimensionless noise intensity.

Using the obtained reduced steady-state probability density one can get $\langle\sin(\varphi)\rangle$ and, thus, the required current-voltage characteristic. For more details you may see the original paper by Ambegaokar and Halperin [11]. I only wish to mention, that due to noise influence even in superconducting state you may observe some nonzero voltage at the Josephson junction, and namely because of this reason the distinction between terms the S-state and the R-state has no sense at nonzero noise intensity.

IV. EXACT TIME CHARACTERISTICS

Let us analyze now influence of fluctuations on the superconductive state life time and the turn-on delay time. The used method for obtaining the required time characteristics was presented in detail in previous lecture and we will not consider it here.

Let me remind that the required time characteristics may be introduced from the probability $P(\varphi_0,t)$ that transition of the phase point from φ_0 outside the considered interval (φ_1,φ_2) will not occur during the time $t>0$: $P(\varphi_0,t) = \int\limits_{\varphi_1}^{\varphi_1} W(\varphi,t)d\varphi$.

By analogy to moments of the First Passage Time (FPT) we can introduce the moments $\tau_n(\varphi_1, \varphi_0, \varphi_1) = \tau_n$ of transition time [21] bearing in mind that the phase point may cross the boundary many times before leaving the considered interval:

$$\tau_n =< t^n >= \frac{\int\limits_0^\infty t^n \frac{\partial P(\varphi_0,t)}{\partial t} dt}{P(\varphi_0,\infty) - P(\varphi_0,0)}, \tag{9}$$

where $P(\varphi_0,\infty) - P(\varphi_0,0) = \int\limits_0^\infty \frac{\partial P(\varphi_0,t)}{\partial t} dt$ is the factor of normalization. In our particular case $P(\varphi_0,0) = 1$, $P(\varphi_0,\infty) = 0$.

Let me remind also that we agreed above to introduce a unite term of the life time of metastable state (or, equivalently, the mean escape time) τ, implying the life time of the S-state at $I < I_c$ and the turn-on delay time at $I > I_c$.

So, using the approach proposed by Malakhov [12] one can get the exact expression of the mean escape time of the random value φ from the interval $[\varphi_1, \varphi_2]$ for an arbitrary potential profile $u(\varphi)$ with $u(-\infty) = +\infty$, $u(+\infty) = -\infty$:

$$\tau = B \left\{ \int\limits_{\varphi_0}^{\varphi_2} e^{u(x)/\gamma} \int\limits_{\varphi_1}^{x} e^{-u(\varphi)/\gamma} d\varphi dx + \int\limits_{\varphi_1}^{\varphi_2} e^{-u(\varphi)/\gamma} d\varphi \cdot \int\limits_{\varphi_2}^{\infty} e^{u(\varphi)/\gamma} d\varphi \right\}. \tag{10}$$

Thus, as it follows from Eq.(10) the life time of the metastable state for the potential profile $u(\varphi) = 1 - \cos\varphi - i\varphi$ has the form:

$$\begin{aligned} \tau = B \left\{ \int\limits_{\varphi_0}^{\varphi_2} e^{-(\cos x + ix)/\gamma} \int\limits_{\varphi_1}^{x} e^{(\cos\varphi + i\varphi)/\gamma} d\varphi dx + \right. \\ \left. + \int\limits_{\varphi_1}^{\varphi_2} e^{(\cos\varphi + i\varphi)/\gamma} d\varphi \cdot \int\limits_{\varphi_2}^{\infty} e^{-(\cos\varphi + i\varphi)/\gamma} d\varphi \right\}. \end{aligned} \tag{11}$$

Let us analyze the formula (11) for different values of the current i and the fluctuations intensity γ. For $0 < i < 1$ and $\gamma \ll 1$ the asymptotic representation of the formula (11) may be also obtained by the Kramers' method [13], [16]:

$$\tau_K = \frac{2\pi}{\omega_c \sqrt{1 - i^2}} e^{\alpha}, \tag{12}$$

where $\alpha = \Delta u/\gamma = (2\sqrt{1 - i^2} + 2i(\arcsin i - \frac{\pi}{2}))/\gamma$ is the dimensionless potential barrier height (Fig. 1). The results of computer simulation of Eq. (11) demonstrate that for $i > 0.3$ formula (12) holds true up to $\alpha \geq 1$ (see Fig. 2, where $\vartheta = \omega_c \tau$, $\vartheta_K = \omega_c \tau_K$, $\varphi_2 = \pi$, $\varphi_0 = \arcsin(i)$, $\varphi_1 = -\pi$, $i = 0.5$). For $i < 0.3$, however, the difference between τ (see Eq. (11)) and τ_K increases, process of diffusion becomes slower because of influence of neighbour potential barriers. For instance, at $i = 0.01$ the ratio $\tau/\tau_K \approx 40$ for $\alpha = 1$ and $\tau/\tau_K \approx 4$ for $\alpha = 10$. Actually, formula (11) is valid only for $i > 0$, because at $i = 0$ the process of diffusion from the initial well is going on very slowly and the definition (9) does not applicable here. The results, presented in paper [14] demonstrate that the time scale of diffusion from a potential well to a flat profile is proportional to $\sim e^{2\alpha}$, where α is the dimensionless depth of the well.

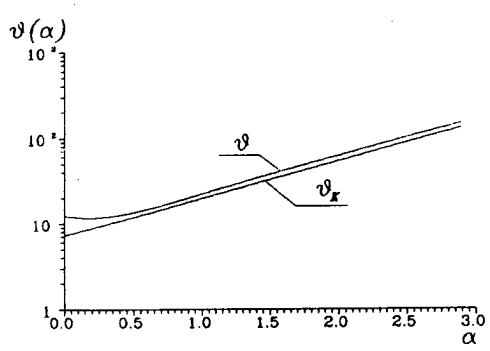

FIG. 2. The exact metastable state life time ϑ and Kramers' time ϑ_K, versus the potential barrier height α ($\vartheta = \omega_c\tau$, $\vartheta_K = \omega_c\tau_K$, $\varphi_2 = \pi$, $\varphi_0 = \arcsin(i)$, $\varphi_1 = -\pi$, $i = 0.5$).

If the intensity of thermal fluctuations is large, $\gamma \gg 1$, both for $i < 1$ and for $i > 1$ the influence of cosinusoidal part of the potential becomes small and we can consider the potential $u(\varphi) \approx 1 - i\varphi$. Then τ approximately equals:

$$\tau \approx \frac{1}{\omega_c}\left[\frac{\varphi_2 - \varphi_0}{i} + \frac{\gamma}{i^2}\left\{1 - e^{i(\varphi_1 - \varphi_0)/\gamma}\right\}\right], \tag{13}$$

i.e. the life time increases proportionally to increasing of the fluctuations intensity. However, at very large γ, $e^{i(\varphi_1-\varphi_0)/\gamma}$ tends to unity and we get the indeterminate form which may be evaluated as follows:

$$\tau \approx \frac{1}{\omega_c}\left[\frac{\varphi_2 - \varphi_1}{i}\right], \tag{14}$$

so τ does not depend on the fluctuations intensity.

For $i > 1$ and $\gamma \ll 1$ one can obtain the following asymptotic representation of the formula (11):

$$\begin{aligned}\tau \approx \frac{1}{\omega_c}\Bigg\{ & \frac{2}{\sqrt{i^2-1}}\arctan\left(\frac{i\tan(x/2)-1}{\sqrt{i^2-1}}\right)\Bigg|_{x=\varphi_0}^{x=\varphi_2} + \\ & +\gamma\left[\frac{1}{2(i-\sin\varphi_2)^2} + \frac{1}{2(i-\sin\varphi_0)^2}\right] + \\ & +\gamma^2\int_{\varphi_0}^{\varphi_2}\left[\frac{3\cos^2 x}{(i-\sin x)^5} - \frac{\sin x}{(i-\sin x)^4}\right]dx + \ldots\Bigg\}.\end{aligned} \tag{15}$$

If the fluctuations intensity is equal to zero ($\gamma = 0$), then formula (15) coincides with the formula obtained without any fluctuations in paper [10] and, in particular, with formula (4) for $\varphi_2 = \pi$ and $\varphi_0 = \pi/2$.

Thus, the representation (15) shows that increasing of the fluctuations intensity for $\gamma \ll 1$ causes increasing of the metastable state life time (see Fig. 3, where $\vartheta = \omega_c\tau$, Figs. 3 and 4 were plotted for $\varphi_2 = \pi$, $\varphi_0 = \pi/2$, $\varphi_1 = -\pi$).

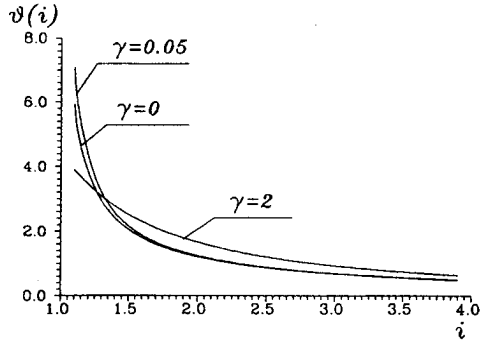

FIG. 3. The turn-on delay time ϑ, versus the current i for different values of γ ($\vartheta = \omega_c \tau$, $\varphi_2 = \pi$, $\varphi_0 = \pi/2$, $\varphi_1 = -\pi$).

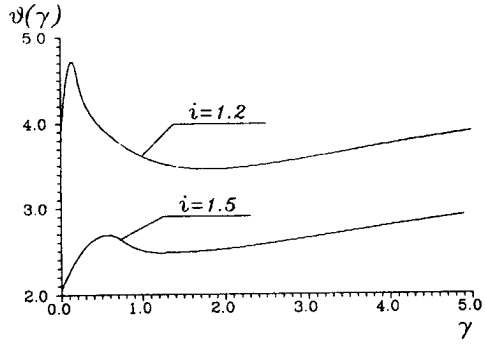

FIG. 4. The turn-on delay time ϑ, versus the intensity of thermal fluctuations γ for different values of i ($\vartheta = \omega_c \tau$, $\varphi_2 = \pi$, $\varphi_0 = \pi/2$, $\varphi_1 = -\pi$)

The effect of turn-on delay increasing may be considered in detail by plotting the dimensionless time ϑ as a function of the fluctuations intensity for different values of the current i. Figure 4 demonstrates three different intervals of $\vartheta(\gamma)$-curve behaviour. It may be explained taking into account the competition of two factors: the variance' increasing with increasing of a temperature and an influence of the returning force of the potential profile (2).

When the phase variance is not so large, the main part of the phase probability distribution is located on the flat part near the point $\varphi = \pi/2$ and the fluctuations influence is more than the returning force influence. Further, when the variance' quantity becomes larger, the returning force quickly increases with the coordinate and we can see decreasing of the turn-on delay time. Finally, when the variance' value becomes large enough, we should take into account an influence of another potential periods and the asymptote of $\vartheta(\gamma)$-curve may be represented by formulae (13), (14). Note, in conclusion, that for $\gamma \ll 1$, as it should, τ both in formulae (12) and (15) does not depend on φ_1 value, because in this case the backward probability current is negligibly small.

Conclusions

Application of JJs as elements of logic devices supposes that the probability of thermally induced errors should be small enough, i.e. the life time of the "correct" state should be much larger than the operation cycle. Simple estimations following from the above presented formulae can demonstrate

the bound of the fluctuations intensity γ below which the logic element will function properly. Considering for the sake of simplicity the turn-on delay time as the main part of an operation cycle, one can see (Fig. 3) that in terms of the dimensionless time $\vartheta = \omega_c \cdot \tau$, the turn-on delay time is approximately equal to unity for $i \geq 2$ and $\vartheta \leq 7$ for $i \geq 1.1$. The prefactor of the formula (12) for $i = 0.8$ is of the order of 10; substituting $\alpha = 10$ into this formula, we get the value of S-state life time equals $10^5 - 10^6$ that is well above than the turn-on delay time. Taking into account that $\Delta u \approx 0.1$ for $i = 0.8$, it is enough to assume $\gamma \leq 0.01$ in order that α to be 10. The influence of thermal fluctuations on the turn-on delay time for $\gamma \leq 0.01$ is well predicted by formula (15).

For example, it is interesting to plot the function $E(i) = (\tau/\tau_d - 1)$ for $\gamma = 0.01$, where τ is the exact turn-on delay time (15) and τ_d is described by formula (4) (see Fig. 5). The function $E(i)$ demonstrates the relative difference between τ and τ_d, and help to choose the interval of the current i, in which the relative error $E(i)$ will be as small as necessary for concrete applications.

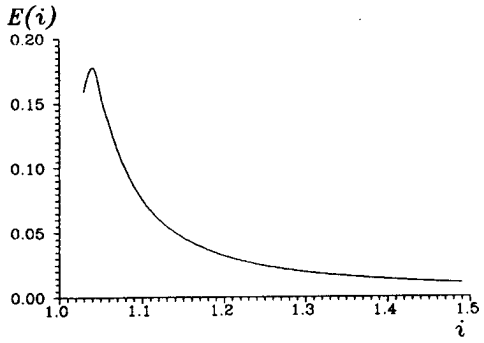

FIG. 5. The relative difference $E(i)$ between τ and τ_d, versus the current i, demonstrating the effect of fluctuations on the turn-on delay time ($\gamma = 0.01$, $\varphi_2 = \pi$, $\varphi_0 = \pi/2$, $\varphi_1 = -\pi$).

V. BISTABLE MEMORY CELL BASED ON SINGLE JUNCTION SQUID

The single junction SQUID [16] (consisting of a superconducting ring enclosed by a Josephson junction) is used for storage of information as the main element of memory cells. When the the SQUID is applied as a bistable memory cell, one of the most important parameters is immunity to thermal fluctuations which can spontaneously switch the memory cell from one state to another. However, because of mathematical difficulties, only approximate evaluations have been done before for such important characteristics as the mean decay time of the "correct" state (or mean time of spontaneous switching), while the variance and higher cumulants of the decay time have not been investigated. Also, it is known that, if the ratio between a potential barrier separating stable states and noise intensity is high, the probability that decay of the "correct" state of the memory cell will not occur until some time t (nondecay probability) is proportional to the exponent: $\sim \exp(-t/\vartheta_K)$ [15], where $\vartheta_K = \tau_K/2$ and τ_K is the approximate mean decay time of the "correct" state (Kramers' time) [16], [13].

Let us consider how it is possible to completely describe noise properties of the bistable memory cell using the approach which we considered in previous lecture [17].

It is known that the dynamics of an overdamped single junction SQUID with fluctuations taken into account is well described by the Langevin equation (1), where the potential have the following form:

$$u(\varphi) = 1 - \cos\varphi + (\varphi - \varphi_e)^2/2\ell, \tag{16}$$

$\varphi = 2\pi\Phi/\Phi_0$ is the dimensionless flux through the ring, Φ_0 is the flux quantum, the quantity φ_e describes the external flux, $\ell = L/L_0$, L is the inductance of the ring, $L_0 = \Phi_0/2\pi I_c$, I_c is the critical current of the junction.

In the case of nonzero noise intensity the flux φ is a random quantity described by the transitional probability density $W(\varphi, t)$, which is governed by the Fokker-Planck equation (5). The initial and boundary conditions for Eq. (5) with the potential (16) are:

$$W(\varphi, 0) = \delta(\varphi - \varphi_0) \quad \text{and} \quad \mathrm{G}(\pm\infty, \mathrm{t}) = 0. \tag{17}$$

The nonlinear dynamical system described by the potential profile (16) may have one or several stable states depending on quantities of parameters ℓ and φ_e. To use the parametric quantron as a memory cell, it is enough to have two stable states [16], which may be realized at $3 < \ell < 8$, $\varphi_e = \pi$. In this particular case the potential (16) has the parabolic barrier separating two wells with parabolic walls, slightly modulated by the cosine term. However, it is difficult to analyze the functioning of such a system because the solution of FPE (5) for the potential (16) is unknown. When the potential barrier separating the stable states is high enough in comparison with the noise intensity, $\Delta u \gg \gamma$, it is possible to approximately obtain the mean decay time of the "correct" state [16] on the basis of the Kramers' method [13] ($\alpha = \Delta u/\gamma$):

$$\tau_K = \frac{2\pi}{b\omega_c} e^{\alpha}, \quad \alpha \gg 1, \tag{18}$$

where $b = \sqrt{b_{min} b_{max}}$, b_{min} and b_{max} are the curvatures of the bottom of the well and the top of the barrier of the potential (16), respectively. In this case the probability $P(\varphi_0, t)$ that decay of the "correct" state will not occur until some time t may be very well approximated by the exponent:

$$P(\varphi_0, t) = \frac{\exp(-t/\vartheta_K) + 1}{2}, \quad \vartheta_K = \tau_K/2. \tag{19}$$

Here φ_0 is the coordinate of the initial delta-shaped probability distribution. Certainly, in the case (18),(19) the probability does not depend on φ_0, but searching further for the exact probability evolution we will keep in mind the initial distribution at φ_0. Formula (19) may be obtained via approach presented in the book by Gardiner [15].

Let, initially, a bit of information be stored in the memory cell by locating the phase point in the left minimum of the potential (16), such that $\varphi_0 \leq \pi$. The decay time of the "correct" state we define as the time needed to cross the barrier top $\varphi = \pi$. It is clear that this decay time is a random value and the problem is how to obtain its mean $\tau = æ_1 =< t >$, variance $D = æ_2 =< t^2 > - < t >^2$ and higher cumulants $æ_n$.

The required time characteristics may be introduced from the probability $P(\varphi_0, t)$ that transition of the phase point from φ_0 outside the considered interval $(-\infty, \pi)$ will not occur during the time $t > 0$: $P(\varphi_0, t) = \int\limits_{-\infty}^{\pi} W(\varphi, t) d\varphi$.

By analogy to moments of the First Passage Time (FPT) [3] we can introduce the moments $\vartheta_n(\varphi_0, \pi) = \vartheta_n$ of transition time [21] bearing in mind that even for an infinitely long time the phase point may still be located within the considered interval because $\lim\limits_{t\to\infty} P(\varphi_0, t) = 1/2$:

$$\vartheta_n =< t^n >= \frac{\int\limits_0^{\infty} t^n \frac{\partial P(\varphi_0, t)}{\partial t} dt}{P(\varphi_0, \infty) - P(\varphi_0, 0)}, \tag{20}$$

where $P(\varphi_0,\infty) - P(\varphi_0,0) = \int\limits_0^\infty \frac{\partial P(\varphi_0,t)}{\partial t} dt$ is the factor of normalization. In our particular case $P(\varphi_0,0) = 1$, $P(\varphi_0,\infty) = 1/2$. Here we can formally denote the derivative of the probability divided by the factor of normalization as $w(\varphi_0,t)$ and thus introduce the probability density of transition time in the following way:

$$w(\varphi_0,t) = \frac{\partial P(\varphi_0,t)}{\partial t[P(\varphi_0,\infty) - P(\varphi_0,0)]}. \tag{21}$$

It is easy to check that the normalization condition is satisfied given with such a definition, $\int\limits_0^\infty w(\varphi_0,t)dt = 1$. The condition of nonnegativity of the probability density $w(\varphi_0,t) \geq 0$ is, actually, the monotonic condition of the probability $P(\varphi_0,t)$.

The above-mentioned cumulants of transition time $æ_n$ are much more useful for our purpose to construct the probability $P(\varphi_0,t)$ that is the integral transformation of the just introduced probability density of transition time $w(\varphi_0,t)$. Unlike the representation via moments, the Fourier transformation of the probability density - the characteristic function - decomposed into a set of cumulants may be inversely transformed into the required probability density. The representation of $æ_n$ via moments ϑ_n is described in the book by Malakhov [18] (see also [19]).

VI. MOMENTS OF DECAY TIME OF "CORRECT" STATE

It is known that there is the recurrent formula [20] for moments of the FPT of the boundary located at $\varphi = c > \varphi_0$ by the phase point under noise perturbation ($u(-\infty) = +\infty$):

$$T_n(\varphi_0,c) = nB \int\limits_{\varphi_0}^{c} e^{u(\varphi)/\gamma} \int\limits_{-\infty}^{\varphi} T_{n-1}(x,c) e^{-u(x)/\gamma} dx d\varphi, \tag{22}$$

which represents the n-th moment of the FPT directly from the function of the potential profile $u(\varphi)$ and the $(n-1)$-th moment. Here $T_0(\varphi_0,c) = 1$ and $T_1(\varphi_0,c)$ is the mean FPT.

Using the duality of time characteristics, proved in [21], it can be demonstrated that all moments of transition time ϑ_n in a symmetric potential over a point of symmetry coincide with the corresponding moments of the First Passage Time of the boundary located at the point of symmetry: $\vartheta_n(\varphi_0,c) = T_n(\varphi_0,c)$ (in our particular case $c = \pi$). Thus, formula (22) is also valid for moments of transition time. When the intensity of thermal fluctuations is much smaller than the barrier height, $\gamma \ll \Delta u$, the following asymptotic representation can be obtained from formula (5) for moments of transition time:

$$\vartheta_n(\varphi_0,c) = n!\vartheta_1^n(\varphi_0,c), \quad \Delta u \gg \gamma. \tag{23}$$

The results of computer simulation demonstrate that expression (23) is valid up to $\Delta u/\gamma \geq 2$. Using the properties of cumulants [18], similar representation can be obtained for $æ_n$:

$$æ_n(\varphi_0,c) = (n-1)!æ_1^n(\varphi_0,c), \quad \Delta u \gg \gamma. \tag{24}$$

It is known that the characteristic function $\Theta(\varphi_0,\omega) = \int\limits_0^\infty w(\varphi_0,t)e^{j\omega t}dt$ ($j = \sqrt{-1}$) can be represented as a set of cumulants:

$$\Theta(\varphi_0,\omega) = \exp\left[\sum_{n=1}^{\infty} \frac{æ_n(\varphi_0,c)}{n!}(j\omega)^n\right].$$

For our particular case (24) this set can be summarized and inverse Fourier transformed, so we get:

$$w(\varphi_0, t) = \frac{e^{-t/\tau}}{\tau}, \quad \Delta u \gg \gamma, \tag{25}$$

where τ is the mean transition time ($\tau(\varphi_0, \pi) \equiv \vartheta_1 \equiv æ_1$):

$$\tau(\varphi_0, \pi) = \frac{1}{\gamma\omega_c} \int\limits_{\varphi_0}^{\pi} e^{u(\varphi)/\gamma} \int\limits_{-\infty}^{\varphi} e^{-u(x)/\gamma} dx d\varphi, \tag{26}$$

with the asymptotic representation ($\alpha = \Delta u/\gamma$):

$$\tau(\varphi_0, \pi) = \tau = \frac{\pi}{b\omega_c} e^{\alpha}, \quad \alpha \gg 1. \tag{27}$$

Formula (25) is, unfortunately, not valid for small periods of time $t \ll \tau$, because it assumes that a quasi-steady-state distribution in the initial well is already reached and then the escape over the barrier happens, so the initial transition to the quasi-steady-state is neglected. Namely, this circumstance will lead to a slight distinction of the numerically simulated probability from its exponential approximation (see the next section). The asymptotical representation of the probability density $w(\varphi_0, t)$ for small periods of time was obtained in [22] and it has been demonstrated that the time of transition to a quasi-steady-state in the initial well is really much smaller than the mean decay time (27).

VII. PROBABILITY EVOLUTION

Integrating probability density (25), with the account of definition (21), we get the following expression for the probability $P(\varphi_0, t)$ that decay of the "correct" state of a memory cell will not occur until some time t ($\alpha = \Delta u/\gamma$):

$$P(\varphi_0, t) = \frac{\exp(-t/\tau) + 1}{2}, \quad \alpha \gg 1, \tag{28}$$

where the mean decay time τ (27) is two times smaller than the Kramers' time (18) and thus formula (28) completely coincides with (19). Actually, the validity of formula (28) coincides with validity of formula (27), and as previous calculations demonstrate, formula (27) is valid up to $\alpha \geq 2$. Our aim was to numerically test this fact for formula (28). We used the usual explicit difference scheme to solve the Fokker-Planck equation (5), assuming the reflecting boundary conditions $G(\pm d, t) = 0$ to be far from the potential minima, instead of natural boundary conditions (17). Note, that we located reflecting boundaries far enough from the potential minima and controlled it carefully, thus even for the large noise intensity (indicated below) the influence of reflecting boundaries on the diffusion process was negligible. Comparing the computer simulation results with formula (28), we have substituted exact mean decay time $\tau(\varphi_0, \pi)$ (26) for asymptotic formula (27) and have found a really close coincidence between the curves, even for a noise intensity larger than unity, where formula (27) is not valid (see Fig.6). Figure 6 presents the numerically simulated nondecay probability $P(\varphi_0, t)$ and the approximate one versus dimensionless time $t^* = \omega_c \cdot t$. The potential barrier height and the dimensionless inductance are, respectively: $\Delta u \approx 1.3$, $\ell = 6$. The maximal difference δ between the corresponding curves is: $\delta < 0.4\%$, $\gamma = 0.2$; $\delta < 1\%$,$\gamma = 0.3$; $\delta \approx 1\%$, $\gamma = 0.4$; $\delta < 1.5\%$, $\gamma = 0.5$; $\delta < 3\%$, $\gamma = 1$; $\delta \approx 2\%$, $\gamma = 2$; $\delta \approx 5\%$, $\gamma = 5$; $\delta \approx 7\%$, $\gamma = 10$.

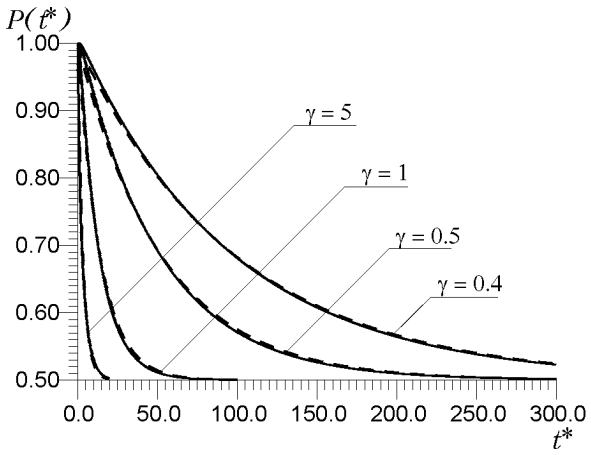

FIG. 6. Evolution of the nondecay probability for different values of noise intensity.

So, we have demonstrated that the approximate model of exponential decay of the "correct" state of a memory cell is applicable with a good precision even for a large noise intensity (large enough for real applications, when the considered system can not already be used for storage of information), if the approximate decay time is replaced by the exact one. The presented theory may be easily used for design and analysis of real devices.

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[1] A.H.Silver, R.R.Phillips and R.D.Sandell, IEEE Trans. Magn., 21 (1985) 204.
[2] G.Oya, M.Yamashita and Y.Sawada, IEEE Trans. Magn., 21 (1985) 880.
[3] K.K. Likharev, O.A. Mukhanov and V.K. Semenov, Mikroelektronika, 17 (1988) 147 (Sov. Microelectronics).
[4] O.A. Mukhanov and V.K. Semenov, Mikroelektronika, 17 (1988) 155 (Sov. Microelectronics).
[5] B.Oelze et al., Appl. Phys. Lett. **68**, 2732 (1996).
[6] B.Oelze et al., IEEE Trans. on Appl. Supercond. **7**, 3450 (1997).
[7] J.H.Kang, J.X.Przybysz, A.H.Worsham and D.L.Miller, Extended Abstracts of ISEC'95, Nagoya, Japan (1995) p. 234.
[8] T.V.Filippov, Supercond.: physics, chemistry, engineering **8**, 147 (1994). (in Russian).
[9] J.Chen, H.Nakamura, H.Myoren, K.Nakajima and T.Yamashita, Extended Abstracts of ISEC'95, Nagoya, Japan (1995) 341.
[10] P.Migny and B.Placais, Electron. Lett., 18 (1982) 777.
[11] V.Ambegaokar and B.I.Halperin, Phys. Rev. Lett., 22 (1969) 1364.
[12] A.N.Malakhov and A.L.Pankratov, Physica C **269**, 46 (1996).
[13] H.Kramers, Physica, 7 (1940) 284.
[14] A.N.Malakhov, Radiophys. and Quant. Electr. 34 (1991) 571.
[15] C.W.Gardiner, Handbook of Stochastic methods (Springer-Verlag, 1985).
[16] K.K.Likharev, Int. Journ. of Theor. Phys. **21**, 311 (1982).
[17] S.P.Nikitenkova and A.L.Pankratov, Physical Review E, **58** (1998) 6964.
[18] A.N.Malakhov, Cumulant analysis of random Non-Gaussian processes and its transformations (Sovetskoe Radio, Moscow, 1978, in Russian).
[19] H.Risken, The Fokker-Planck equation (Springer Verlag, Berlin, 1985).
[20] V.I.Tikhonov and M.A.Mironov, Markovian processes (Sovetskoe Radio, Moscow, 1978, in Russian).
[21] A.L.Pankratov, Physics Letters A **234**, 329 (1997).
[22] A.L.Pankratov, Extended Abstracts of 6th Int. Superconductive Electronics Conference (ISEC'97), Berlin, Germany, 1997, v.**2**, p.365.

Stochastic processes and applications
Lecture 9

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I. STOCHASTIC RESONANCE: INTRODUCTION

Over the last two decades, stochastic resonance has continuously attracted considerable attention. The term is given to a phenomenon that is manifest in nonlinear systems whereby generally feeble input information (such as a weak signal) can be amplified and optimized by the assistance of noise. Following the review [1], the effect requires three basic ingredients: (i) an energetic activation barrier or, more generally, a form of threshold; (ii) a weak coherent input (such as a periodic signal); (iii) a source of noise that is inherent in the system, or that adds to the coherent input. Given these features, the response of the system undergoes resonance-like behavior as a function of the noise level; hence the name "stochastic resonance". The underlying mechanism is fairly simple and robust. As a consequence, stochastic resonance has been observed in a large variety of systems, including bistable ring lasers, semiconductor devices, chemical reactions, and mechanoreceptor cells in the tail fan of a crayfish.

In the present lecture we consider some basic statements of theory of stochastic resonance, following fresh review [1]. It is necessary to mention, that as was recently demonstrated [2], the existance of a threshold is not necessary for observation of stochastic resonance.

II. STOCHASTIC RESONANCE: BRIEF DESCRIPTION

The mechanism of stochastic resonance is simple to explain. Consider a heavily damped particle of mass m and viscous friction h, moving in a symmetric double-well potential $V(x)$ (see Fig. 1(a), where given a sketch of the double-well potential $V(x) = (1/4)bx^4 - (1/2)ax^2$; the minima are located at $\pm x_m$, where $x_m = \sqrt{a/b}$; these minima are separated by a potential barrier with the height given by $\Delta V = a^2/(4b)$, the barrier top is located at $x_b = 0$). The particle is subject to fluctuational forces that are, for example, induced by coupling to a heat bath. Such a model we considered during our course. The fluctuational forces cause transitions between the neighboring potential wells with a rate given by the Kramers rate [3] (inverse of the Kramers' time, see lecture 5), i.e.,

$$r_K = \frac{\sqrt{V''(x_m)|V''(x_b)|}}{2\pi h} e^{-\Delta V/D}, \tag{1}$$

where $\Delta V = V(x_b) - V(x_m)$ is the height of the potential barrier separating the two minima, as D is denoted the noise intensity $D = kT$ (let me mention, that noise intensity should also depend on viscosity, but in the present consideration under noise intensity we will mean namely this quantity D).

If we apply a weak periodic forcing to the particle, the double-well potential $V(x,t) = V(x) - A_0 x \cos(\Omega t)$ is tilted asymmetrically up and down, periodically raising and lowering the potential barrier, this cyclic variation is shown in Fig. 1(b). Although the periodic forcing is too weak to let the particle roll periodically from one potential well into the other one, noise-induced hopping between the potential wells can become synchronized with the weak periodic forcing (strictly speaking, this

holds true only in the statistical average). This statistical synchronization takes place when the average waiting time (Kramers' time) $\tau_K(D) = 1/r_K$ between two noise-induced interwell transitions is comparable with half the period T_Ω of the periodic forcing. This yields the time-scale matching condition for stochastic resonance, i.e.,

$$2\tau_K(D) = T_\Omega. \tag{2}$$

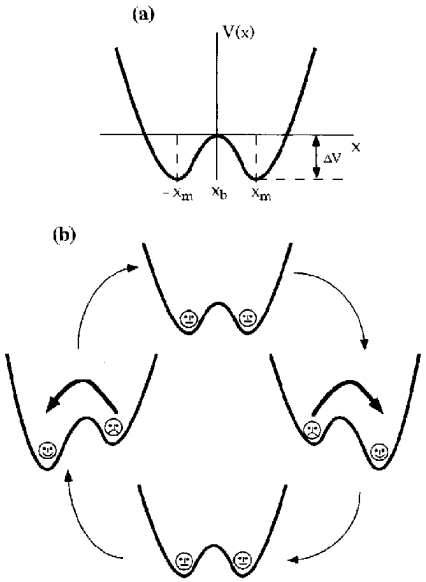

FIG. 1. Symmetric double-well potential: a) without applied periodic force and b) with applied periodic force.

In short, stochastic resonance in a symmetric double-well potential manifests itself by a synchronization of activated hopping events between the potential minima with the weak periodic forcing [4]. For a given period of the forcing T_Ω, the time-scale matching condition can be fulfilled by tuning the noise level D_{max} to the value determined by Eq. (2).

The concept of stochastic resonance was originally put forward in the seminal papers by Benzi and collaborators (see, e.g., [5], [6]) wherein they address the problem of the periodically recurrent ice ages. This very suggestion that stochastic resonance might rule the periodicity of the primary cycle of recurrent ice ages was raised independently by C. Nicolis and G. Nicolis ([7], [8], [9]; [10]). A statistical analysis of continental ice volume variations over the last 10^6 yr shows that the glaciation sequence has an average periodicity of about 10^5 yr. This conclusion is intriguing because the only comparable astronomical time scale in earth dynamics known so far is the modulation period of its orbital eccentricity caused by planetary gravitational perturbations. The ensuing variations of the solar energy influx (or solar constant) on the earth surface are exceedingly small, about 0.1%. The question climatologists (still) debate is whether a geodynamical model can be devised, capable of enhancing the climate sensitivity to such a small external periodic forcing. Stochastic resonance provides a simple, although not conclusive answer to this question. In the model of Benzi et al., the global climate is represented by a double-well potential, where one minimum represents a small temperature corresponding to a largely ice-covered earth. The small modulation of the earth's orbital eccentricity is represented by a weak periodic forcing. Short-term climate fluctuations, such as the annual fluctuations in solar radiation, are modeled by Gaussian white noise. If the noise is tuned according to Eq. (2), synchronized hopping between the cold and warm climate could significantly

enhance the response of the earth's climate to the weak perturbations caused by the earth's orbital eccentricity, according to arguments by Benzi et al. A first experimental verification of the stochastic resonance phenomenon was obtained by Fauve and Heslot [11], who studied the noise dependence of the spectral line of an ac-driven Schmitt trigger. The field then remained somewhat dormant until the modern age of stochastic resonance was ushered in by a key experiment in a bistable ring laser. Soon after, prominent dynamical theories in the adiabatic limit and in the full nonadiabatic regime have been proposed. Moreover, descriptions in terms of the linear-response approximation have frequently been introduced to characterize stochastic resonance.

Over time, the notion of stochastic resonance has been widened to include a number of different mechanisms. The unifying feature of all these systems is the increased sensitivity to small perturbations at an optimal noise level. Under this widened notion of stochastic resonance, the first non-bistable systems discussed were excitable systems. In contrast to bistable systems, excitable systems have only one stable state (the rest state), but possess a threshold to an excited state which is not stable and decays after a relatively long time (in comparison to the relaxation rate of small perturbations around the stable state) to the rest state. Soon afterwards, threshold detectors were discovered as a class of simple systems exhibiting stochastic resonance. In the same spirit, stochastic-resonance-like features in purely autonomous systems have been reported. The framework developed for excitable and threshold dynamical systems has paved the way for stochastic resonance applications in neurophysiology: stochastic resonance has been demonstrated in mechanoreceptor neurons located in the tail fan of crayfish and in hair cells of crickets.

In the course of an ever-increasing flourishing of stochastic resonance, new applications with novel types of stochastic resonance have been discovered, and there seems to be no end in sight. Most recently, the notion of stochastic resonance has been extended into the domain of microscopic and mesoscopic physics by addressing the quantum analog of stochastic resonance and also into the world of spatially extended, pattern-forming systems (spatiotemporal stochastic resonance). Other important extensions of stochastic resonance include stochastic resonance phenomena in coupled systems and stochastic resonance in deterministic systems exhibiting chaos. Stochastic resonance is by now a well-established phenomenon.

III. CHARACTERIZATION OF STOCHASTIC RESONANCE: A GENERIC MODEL

Having elucidated the main physical ideas of stochastic resonance in the preceding section, we next define the observables that actually quantify the effect. These observables should be physically motivated, easily measurable, and/or be of technical relevance. In the seminal paper [5], stochastic resonance was quantified by the intensity of a peak in the power spectrum. Observables based on the power spectrum are indeed very convenient in theory and experiment, since they have immediate intuitive meaning and are readily measurable. In the neurophysiological applications of stochastic resonance another measure has become fashionable, namely the interval distributions between activated events such as those given by successive neuronal firing spikes or consecutive barrier crossings. We follow here the historical development of stochastic resonance and discuss important quantifiers of stochastic resonance based on the power spectrum.

We consider the overdamped motion of a Brownian particle in a bistable potential in the presence of noise and periodic forcing:

$$\frac{dx}{dt} = -V'(x) + A_0 \cos(\Omega t + \varphi) + \xi(t), \tag{3}$$

where $V(x)$ denotes the reflection-symmetric quartic potential

$$V(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4. \tag{4}$$

By means of an appropriate scale transformation, the potential parameters a and b can be eliminated such that Eq. (4) assumes the dimensionless form

$$V(x) = -\frac{1}{2}x^2 + \frac{1}{4}x^4. \tag{5}$$

In Eq. (3) $\xi(t)$ denotes a zero-mean, Gaussian white noise with autocorrelation function

$$< \xi(t)\xi(0) >= 2D\delta(t), \tag{6}$$

and intensity D. The potential $V(x)$ (5) is bistable with minima located at $\pm x_m$, with $x_m = 1$. The height of the potential barrier between the minima is given by $\Delta V = 1/4$ (see Fig. 1(a)). In the absence of periodic forcing, $x(t)$ fluctuates around its local stable states with a statistical variance proportional to the noise intensity D. Noise-induced hopping between the local equilibrium states with the Kramers rate

$$r_K = \frac{1}{\sqrt{2}\pi} e^{-\Delta V/D}, \tag{7}$$

enforces the mean value $< x(t) >$ to vanish.

In the presence of periodic forcing, the reflection symmetry of the system is broken and the mean value $< x(t) >$ does not vanish. This can be intuitively understood as the consequence of the periodic biasing towards one or the other potential well.

A. The periodic response

For convenience, we choose the phase of the periodic driving $\varphi = 0$, i.e., the input signal reads explicitly $A(t) = A_0 \cos(\Omega t)$. The mean value $< x(t)|x_0, t_0 >$ is obtained by averaging the inhomogeneous process $x(t)$ with initial conditions $x_0 = x(t_0)$ over the ensemble of the noise realizations. Asymptotically ($t_0 \to \infty$), the memory of the initial conditions gets lost and $< x(t)|x_0, t_0 >$ becomes a periodic function of time, i.e., $< x(t) >_{as} = < x(t + T_\Omega) >_{as}$ with $T_\Omega = 2\pi/\Omega$. For small amplitudes, the response of the system to the periodic input signal can be written as

$$< x(t) >_{as} = \bar{x} \cos(\Omega t - \bar{\phi}), \tag{8}$$

with amplitude $\bar{x}$ and a phase lag $\bar{\phi}$. Approximate expressions for the amplitude and phase shift read

$$\bar{x}(D) = \frac{A_0 < x^2 >_0}{D} \frac{2r_K}{\sqrt{4r_K^2 + \Omega^2}}, \tag{9}$$

and

$$\bar{\phi}(D) = \arctan\left(\frac{\Omega}{2r_K}\right), \tag{10}$$

where $< x^2 >_0$ is the D-dependent variance of the stationary unperturbed system ($A_0 = 0$). Equations (9),(10) have been shown to hold in leading order of the modulation amplitude $A_0 x_m/D$ for both discrete and continuous one-dimensional systems [1]. Let us notice here that Eq. (9) allows

within the two-state approximation, i.e., $< x^2 >_0 = x_m^2$, a direct estimate for the noise intensity D_{SR} that maximizes the output $\bar{x}$ versus D for fixed driving strength and driving frequency.

The first and most important feature of the amplitude $\bar{x}$ is that it depends on the noise strength D, i.e., the periodic response of the system can be manipulated by changing the noise level. At a closer inspection of Eqs. (9),(10), we note that the amplitude $\bar{x}$ first increases with increasing noise level, reaches a maximum, and then decreases again. This is the celebrated stochastic resonance effect. In Fig. 2, we show the result of a simulation of the double-well system (Eqs. (3)–(6)) for several weak amplitudes of the periodic forcing A_0. Upon decreasing the driving frequency Ω, the position of the peak moves to smaller noise strength.

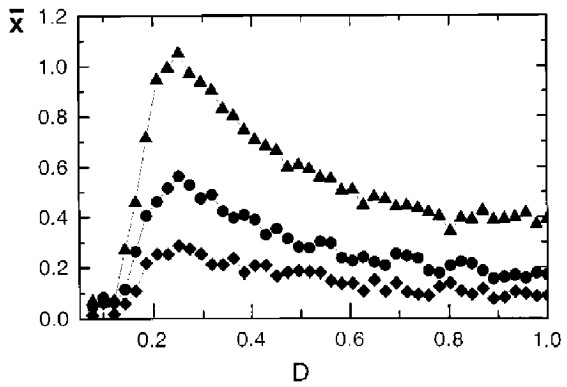

FIG. 2. Amplitude $\bar{x}(D)$ of the periodic component of the system response vs the noise intensity D (in units of ΔV) for the following values of the input amplitude: $A_0 x_m/\Delta V = 0.4$ (triangles), $A_0 x_m/\Delta V = 0.2$ (circles), and $A_0 x_m/\Delta V = 0.1$ (diamonds) in the quartic double-well potential with $a = 10^4 s^{-1}$, $x_m = 10$ (in units $[x]$ used in the experiment), and $\Omega = 100 s^{-1}$.

Next we attempt to assign a physical meaning to the value of D_{SR}. The answer was given originally by Benzi and co-workers [5], [6]: an unperturbed bistable system with $A_0 = 0$ switches spontaneously between its stable states with rate r_K. The input signal modulates the symmetric bistable system, making successively one stable state less stable than the other over half a period of the forcing. Tuning the noise intensity so that the random-switching frequency r_K is made to agree closely with the forcing angular frequency Ω, the system attains the maximum probability for an escape out of the less stable state into the more stable one, before a random back switching event takes place. When the noise intensity D is too small ($D \ll D_{SR}$), the switching events become very rare; thus the periodic component(s) of the interwell dynamics are hardly visible. Under such circumstances, the periodic component of the output signal $x(t)$ is determined primarily by motion around the potential minima – the intrawell motion. A similar loss of synchronization happens in the opposite case when $D \gg D_{SR}$: The system driven by the random source flips too many times between its stable states within each half forcing period for the forced components of the interwell dynamics to be statistically relevant.

In this spirit, the time-scale matching condition in Eq. (1), which with $\tau_K = 1/r_K$ is recast as $\Omega = \pi r_K$, provides a reasonable condition for the maximum of the response amplitude $\bar{x}(D)$. Although the time-scale matching argument yields a value for D_{SR} that is reasonably close to the exact value it is important to note that it is not exact. Within the two-state model, the value D_{SR} obeys the transcendental equation

$$4r_K^2(D_{SR}) = \Omega^2(\Delta V/D_{SR} - 1), \tag{11}$$

obtained from Eq. (9). The time-scale matching condition obviously does not fulfill Eq. (11); thus

underpinning its approximate nature.

The phase lag $\bar{\phi}$ exhibits a transition from $\bar{\phi} = \pi/2$ at $D = 0^+$ to $\bar{\phi} \propto \Omega$ in the vicinity of D_{SR}. By taking the second derivative of the function $\bar{\phi}$ in Eq. (10) and comparing with Eq. (11) one easily checks that D_{SR} lies on the right-hand side of the point of inflection of $\bar{\phi}$, being $\bar{\phi}''(D_{SR}) > 0$.

It is important to note that the variation of the angular frequency Ω at a fixed value of the noise intensity D does not yield a resonance-like behavior of the response amplitude. This behavior is immediately evident from Eq. (9) and also from numerical studies (for those who don't trust the theory).

Finally, we introduce an alternative interpretation of the quantity $\bar{x}(D)$ due to Jung and Hanggi: the integrated power p_1 stored in the delta-like spikes of spectral density $S(\omega)$ at $\pm\Omega$ is $p_1 = \pi\bar{x}^2(D)$. Analogously, the modulation signal carries a total power $p_A = \pi A_0^2$. Hence the spectral amplification reads

$$\eta = p_1/p_A = (\bar{x}(D)/A_0)^2. \tag{12}$$

In the linear-response regime (9),(10), η is independent of the input amplitude.

B. Signal-to-noise ratio

Instead of taking the ensemble average of the system response, it sometimes can be more convenient to extract the relevant phase-averaged power spectral density $S(\omega)$, defined here as

$$S(\omega) = \int_{-\infty}^{+\infty} e^{-i\omega\tau} << x(t+\tau)x(t) >> d\tau, \tag{13}$$

where the inner brackets denote the ensemble average over the realizations of the noise and outer brackets indicate the average over the input initial phase φ. In Fig. 3(a) we display a typical example of $S(\nu)$ ($\omega = 2\pi\nu$) for the bistable system. Qualitatively, $S(\omega)$ may be described as the superposition of a background power spectral density $S_N(\omega)$ and a structure of delta spikes centered at $\omega = (2n+1)\Omega$ with $n = 0, \pm 1, \pm 2, \ldots$. The generation of only odd higher harmonics of the input frequency are typical fingerprints of periodically driven symmetric nonlinear systems [12]. Since the strength (i.e., the integrated power) of such spectral spikes decays with n according to a power law such as A_0^{2n}, we can restrict ourselves to the first spectral spike, being consistent with the linear-response assumption implicit in Eq. (8). For small forcing amplitudes, $S_N(\omega)$ does not deviate much from the power spectral density $S_N^0(\omega)$ of the unperturbed system. For a bistable system with relaxation rate $2r_K$, the hopping contribution to $S_N^0(\omega)$ reads

$$S_N^0(\omega) = 4r_K < x^2 >_0 /(4r_K^2 + \omega^2). \tag{14}$$

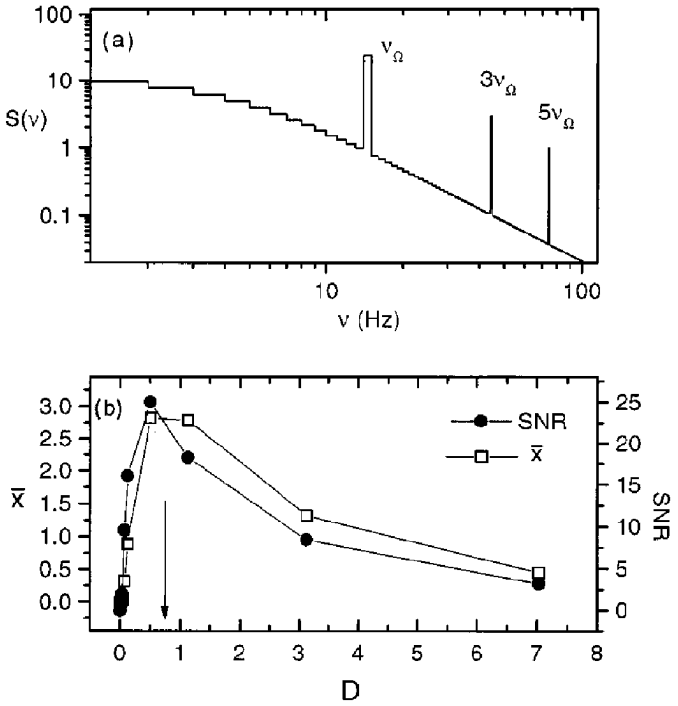

FIG. 3. Characterization of stochastic resonance. (a) A typical power spectral density $S(\nu)$ vs frequency ν for the case of the quartic double-well potential. The delta-like spikes at $\nu = (2n+1)\nu_\Omega$, $\Omega = 2\pi\nu_\Omega$, with $n = 0$, 1, and 2, are displayed as finite-size histogram bins. (b) Strength of the first delta spike, and the signal-to-noise ratio SNR, vs D (in units of ΔV). The arrow denotes the D value corresponding to the power spectral density plotted in (a). The other parameters are $Ax_m/\Delta V = 0.1$, $a = 10^4 s^{-1}$, and $x_m = 10$ (in units [x] used in the experiment).

The spectral spike at Ω was verified experimentally (see references in [1]) to be a delta function, thus signaling the presence of a periodic component with angular frequency Ω in the system response (Eq. (8)). In fact, for $Ax_m \ll \Delta V$ we are led to separate $x(t)$ into a noisy background (which coincides, apart from a normalization constant, with the unperturbed output signal) and a periodic component with $< x(t) >_{as}$ as given by Eq. (8) [12]. On adding the power spectral density of either component, we easily obtain

$$S(\omega) = (\pi/2)\bar{x}^2(D)[\delta(\omega - \Omega) + \delta(\omega + \Omega)] + S_N(\omega), \tag{15}$$

with $S_N(\omega) = S_N^0(\omega) + O(A_0^2)$ and $\bar{x}(D)$ given in Eq. (9). In Fig. 3(b) the strength of the delta-like spike of $S(\omega)$ (more precisely $\bar{x}(D)$) is plotted as a function of D. Stochastic resonance can be envisioned as a particular problem of signal extraction from background noise. It is quite natural that a number of authors tried to characterize stochastic resonance within the formalism of data analysis, most notably by introducing the notion of signal-to-noise ratio (SNR) (see references in [1]). We adopt here the following definition of the signal-to-noise ratio

$$SNR = 2 \left[\lim_{\Delta\omega \to 0} \int_{\Omega - \Delta\omega}^{\Omega + \Delta\omega} S(\omega) d\omega \right] \Big/ S_N(\Omega). \tag{16}$$

Hence on combining Eqs. (14) and (15), the SN ratio for a symmetric bistable system reads in leading order

$$SNR = \pi (A_0 x_m / D)^2 r_K. \tag{17}$$

Note that the factor of 2 in the definition (16) was introduced for convenience, in view of the power spectral density symmetry $S(\omega) = S(-\omega)$. The SN ratio SNR for the power spectral density plotted in Fig. 3(a) versus frequency ν ($\omega = 2\pi\nu$) is displayed in Fig. 3(b). The noise intensity $\bar{D}_{SR}$ at which SNR assumes its maximum does not coincide with the value D_{SR} that maximizes the response amplitude $\bar{x}$, or equivalently the strength of the delta spike in the power spectrum given by Eq. (15). As a matter of fact, if the prefactor of the Kramers rate is independent of D, we find that the SN ratio of Eq. (17) has a maximum at

$$\bar{D}_{SR} = \Delta V/2. \tag{18}$$

There are exist two generic models of stochastic resonance: the periodically driven bistable two-state system and the double-well system. The first one may be described by master equation and the second one may be described in the terms of the Fokker-Planck equation. In the Fokker-Planck description of stochastic resonance the Floquet approach and Linear-Response Theory are usually used. For detailed description of these approaches one may see the review [1].

Finally, I wish to present figure from this review, demonstrating example of input/output synchronization in the symmetric bistable system described by (3)-(4).

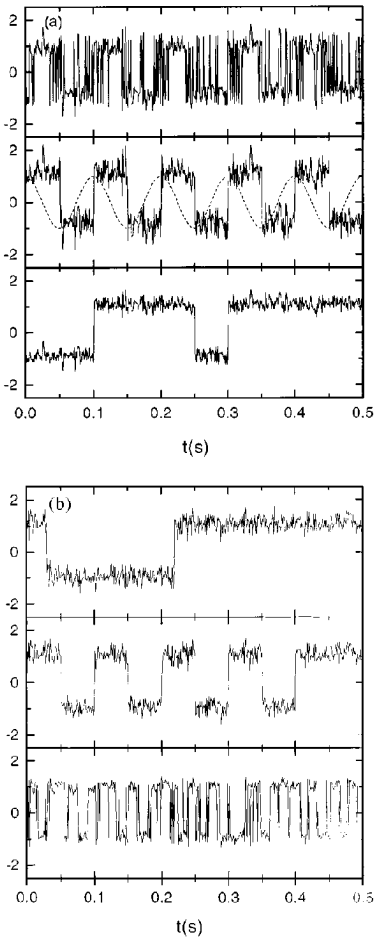

FIG. 4. Example of input/output synchronization in the symmetric bistable system of Eqs. (3)-(4). (a) Varying the noise intensity D with Ω held constant. The sampled signal shown with dashes is the input $A(t)$ (arbitrary units). The remaining trajectories are the corresponding system output (in units of x_m) for increasing D values (from bottom to top). (b) Effect of varying Ω with D held constant. The three outputsamples $x(t)$ (in units of x_m) are displayed for increasing Ω values (from top to bottom). The parameters for (a) and (b) are $A_0 x_m/\Delta V = 0.1$, $a = 10^4 s^{-1}$ and $x_m = (a/b)^{1/2} = 10$, cf. in Fig. 2.

IV. WHAT STOCHASTIC RESONANCE CAN AND CANNOT DO

Because in past years there were a lot of speculations about stochastic resonance, as a conclusion I wish to refer to the recent paper published by Dykman and McClintock in Nature. The title of the paper is just "What stochastic resonance can and cannot do".

An important consequence of Linear-Response Theory, apposite to the recent correspondence [14], [15] is that, for a system driven by a signal and Gaussian noise, the SNR at the output, $R_{\rm out}$, does not exceed that at the input, $R_{\rm in}$. For a linear system $R_{\rm out} = R_{\rm in}$, and the SNR decreases with the increasing noise intensity. For a nonlinear system the ratio $R_{\rm out}/R_{\rm in}$ may be small, and then the provision of additional noise can sometimes help to increase the SNR at the output, back towards its value at the input. It is this latter effect which constitutes Stochastic Resonance.

Stochastic Resonance can ameliorate quite dramatically the SNR degradation of a noisy signal caused by its transduction through a nonlinear element. It does not, however, provide a mechanism whereby the SNR of the input signal can meaningfully be enhanced.

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[1] L.Gammaitoni, P.Hanggi, P.Jung and F.Marchesoni, Rev. Mod. Phys., 70 (1998) 223.
[2] S.M.Bezrukov and I.Vodyanoy, Nature, 385 (1987) 319.
[3] H.Kramers, Physica, 7 (1940) 284.
[4] L.Gammaitoni, F.Marchesoni, et al., Phys. Rev. Lett., 62 (1989) 349.
[5] R.Benzi, A.Sutera and A.Vulpiani, J. Phys. A, 14 (1981) L453.
[6] R.Benzi et al., Tellus, 34 (1982) 10.
[7] C.Nicolis, Sol.Phys, 74 (1981) 473.
[8] C.Nicolis, Tellus, 34 (1982) 1.
[9] C.Nicolis, J.Stat.Phys, 70 (1993) 3.
[10] C.Nicolis and G.Nicolis, Tellus, 33 (1981) 225.
[11] S.Fauve and F.Heslot, Phys. Lett. A, 97 (1983) 5.
[12] P.Jung and P.Hanggi, Europhys. Lett., 8 (1989) 505.
[13] M.I.Dykman and P.V.E.McClintock, Nature, 391 (1998) 344.
[14] R.D.Astumian, R.K.Adair and J.C.Weaver, Nature, 388 (1997) 632.
[15] S.M.Bezrukov and I.Vodyanoy, Nature, 388 (1997) 633.

Stochastic processes and applications
Lecture 10

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I. RATCHET EFFECT: INTRODUCTION

In the present lecture we briefly consider the effect, attracting now significant attention. This effect is called as "ratchet effect" and is also known as "molecular motor" or "Brownian motor". The present lecture is based on recent reviews [1], [2].

A "stochastic ratchet" is a process in which unoriented nonequilibrium fluctuations and a spatially anisotropic periodic potential conspire to produce direct motion. Transport in ratchet-like potentials provides a mechanism for the transformation of nonequilibrium fluctuations into useful work. By "ratchet-like" we mean a potential that is periodic, but spatially anisotropic. Under the influence of the fluctuations in the environment, the potential felt by a particle randomly switches between two or more possible configurations. The resulting current generated by these systems depends not only on the spatial asymmetry of the potenital, but also on the statistical properties of the nonequilibrium fluctuations.

Recent motivation of study these types of systems comes from the theoretical modeling of the molecules kinesin and myosin, which posesses the ability to move unidirectionaly along structural filaments such as microtubulin and actin. Modern biology has shown that an important number of biological processes are governed by the action of molecular complexes reminiscent in some way of macroscopic machines [3], [4]. For instance, the words "channels" and "pumps" are commonly used to describe protein aggregates promoting, respectively, passive and active transport of ions and molecules across biological membranes, whereas the word "motor" is used for proteins or protein complexes that transduce at a molecular scale chemical energy into mechanical work. Both rotatory and translationary motors are known to exist. In this lecture, we briefly give qualitative and simple description, which allows one to extract the main features of the physics involved, deliberately avoiding the biological complexity.

From a theoretical point of view, molecular motors are microscopic objects that unidirectionally move along one-dimensional periodic structures. The problem of explaining this unidirectionality belongs to a larger class of such problems involving rectifying processes at small scale. A simple model of such a process is a generalization of Feynman's famous "thermal ratchet" [5]. Buttiker [6] and Landauer [7] showed that a periodic distribution of temperatures with the proper asymmetry was sufficient to induce macroscopic motion of a particle in a periodic potential via a rectification mechanism of the random Brownian forces. However, any temperature inhomogeneity at the scale of a few tens of nanometers decays on time scales of microseconds, so that even though the developed concept is very attractive it cannot be retained for describing motors at the nanometer scale. Various isothermal rectifying processes have been discussed. For instance in the context of biophysics they were invoked both for the function of ion pumps [8] and for the translocation of proteins [9]. Periodic isothermal ratchets have been discussed from different perspectives [10], [11]. We can distinguish three different approaches.

(i) *Fluctuating forces*: a pointlike particle is placed in a periodic, asymmetric potential $W(x)$ and is submitted to a fluctuating force that does not satisfy a fluctuation-dissipation theorem. Typically the particle motion is described by the Langevin equation

$$\xi \frac{dx}{dt} = -W'(x) + F(t), \tag{1}$$

where ξ is a constant friction coefficient, x is the position of the particle, and $W(x)$ is the potential energy it experiences. The fluctuating force $F(t)$ has zero averaged value, $< F(t) >= 0$, but has richer correlation functions than a simple Gaussian white noise. These correlations of the fluctuating forces reflect the energy source: their structure depends for example on the complexity of an underlying chemical process. As soon as the fluctuation-dissipation theorem is broken, a rectified motion sets in with a direction that depends in a subtle manner on the details of the statistics. In principle, inertial terms could be added in Eq. (1). The motion of a massive particle subject to a fluctuating force is a beautiful theoretical problem. We shall not go into this subject here: indeed, the characteristic crossover time between underdamped and overdamped behavior is of the order of a few picoseconds on the 10-nm scale.

(ii) *Fluctuating potentials*: A pointlike particle is placed in a periodic, asymmetric potential with a value that depends on time:

$$\xi \frac{dx}{dt} = -W'(x) + f(t), \tag{2}$$

x, ξ, and W keep the same meaning as in Eq. (1) but the potential W depends explicitly on time, and the random forces $f(t)$ are Gaussian white noise which obeys a fluctuation-dissipation theorem:

$$< f(t) >= 0, \quad < f(t)f(t') >= 2\xi k_B T \delta(t - t'). \tag{3}$$

The energy source is now implicit in the time dependence of the potential W. Most works have considered the case in which $W(x,t) = A(t)V(x)$ (see references given in [1]). If $A(t)$ is a random variable which can adopt two different values and if the distribution of residence times at each value is given by a Poisson distribution, Eq. (2) corresponds to the motion of a particle fluctuating between different states for which the transition rates between states are constant.

(iii) *Particle fluctuating between states*: In each of the states, the "particle" experiences a classical Langevin equation:

$$\xi_i \frac{dx}{dt} = -W_i'(x) + f_i(t). \tag{4}$$

Here, the index i refers to the considered state, $i = 1, ..., N$, and $f_i(t)$ satisfies a fluctuation-dissipation theorem:

$$< f_i(t) >= 0, \quad < f_i(t)f_j(t') >= 2\xi_i k_B T \delta(t - t')\delta_{ij}. \tag{5}$$

The dynamics of transitions between the states have to be added independently, which is most conveniently done in a Fokker-Planck formalism, as will be discussed below. Rectification is obtained only to the extent that at least one of the transitions does not satisfy detailed balance. Although approaches (i) to (iii) may differ in the details of the rectification process, they share in common their main features. Aiming at a more realistic description on the molecular level, several authors have added internal variables (which become necessary if the time required to achieve, for instance, a conformational change is not small compared to other time scales), in particular in order to quantify the significance of correlations between the two heads of the motors (see [12]- [15]). Such models often aim at describing more closely specific features of particular biological motors, such as the two-head walk of kinesin or the power stroke of myosin.

II. A TWO-STATE MODEL FOR A SINGLE MOTOR

We shall now discuss a concrete model for force generation and motion of linear molecular motors. We restrict our analysis to a two-state model [1], in which the fuel consumption triggers a conformational change between two states 1 and 2. Transitions between these states are described by standard chemical kinetics. For each of the states, a position-dependent one-dimensional potential can be defined in the following way: The motor is allowed to find its equilibrium position close to the filament with the constraint that the x coordinate of the center of mass is given. The free energy of the motor in state i confined at point x defines the potential $W_i(x)$. This definition implies that the symmetry of the filament is reflected in the symmetry of the potentials: $W_i(x)$ is both periodic and asymmetric. Note that this potential is defined for any x, irrespective of the range of interactions involved. The variations of this potential can in principle be estimated by measuring the force required to maintain the particle at the prescribed position x. An experiment along these lines suggests that the distance between minimum and maximum is of the order of 3 nm for actin/myosin (Nishizaka et al., 1995), but in general the potential shape is unknown.

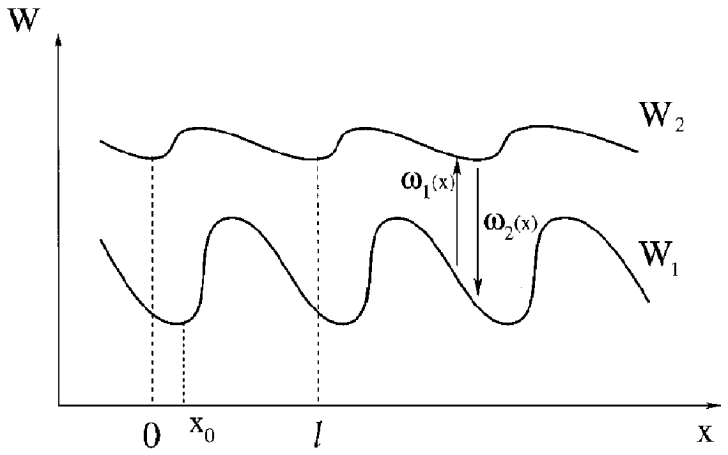

FIG. 1. Schematic picture of the two l-periodic asymmetric potentials. Although the two potentials are flat on a larger scale, motion is expected when the ratio of transition rates ω_1/ω_2 is driven away from its equilibrium value given by Eq. (11).

In order to develop a stochastic description of the dynamics, we introduce the probability density $P_i(x,t)$ for the motor to be at position x at time t in state i. This periodic system with period l is shown schematically in Fig. 1. The evolution of the system can be described by two Fokker-Planck equations with source terms:

$$\partial_t P_1 + \partial_x J_1 = -\omega_1(x)P_1 + \omega_2(x)P_2, \tag{6}$$

$$\partial_t P_2 + \partial_x J_2 = \omega_1(x)P_1 - \omega_2(x)P_2, \tag{7}$$

where the currents result from diffusion, interaction with the filament, and the action of a possible external force f_{ext}:

$$J_i = \mu_i[-k_B T \partial_x P_i - P_i \partial_x W_i + P_i f_{ext}]. \tag{8}$$

Here μ_i is the chemical potential.

The source terms are determined by the rates $\omega_i(x)$ at which the motor switches from one state to the other. The functions $\omega_i(x)$ again have the symmetry properties of the filament. The set of Eqs.

(6)-(8) can be used not only to illustrate the motion of molecular motors but also to show explicitly in terms of an effective one-dimensional equation how this motion and force generation emerge. This effective description is obtained by evaluating the steady-state particle current $J = J_1(x) + J_2(x)$ for l-periodic $P_i(x)$. Introducing $P = P_1 + P_2$ and $\lambda(x) = P_1(x)/P(x)$, it takes the form

$$J = \mu_{eff}[-k_B T \partial_x P - P\partial_x W_{eff} + P f_{ext}]. \tag{9}$$

with an effective mobility given by $\mu_{eff} = \mu_1\lambda + \mu_2(1-\lambda)$ and an effective potential that reads

$$W_{eff}(x') - W_{eff}(0) = \int_0^{x'} dx \frac{\mu_1\lambda\partial_x W_1 + \mu_2(1-\lambda)\partial_x W_2}{\mu_1\lambda + \mu_2(1-\lambda)} + k_B T[\ln(\mu_{eff})]_0^{x'}. \tag{10}$$

One can show that, with periodic boundary conditions, $\lambda(x)$ has the potential symmetry. So if the potential is symmetric, the integrand in Eq. (10) is antisymmetric and the effective potential is periodic: $W_{eff}(nl) = W_{eff}(0)$ for integer n. It is thus flat on large scales and cannot generate motion.

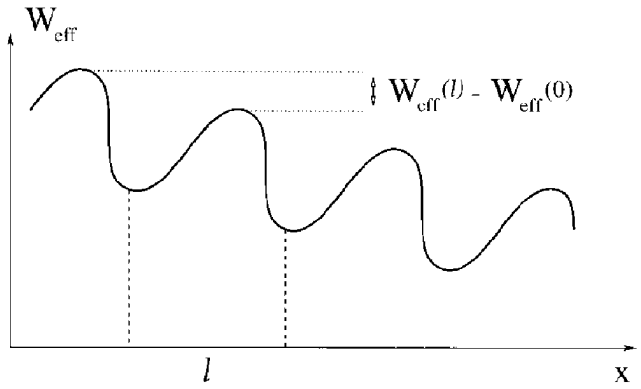

FIG. 2. Schematic picture of the effective potential $W_{eff}(x)$ acting on the particle if the transition rates between the two states do not obey detailed balance.

For asymmetric potentials, the effective potential generically has a nonzero average slope $[W_{eff}(l) - W_{eff}(0)]/l$ on large scales (see Fig. 2), although W_1 and W_2 are flat on large scales (see Fig. 1). This average slope corresponds to an average force that the motor develops, able to generate motion against weaker external forces f_{ext}. However, this average force exists (i.e., the system operates as a motor) only if the system consumes chemical energy. If no energy is provided to the system, detailed balance has to be satisfied:

$$\omega_1(x) = \omega_2(x) \exp\left[\frac{W_1(x) - W_2(x)}{k_B T}\right]. \tag{11}$$

As a consequence $\lambda = (1 + \exp[(W_1(x) - W_2(x))/k_B T])^{-1}$ and W_{eff} is the l-periodic free energy of the motor, which is obviously flat on large scales. Thus breaking detailed balance is also a clear requirement for spontaneous motion.

As already discussed, in biological systems detailed balance is broken most of the time by ATP hydrolysis. Let us assume that an hydrolysis event triggers, say, the change of the motor from state 1 to state 2 (the other choice would give similar results). Let us construct a quantity measuring the local deviation from detailed balance:

$$\Omega(x) = \omega_1(x) - \omega_2(x) \exp\left[\frac{W_1(x) - W_2(x)}{k_B T}\right]. \tag{12}$$

For practical purposes, we write $\Omega(x) = \Omega\theta(x)$, where the perturbation amplitude Ω measures the distance to equilibrium and $\int_0^l \theta(x)dx$ is normalized to one.

As a result of broken detailed balance, the motor begins to move on average and can work mechanically against a load as described by Eqs. (9) and (10). Its average velocity v is determined by $J = v \int_0^l dx P(x)/l$. However, to get explicit expressions for the velocity and the efficiency of the process, one needs to calculate $\lambda(x)$ and thus solve Eqs. (6)-(8). It is then necessary to specify the potential shapes in order to get specific results.

Two interesting limits can be identified: a homogeneous perturbation $\theta(x) = 1/l$, or a perturbation "localized" in the vicinity of the minima of W_1, $\theta(x) = \sum_n \delta(x - x_0 + nl)$. The latter case corresponds to the notion of "active sites" in biology: it tells us that the (ATP-assisted) transition from state 1 to 2 is basically impossible, except when the protein is at a specific location along the filament. Independent of any detailed calculation, it is easy to show that the behavior of the spontaneous velocity v ($f_{ext} = 0$) as a function of the excitation rate Ω differs fundamentally in these two cases (Fig. 3).

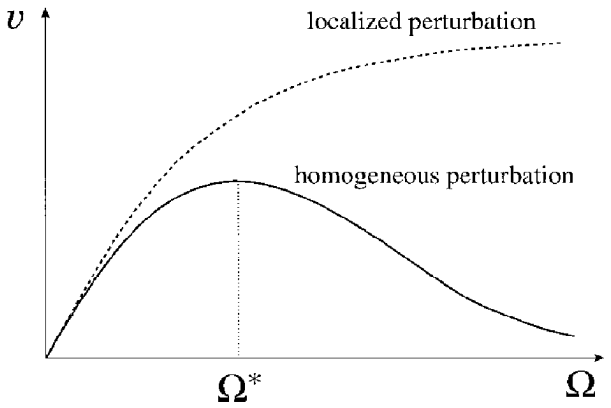

FIG. 3. Schematic diagram of the spontaneous average velocity v (for zero external force $f_{ext} = 0$) of the particle as a function of Ω, which measures the departure from equilibrium and is related to the fuel concentration.

In the first case of a homogeneous perturbation, a well-defined velocity maximum occurs at a given value of Ω. Indeed, for low excitation rates, the system is close to thermodynamic equilibrium and v grows linearly with Ω starting from zero at $\Omega = 0$ in agreement with linear-response theory. At very large Ω, only state 2 is populated, which restores a Boltzmann distribution in this state, so that in the absence of an external force the velocity vanishes as $1/\Omega^3$. The maximum velocity is obtained when two pairs of characteristic times are matched. This can be understood in the case of a constant potential W_2 (Fig. 4): suppose the particle starts from an energy minimum of the ground state 1 and gets excited to state 2. In this state it will undergo a diffusion process, which will lead after a time t to a Gaussian probability distribution with halfwidth $(2k_B T \mu_2 t)^{1/2}$. After a typical lifetime $\tau_2 = \omega_2^{-1}$, the particle will return to the ground state. Depending on whether this transition takes place on the right or the left of the maximum of $W_1(x)$, the process will contribute to net motion (to the right) or not, as shown in Fig. 4. We want the number of favorable events contributing to the net motion

to be as large as possible: A short lifetime τ_2 would yield a small contribution to motion but letting the diffusive stage last too long would allow the particle to jump to the left with an appreciable probability too. So, in scaling form, optimal conditions read $\tau_2 \approx a^2/(k_B T \mu_2)$ (for the definition of the length a, see Fig. 4). Now we want the particle that moved over the barrier to have sufficient time in state 1 to drift down the potential slope to reach the next minimum. Since waiting there would lead to a loss of time, the second time matching for optimization is $\tau_1 = \omega_1^{-1} = \Omega^{-1} \approx b^2/(m u_1 W_1)$. This determines the value Ω^* at which the maximum velocity is reached in Fig. 3.

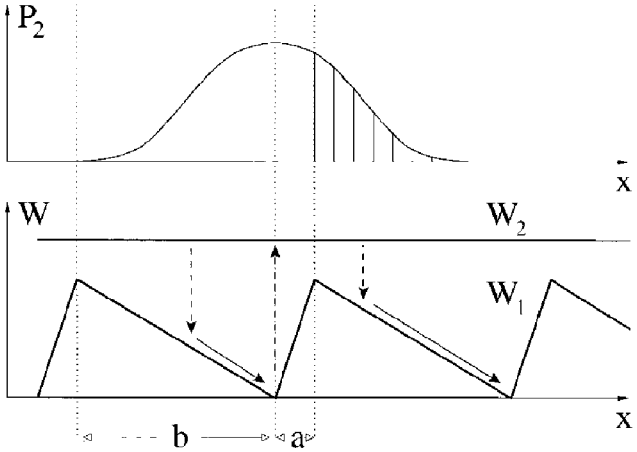

FIG. 4. Motion generation for $W_2 = const$ and $f_{ext} = 0$: A particle trapped in state 1 is excited to state 2, where it diffuses freely. It returns to state 1 after a typical lifetime ω_2^{-1} when it has a Gaussian probability distribution P_2. With a probability proportional to the hatched area of the Gaussian distribution, it arrives at the next minimum of W_1 provided it has sufficient time in state 1 to slide to that minimum.

In the second case of highly localized excitations, there is no maximum in the $v(\Omega)$ curve. Indeed, while the previously mentioned time matching in state 2 is still needed, particles will now always drift downhill to the energy minimum of state 1 before being reexcited to state 2. The less time spent in the minimum, the faster the cycle and the larger the velocity. Thus the maximum is pushed towards $\Omega = \infty$.

Note that in both cases a diffusive step is needed. This is due to the fact that in the situation of Fig. 3, the particle has to escape from a valley by diffusion in either state 1 or state 2. Thus the case considered in Fig. 4, where one of the potentials is flat, allows for the fastest escape. If the mobilities μ_1 and μ_2 are comparable, the velocity scale is consequently limited by the "slow" diffusive step, so that a typical value is $v_{typical} = (\mu_2 \omega_2 / k_B T)^{1/2}$, which under optimal conditions is equivalent to $v_{typical} \approx a/\tau_2 \approx \mu_2 k_B T/a$. Using the approximations described above to get analytical results, one can show that the maximum velocity is about twice as large for a localized perturbation as for a homogeneous one, everything else being kept alike. Indeed, not every drift event down towards the potential minimum is efficient in the case of homogeneous perturbations, where particles may be excited before actually reaching the minimum, whereas they are all efficient in the other case.

Note finally, that we have discussed here two extremes: a homogeneous perturbation $\theta(x) = 1/l$ and a perturbation localized to a point $\theta(x) = \delta(x \bmod l)$, whereas in generalone expects a smoother function of x. In this intermediate case, a maximum of the velocity still exists for finite Ω, but the velocity does not vanish for large Ω.

[1] F.Julicher, A.Ajdary and J.Prost, Rev. Mod. Phys., 69 (1997) 1269.
[2] C.R.Doering, Physica A, 254 (1998) 1.
[3] T.Kreis and R.Vale, *Cytoskeletal and motor proteins*, 1993 (Oxford University Press, New York).
[4] B.Alberts et al., *The molecular biology of the cell*, 1994 (Garland, New York).
[5] R.P.Feynman, R.B.Leighton and M.Sands, *The Feynman Lectures on Physics*, 1966 (Addison-Wesley, Reading, MA), Vol I, Chap. 46.
[6] M.Buttiker, Z.Phys. B, 68 (1987) 161.
[7] R.Landauer, J.Stat.Phys., 53 (1988) 233.
[8] D.Astumian et al., Proc. Natl. Acad. Sci. USA, 84 (1987) 434.
[9] S.Simon, C.Peskin and G.Oster, Proc. Natl. Acad. Sci. USA, 89 (1992) 3770.
[10] C.R.Doering, Nuovo Cimento, 17 (1995) 685.
[11] R.D.Astumian, Science, 276 (1997) 917.
[12] A.Ajdari, J.Phys. I, 4 (1994) 1577.
[13] C.S.Peskin and G.F.Oster, Biophys. J. 68 (1995) 202.
[14] I.Derenyi and T.Vicsek, Proc. Natl. Acad. Sci. USA, 93 (1996) 6755.
[15] T.Duke and S.Leibler, Biophys. J., 71 (1996) 1235.

Шумы и флуктуации в джозефсоновских системах
Лекция 11. Флуктуации в автоколебательных системах, форма и ширина линии генерации

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The determination of the spectral form of the oscillator signal may be considered in certain cases as the final goal of investigation of influence of random forces on an oscillator. The existence of a continuous part of the spectrum, even when it contains a quasi-monochromatic line, may restrict, e.g., the detection of small signals located close to the oscillator frequency. The necessity of a relatively exact knowledge of the spectrum is obvious in this case.

On the other hand, in a number of physical tasks the mechanism of broadening of the spectral line is considered on the basis of a random frequency modulation. Therefore, the determination of the spectral form of a signal with fluctuations in both amplitude and frequency is of independent importance.

A unified method for finding the shape and the linewidth of the signal, in general having correlated amplitude and frequency fluctuations, will be considered. The analysis is performed both for stationary and nonstationary fluctuations in amplitude and frequency. The frequency fluctuations will be considered in detail and the influence of correlated amplitude and frequency fluctuations on the form of spectral line will be described.

A. Setup of the problem

1. The oscillation of any real oscillator has fluctuations of both amplitude and frequency. In general case there is a correlation between these fluctuations. Existence of these fluctuations lead to the fact, that the spectrum of the oscillator is not any more monochromatic line. The spectral line of the signal takes certain, nonzero width and definite "form some definite dependence of spectral power density as function of frequency.

Our task is determination of the form and the width of the spectral line of an oscillation on the basis of given statistical characteristics of amplitude and frequency fluctuations.

2. Let us consider the oscillation of the form [1]:

$$z(t) = R_0[1 + \alpha(t)]\cos[\omega_0 t + \varphi(t)], \tag{1}$$

where R_0, ω_0 - mean constant values of the amplitude and the frequency. In order to consider $z(t)$ as a sinusoidal oscillation with variable amplitude and phase the functions $\alpha(t)$ and $\varphi(t)$ should be slow functions of time in comparison with $\cos(\omega_0 t)$, that we will imply fulfilled. The random function $\alpha(t)$ represents relative fluctuations of the amplitude and $\varphi(t)$ - fluctuations of the phase that are equal to:

$$\varphi(t) = \int\limits_{t_0}^{t} \nu(t)dt, \tag{2}$$

where ν are fluctuations of frequency. Let us suppose that $< \alpha(t) >=< \varphi(t) >=< \nu(t) >= 0$, and that we know correlation (or structural) functions $\Phi_\alpha(\tau)$, $\Phi_\nu(\tau)$, $\Phi_{\alpha\nu}(\tau)$ and the corresponding spectral densities $S_\alpha(\omega)$, $S_\nu(\omega)$, $S^0_{\alpha\nu}(\omega)$, $S^1_{\alpha\nu}(\omega)$.

Our final goal is obtaining the spectral density $S_z(\omega)$ of the oscillation $z(t)$. This spectral density, that is counted from $\omega = \omega_0$, we will also call the shape of spectral line, which will be considered in the frequency range much smaller than ω_0 due to slowness of α and φ.

Let us calculate the correlation function of the signal $z(t)$, which is the signal of the second group.

• We will speak, that the signal $z(t)$ belongs to the second group if its energy is infinite and the quantity

$$S_z = \lim_{T\to\infty} \frac{1}{2T} \int\limits_{-T}^{+T} < z^2(t) > dt, \tag{3}$$

called the power of the signal, is a finite quantity. Few examples of the signal of the second group are constant, sinusoidal signal, random stationary function and so on.

For the signal $z(t)$ one has to introduce the correlation function of the second order that is defined as:

$$\Phi_z(\tau) = \lim_{T\to\infty} \frac{1}{2T} \int\limits_{-T}^{+T} K[t, t+\tau]dt. \tag{4}$$

We define the power spectral density of the signal $z(t)$ as

$$S_z(\omega) = \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} \Phi_z(\tau)\cos(\omega\tau)d\tau. \tag{5}$$

If $z(t)$ is a random stationary process with the given correlation function $K_z[\tau]$, then the correlation function of the second order looks like: $\Phi_z(\tau) = K_z[\tau]$, i.e. coincide with the correlation function.

With the help of the formula (4), defining $t+\tau = t'$, $\alpha(t') = \alpha'$, $\varphi(t') = \varphi'$, $\varphi' - \varphi = \Delta\varphi$, we find:

$$\Phi_z(\tau) = \lim_{T\to\infty} \frac{1}{2T} \int\limits_{-T}^{+T} \left\langle \frac{1}{2} R_0^2 (1+\alpha+\alpha'+\alpha\alpha')[\cos(\omega_0\tau+\Delta\varphi) + \cos[\omega_0(t+t')+\varphi+\varphi']] \right\rangle dt. \tag{6}$$

It is easy to see, that the second term (cosine of sum) will not give contribution into $\Phi_z(\tau)$, since it visibly contains the current time. Transforming cosine, we get:

$$\Phi_z(\tau) = A^0(\tau)\cos(\omega_0\tau) - A^1(\tau)\sin(\omega_0\tau), \tag{7}$$

where

$$A^0(\tau) = \frac{1}{2} R_0^2 \lim_{T\to\infty} \frac{1}{2T} \int\limits_{-T}^{+T} \langle (1+\alpha+\alpha'+\alpha\alpha')\cos(\Delta\varphi)\rangle \, dt \tag{8}$$

and

$$A^1(\tau) = \frac{1}{2} R_0^2 \lim_{T\to\infty} \frac{1}{2T} \int\limits_{-T}^{+T} \langle (1+\alpha+\alpha'+\alpha\alpha')\sin(\Delta\varphi)\rangle \, dt \tag{9}$$

are even and odd functions of τ, respectively.

We have got general definition of functions $A^0(\tau)$ and $A^1(\tau)$, valid both for stationary and nonstationary fluctuations $\alpha(t)$ and $\Delta\varphi$. The phase increment $\Delta\varphi$ is equal to:

$$\Delta\varphi = \Delta\varphi(t) = \varphi(t+\tau) - \varphi(t) = \int\limits_{t}^{t+\tau} \nu(\xi)d\xi \tag{10}$$

and in general case of arbitrary fluctuations of frequency is nonstationary function of time.

If $\alpha(t)$ and $\Delta\varphi$ are stationary and stationary conjuncted then instead of (8), (9) we have:

$$A^0(\tau) = \frac{1}{2}R_0^2 \left\langle (1 + \alpha + \alpha' + \alpha\alpha') \cos(\Delta\varphi) \right\rangle , \tag{11}$$

$$A^1(\tau) = \frac{1}{2}R_0^2 \left\langle (1 + \alpha + \alpha' + \alpha\alpha') \sin(\Delta\varphi) \right\rangle . \tag{12}$$

3. Substituting (7) into (4), introducing frequency $\Omega = \omega - \omega_0$ and neglecting due to slowness of α and φ by terms with $\cos(\omega_0 + \omega)\tau$ and $\sin(\omega_0 + \omega)\tau$, we get:

$$S_z(\omega_0 + \Omega) = \frac{1}{4\pi} \int\limits_{-\infty}^{+\infty} A^0(\tau) \cos(\Omega\tau) d\tau + \frac{1}{4\pi} \int\limits_{-\infty}^{+\infty} A^1(\tau) \sin(\Omega\tau) d\tau.$$

Let us proceed from the spectral density $S_z(\omega)$, extended both to positive and negative frequency axes to the spectral density $G_z(\omega)$ defined only for positive frequency:

$$G_z(\omega) = \begin{cases} 0, & \omega < 0, \\ 2S_z(\omega), & \omega \geq 0. \end{cases}$$

Defining $W_z(\Omega) = G_z(\omega_0 + \Omega)$, we get the following final expression for spectral density $W_z(\Omega)$ – the form of spectral line of the oscillation:

$$W_z(\Omega) = W_z^0(\Omega) + W_z^1(\Omega), \tag{13}$$

where

$$W_z^0(\Omega) = \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} A^0(\tau) \cos(\Omega\tau) d\tau, \tag{14}$$

$$W_z^1(\Omega) = \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} A^1(\tau) \sin(\Omega\tau) d\tau. \tag{15}$$

It is seen from (13) that in general case $W_z(\Omega)$ is not an even function of Ω, i.e. in general case the spectral line of the signal is asymmetric relatively $\Omega = 0$ (relatively the central frequency ω_0), and even $W_z^0(\Omega)$ and odd $W_z^1(\Omega)$ parts can be extracted.

It follows from (15) that asymmetry of the spectral line takes place for $A^1(\tau) \neq 0$. Analyzing (9), it is easy to see that if fluctuations of amplitude and frequency are statistically independent, then:

$$A^1(\tau) = \frac{1}{2}R_0^2 \lim_{T\to\infty} \frac{1}{2T} \int\limits_{-T}^{+T} (1 + K_\alpha[t, t + \tau]) \left\langle \sin(\Delta\varphi) \right\rangle dt,$$

and this expression is different from zero if $\langle \sin(\Delta\varphi) \rangle$ is different from zero. The latter depends on the law of distribution of fluctuations of $\nu(t)$. If probabilistic distribution of fluctuations of frequency is symmetric, it can be demonstrated that $\langle \sin(\Delta\varphi) \rangle = 0$. Therefore, the function $A^1(\tau)$ may be not equal to zero for asymmetric distribution of frequency fluctuations.

So, asymmetry of distribution of frequency fluctuations lead to asymmetry of the form of spectral line of oscillations.

If the distribution of $\nu(t)$ is symmetric (that is often true in practice) then only correlation between $\alpha(t)$ and $\nu(t)$ may lead to $A^1(\tau) \neq 0$ and, correspondingly, to asymmetric form of spectral line.

Let us note, that formulas (14) and (15) are presented in the most general form and they are valid for any laws of distribution of α and ν and, therefore, it is rather difficult to make any concrete conclusions about functions $A^0(\tau)$ and $A^1(\tau)$. The analysis of these functions and, correspondingly, of $W_z(\Omega)$ is possible to perform for a few particular cases only, most of which will be considered below.

B. Spectrum of a signal, having fluctuations of amplitude.

1. Let us consider for generality of presentation the simplest case when only amplitude fluctuations of $z(t)$ are present (fluctuations of frequency are absent, $\nu = 0$):

$$z(t) = R_0[1 + \alpha(t)]\cos(\omega_0 t).$$

In this case $\Delta\varphi = 0$ and it follows from (8), (9) that

$$A^0(\tau) = \frac{1}{2}R_0^2[1 + \Phi_\alpha(\tau)],$$

$$A^1(\tau) = 0.$$

Due to this, the spectrum $W_z(\Omega)$ of the signal is symmetric and is equal to:

$$W_z(\Omega) = W_z^0(\Omega) = \frac{R_0^2}{2}\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}\cos(\Omega\tau)d\tau + \frac{R_0^2}{2}\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}\Phi_\alpha(\tau)\cos(\Omega\tau)d\tau.$$

The first integral is delta-function and the second one is equal to the spectral density of amplitude fluctuations $S_\alpha(\Omega)$. Therefore:

$$W_z(\Omega) = \frac{R_0^2}{2}\delta(\Omega) + \frac{R_0^2}{2}S_\alpha(\Omega). \tag{16}$$

In the expression obtained the first term represents monochromatic spectral line with the power $R_0^2/2$, and the second one – the symmetric pedestal of the line due to amplitude fluctuations. Therefore, for $R_0 \neq 0$ amplitude fluctuations do not "wash out"the spectral line (its width remains equal to zero) but only adds to the monochromatic line some pedestal with the form coinciding with the form of spectrum of amplitude fluctuations.

Let now $R_0 = 0$, but amplitude fluctuations do exist. This case may occur, in particular, when oscillator is at the oscillation threshold and the mean amplitude is equai to zero. In this case for obtaining the spectral density, instead of $\alpha(t)$ one should consider $\Delta R(t)$, because

$$R = R_0 + \Delta R(t).$$

Since $R_0 = 0$, performing calculations, we get that the spectrum of the signal coincides in form with the spectrum of amplitude fluctuations. In this case it is generally possible to say that the spectral line has a width equals the width of the spectrum of amplitude fluctuations.

C. Spectrum of a signal, having random phase.

1. Let us consider the signal having only phase fluctuations:

$$z(t) = R_0 \cos(\omega_0 t + \varphi(t)).$$

In accordance with (8)-(9) we have:

$$\begin{aligned} A^0(\tau) &= \frac{R_0^2}{2} \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{+T} \langle \cos(\Delta\varphi)\rangle \, dt, \\ A^1(\tau) &= \frac{R_0^2}{2} \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{+T} \langle \sin(\Delta\varphi)\rangle \, dt. \end{aligned} \tag{17}$$

Let us suppose, that the probabilistic distribution is normal (Gaussian). Then (since $\langle \Delta\varphi \rangle = 0$)

$$\begin{aligned} &\langle \sin(\Delta\varphi)\rangle = 0, \\ &\langle \cos(\Delta\varphi)\rangle = \exp\left[-\tfrac{1}{2}\langle \Delta\varphi^2\rangle\right] = \exp\left[-d_\varphi[t,t;\tau]\right], \end{aligned} \tag{18}$$

where $d_\varphi[t,t;\tau]$ is a statistical structural function:

$$d_z[t_1,t_2;\tau] = \frac{1}{2}\left\langle [z(t_1+\tau)-z(t_1)][z(t_2+\tau)-z(t_2)]\right\rangle. \tag{19}$$

In this case

$$A^1(\tau) = 0, \;\; A^0(\tau) = \frac{R_0^2}{2} \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{+T} \exp[-d_\varphi[t,t;\tau]]dt \tag{20}$$

and the form of spectral line is symmetric. Let now fluctuations of phase have stationary increments ($\Delta\varphi$ is a stationary process); then

$$d_\varphi[t,t;\tau] = d_\varphi[0;\tau] = \Delta_\varphi(0,\tau) \equiv \chi(\tau), \tag{21}$$

and, correspondingly,

$$A^0(\tau) = A^0_\chi(\tau) = \frac{R_0^2}{2}\exp[-\chi(\tau)], \tag{22}$$

where

$$\Delta_z(\theta,\tau) = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{+T} d_z[t,t+\theta;\tau]dt \tag{23}$$

is a structural function of the second kind. For random process with stationary increments

$$\Delta_z(\theta,\tau) = d_z[\theta;\tau]. \tag{24}$$

The form of the spectral line is, therefore:

$$W_z(\Omega) = W_z^0(\Omega) = \frac{R_0^2}{4\pi} \int_{-\infty}^{+\infty} \exp[-\chi(\tau)]\cos(\Omega\tau)d\tau \tag{25}$$

and is completely determined by the function $\chi(\tau)$ – structural function of the second kind of frequency fluctuations (variance of drift of the phase during the time τ).

The structural function $\chi(\tau)$ has the following properties:

1) $\chi(0) = 0$,

2) $\chi(\tau) \geq 0$,

3) $\chi(\tau) = \chi(-\tau)$.

The behaviour of $\chi(\tau)$ for $\tau \to \infty$ significantly depends on the character of phase fluctuations. For example, for stationary phase fluctuations, for which the correlation function exists for any τ, the function $\chi(\tau)$ is always restricted. For nonstationary phase fluctuations $\chi(\tau)$ may infinitely grow for $\tau \to \infty$. In the present paragraph we will consider the case of restricted $\chi(\tau)$.

2. Let stationary fluctuations of the phase have finite intensity $\langle\varphi^2\rangle = \Phi_\varphi(0)$. Then on the basis of definition of $\chi(\tau)$ we have:

$$\chi(\tau) = \Phi_\varphi(0) - \Phi_\varphi(\tau).$$

Therefore, the function $\chi(\tau)$ is restricted due to restricted $\langle\varphi^2\rangle$. The width of the function $\chi(\tau)$ may be expressed as $2\tau_0$, where τ_0 is actually correlation time of phase fluctuations. For the considered case of restricted $\chi(\tau)$ it is expedient to slightly change notations of functions $A^0_\chi(\tau)$ and $W^0_{z\chi}(\tau)$. We will write them as $A^0_\varphi(\tau)$ and $W^0_{z\varphi}(\tau)$. The sense of these notations will become clear a bit below.

Let us represent the exponent in (25) in the form:

$$e^{-\chi(\tau)} = e^{-\Phi_\varphi(0)+\Phi_\varphi(\tau)} = e^{-<\varphi^2>+\Phi_\varphi(\tau)} - e^{-<\varphi^2>} + e^{-<\varphi^2>} = e^{-<\varphi^2>}\left[e^{\Phi_\varphi(\tau)} - 1\right] + e^{-<\varphi^2>}. \quad (26)$$

Then the integral (25) takes the form:

$$W_z(\Omega) = W^0_z(\Omega) = \frac{R_0^2}{2}e^{-<\varphi^2>}\delta(\Omega) + \frac{R_0^2}{2}e^{-<\varphi^2>}\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty}\left[e^{\Phi_\varphi(\tau)} - 1\right]\cos(\Omega\tau)d\tau. \quad (27)$$

It is seen, that the spectrum of the signal consists from the monochromatic line of the power $\frac{R_0^2}{2}e^{-<\varphi^2>}$ and the pedestal equals the second term in (27).

Thus, stationary phase fluctuations as well as amplitude fluctuations do not dither spectral line and create only an additional pedestal.

D. Spectrum of a signal, having fluctuations of frequency.

Distinguishing of cases of phase fluctuations $\varphi(t)$ and frequency fluctuations $\nu(t)$ into two different paragraphs is in some way nominal, since they are connected by relation:

$$\varphi(t) = \int \nu(t)dt$$

and always simultaneously exist. Nevertheless, such distinguishing may be justified by the fact, that spectra of signals, having fluctuations of phase and frequency with the same statistical characteristics are significantly different. In the previous paragraph we have seen that stationary fluctuations of the phase lead to the spectrum, consisting of monochromatic line and pedestal. It will be demonstrated in the present paragraph that stationary fluctuations of frequency lead to dithering of spectral line; the line is not any more monochromatic, but has some width $\Delta\Omega > 0$. This is due to infinity of the function $\chi(\tau)$ or infinity of more general characteristic – $d_\varphi[t, t; \tau]$ for $\tau \to \infty$.

Thus, the present paragraph will be different from the previous one: we will deal with such $d_\varphi[t, t; \tau]$ which infinitely grows for $\tau \to \infty$.

1. So, let us consider the signal, having frequency fluctuations:

$$z(t) = R_0 \cos\left[\omega_0 t + \int \nu(t)dt\right].$$

Functions $A^0(\tau)$, $A^1(\tau)$ are given by formulas (17), $\Delta\varphi$ – phase increment durinng time τ – by formula (10).

Let us suppose that fluctuations of frequency (or phase) are such, that there exists nonzero linewidth $\Delta\Omega$. This linewidth may be defined by different ways. From the point of view of mathematical analysis, the most efficient is the energetic definition. For that it is enough to define the linewidth on the basis of even part of shape of the spectral line $W_z^0(\Omega)$. Let us substitute $W_z^0(\Omega)$ by the rectangle with the equal square with the height $W_z^0(0)$. Then the width of this rectangle we take as the width of the spectral line $\Delta\Omega$.

The whole square under the curve $W_z^0(\Omega)$ (that is equal to the square under the curve $W_z(\Omega)$) is the energy of the signal $z(t)$, equals $R_0^2/2$. Therefore (see (14)),

$$\Delta\Omega = \frac{R_0^2}{2W_z^0(0)} = \frac{\pi R_0^2}{2\int\limits_0^\infty A_0(\tau)d\tau} = \frac{\pi}{\int\limits_0^\infty d\tau \lim_{T\to\infty} \int\limits_{-T}^{+T} \langle\cos(\Delta\varphi)\rangle\, dt}. \tag{28}$$

If fluctuations of phase have stationary increments, then

$$\Delta\Omega = \frac{\pi}{\int\limits_0^\infty < \cos(\Delta\varphi) > d\tau}. \tag{29}$$

If in addition fluctuations are normally distributed, then:

$$\Delta\Omega = \frac{\pi}{\int\limits_0^\infty \exp[-\chi(\tau)]d\tau}. \tag{30}$$

The latter formula allows to find a condition for $\chi(\tau)$, required for existence of dithering of a linewidth.

If, e.g., $\chi(\tau)$ is restricted for $\tau \to \infty$ (i.e. exist $\chi_\infty < \infty$), then it is easy to see, that the integral in (30) diverges and, correspondingly, the width of the spectral line $\Delta\Omega$ becomes zero. As it has been demonstrated in previous paragraphs, this corresponds to monochromatic line in the spectrum of $z(t)$. Therefore, we indeed have $\Delta\Omega = 0$, if the spectrum of the signal contains a monochromatic line.

In order to have $\Delta\Omega > 0$, the finity of the integral $\int\limits_0^\infty \exp[-\chi(\tau)]d\tau$ is needed, which leads to infinite $\chi(\tau)$ for $\tau \to \infty$. **Therefore, the spectral width is dithered only in the case when $\chi(\tau) \to \infty$ for $\tau \to \infty$.**

This means that the spectral line may be dithered only by nonstationary phase fluctuations. Indeed, since $\chi(\tau) = d_\varphi[0;\tau] = \frac{1}{2}\langle[\varphi(t+\tau) - \varphi(t)]^2\rangle$, supposing, e.g., $t = 0$ and $\varphi(0) = 0$, we find $\chi(\tau) = \frac{1}{2}\langle\varphi(\tau)^2\rangle$. Indefinite increase of $\chi(\tau)$ for $\tau \to \infty$ means here time dependence of $\langle\varphi(\tau)^2\rangle$ for any τ as function of τ (nonstationarity of phase fluctuations).

Let us note also: higher increase of $\chi(\tau)$ with τ – smaller integral in the denominator of (30) and wider linewidth $\Delta\Omega$.

2. Let us start the analysis from the case when $\varphi(t)$ is a process with stationary increments and distribution of $\nu(t)$ is an arbitrary function. In this case

$$A^0(\tau) = \frac{R_0^2}{2}\langle\cos\Delta\varphi\rangle,\ A^1(\tau) = \frac{R_0^2}{2}\langle\sin\Delta\varphi\rangle \tag{31}$$

and components of the spectral line equal:

$$W_z^0(\Omega) = \frac{R_0^2}{4\pi}\int\limits_{-\infty}^{+\infty} \langle \cos\Delta\varphi\rangle \cos\Omega\tau d\tau,$$
$$W_z^1(\Omega) = \frac{R_0^2}{4\pi}\int\limits_{-\infty}^{+\infty} \langle \sin\Delta\varphi\rangle \sin\Omega\tau d\tau. \quad (32)$$

Let us consider the first limiting case: frequency fluctuations ν represents as slow as possible stationary process. Let the distribution law of ν is arbitrary and the probability density equals $W_\nu(\nu)$. For as slow as possible process

$$\Delta\varphi = \int\limits_t^{t+\tau} \nu(\xi)d\xi = \nu\tau.$$

From this we get:

$$A^0(\tau) = \frac{R_0^2}{2} < \cos\nu\tau >= \frac{R_0^2}{2}\int \cos\nu\tau W_\nu(\nu)d\nu = \frac{R_0^2}{2}\int W_\nu^0(\nu)\cos\nu\tau d\nu,$$
$$A^1(\tau) = \frac{R_0^2}{2} < \sin\nu\tau >= \frac{R_0^2}{2}\int \sin\nu\tau W_\nu(\nu)d\nu = \frac{R_0^2}{2}\int W_\nu^1(\nu)\sin\nu\tau d\nu,$$

where $W_\nu^0(\nu)$ and $W_\nu^1(\nu)$ are even and odd components of the probability density $W_\nu(\nu) = W_\nu^0(\nu) + W_\nu^1(\nu)$. The obtained expressions demonstrate that $A^0(\tau)$ is Fourier conjugated of $W_\nu^0(\nu)$, and $A^1(\tau)$ - Fourier conjugated of $W_\nu^1(\nu)$. On the other hand, formulas (14) and (15) shows that $A^0(\tau)$ and $A^1(\tau)$ are Fourier conjugated of $W_z^0(\Omega)$ and $W_z^1(\Omega)$. Therefore, $W_z^0(\Omega)$ and $W_z^1(\Omega)$ are proportional to $W_\nu^0(\nu)$ and $W_\nu^1(\nu)$, respectively. Defining the proportionality coefficient from the normalization conditions, we get:

$$W_z^0(\Omega) = \frac{R_0^2}{2}W_\nu^0(\nu),\ W_z^1(\Omega) = \frac{R_0^2}{2}W_\nu^1(\nu).$$

Summing these equalities we get:

$$W_z(\Omega) = \frac{R_0^2}{2}W_\nu(\nu). \quad (33)$$

The form of spectral line of the signal, having as slow as possible frequency fluctuations, coincides with the shape of their probability distribution. This case may be called "case of technical fluctuations of frequency because, as it will be seen below, in oscillators slow quasistatic fluctuations of frequency are mainly originated from flicker noise – "technical"reasons. On the basis of (28) the width of spectral line is equal to $\Delta\Omega = W_\nu^{-1}(0)$.

With the usual assumption of Gaussian frequency fluctuations we get well-known Doppler form (or Gaussian, or technical form) of the spectral line equals

$$W_z(\Omega) = \frac{R_0^2}{2}\frac{1}{\sqrt{2\pi\langle\nu^2\rangle}}e^{-\frac{1}{2}\frac{\Omega^2}{\langle\nu^2\rangle}} \quad (34)$$

with the width

$$\Delta\Omega = \sqrt{2\pi\langle\nu^2\rangle}, \quad (35)$$

where $\langle \nu^2 \rangle$ is a variance of frequency fluctuations which is supposed to be known.

Let us consider now the second limiting case. Let us suppose, that fluctuations of frequency is a delta-correlated stationary random process with the correlation function:

$$\Phi_\nu(\tau) = D\delta(\tau);$$

and the distribution function of ν is arbitrary. In this case the phase increment $\Delta\varphi$, given by Eq. (10) represents a sum of infinitely large number of independent variables and therefore has normal distribution independently of distribution of $\nu(t)$.

If frequency fluctuations $\nu(\tau)$ represents stationary process and almost for all τ exist $\Phi_\nu(\tau)$, then it is not difficult to express $\chi(\tau)$ via $\Phi_\nu(\tau)$. It can be demonstrated that:

$$\chi(\tau) = \frac{1}{2}\left\langle \Delta\varphi^2 \right\rangle = \frac{1}{2}\int\limits_t^{t+\tau}\int\limits_t^{t+\tau} \Phi_\nu(\xi-\eta)d\xi d\eta = \frac{1}{2}\int\limits_{-\tau}^{+\tau}(\tau - |\xi|)\Phi_\nu(\xi)d\xi. \tag{36}$$

It is not difficult to express $\chi(\tau)$ via spectral density $S_\nu(\omega)$ of frequency fluctuations. Substituting into Eq. (36) the expression $\Phi_\nu(\tau)$ via $S_\nu(\omega)$ and integrating over τ we get

$$\frac{1}{2}\left\langle \Delta\varphi^2 \right\rangle = \chi(\tau) = \int\limits_{-\infty}^{+\infty}\frac{1-\cos\omega\tau}{\omega^2}S_\nu(\omega)d\omega = 2\int\limits_{-\infty}^{+\infty}\sin^2\frac{\omega\tau}{2}S_\nu(\omega)\frac{d\omega}{\omega^2}. \tag{37}$$

Besides properties of the function $\chi(\tau)$, mentioned in the previous paragraph, on the basis of (36), it is easy to discover the following properties:

$$\frac{d}{d\tau}\chi(\tau) = \int\limits_0^\tau \Phi_\nu(\tau)d\tau, \quad \left[\frac{d}{d\tau}\chi(\tau)\right]_{\tau=0} = 0. \tag{38}$$

$$\frac{d^2}{d\tau^2}\chi(\tau) = \Phi_\nu(\tau), \quad \left[\frac{d^2}{d\tau^2}\chi(\tau)\right]_{\tau=0} = \left\langle \nu^2 \right\rangle. \tag{39}$$

For delta-correlated frequency fluctuations we have from (36)

$$\chi(\tau) = \frac{1}{2}D|\tau|.$$

This formula expresses the so-called diffusive law of phase fluctuations – the mean square of phase increment during time τ is proportional to τ.

Due to Gaussian distribution of $\Delta\varphi$ we have

$$\langle\cos(\Delta\phi)\rangle = \exp\left[-\frac{D}{2}|\tau|\right], \ \langle\sin(\Delta\phi)\rangle = 0.$$

Taking into account (32), one can finally obtain:

$$W_z(\Omega) = \frac{R_0^2}{4\pi}\int\limits_{-\infty}^{+\infty}\exp\left[-\frac{1}{2}D|\tau|\right]\cos\Omega\tau d\tau = \frac{R_0^2}{2\pi}\frac{D/2}{(D/2)^2+\Omega^2}. \tag{40}$$

The obtained form of the line is well-known Lorentzian or resonant (or natural) form of spectral line. As follows from the above presented, for its realization it is only necessary to assume delta-correlated frequency fluctuations. On the basis of (30), the linewidth of this spectral line is equal to:

$$\Delta\Omega = \frac{\pi D}{2}. \tag{41}$$

The consideration of the form of spectral line for arbitrary law of distribution of frequency fluctuations is restricted by the two above mentioned cases.

3. Significantly more detailed analysis may be performed for normally distributed stationary fluctuations of frequency. Let us consider this case. Let fluctuations of frequency $\nu(t)$ are stationary and normally distributed, $\langle\nu(t)\rangle = 0$ with the given correlation function $\Phi_\nu(\tau)$ and spectral density $S_\nu(\Omega)$. On the basis of (10) the phase increment $\Delta\varphi$ will be stationary process, having normal symmetric distribution. Therefore, the shape of spectral line will be described by Eq. (25) and the width – by Eq. (30).

Combining (25) and (36) we get the following expression for the shape of spectral line:

$$W_z(\Omega) = \frac{R_0^2}{4\pi}\int\limits_{-\infty}^{+\infty}\exp\left[-\int\limits_0^\tau(\tau-\xi)\Phi_\nu(\xi)d\xi\right]\cos\Omega\tau d\tau, \tag{42}$$

which we will analyze.

Let us consider, how different characteristics of frequency fluctuations influence the form of the line $W_z(\Omega)$. Let us define the correlation time τ_0 as:

$$\tau_0 = \frac{1}{2\Phi_\nu(0)}\int\limits_{-\infty}^{+\infty}\Phi_\nu(\tau)d\tau = \frac{\pi S_\nu(0)}{\langle\nu^2\rangle}. \tag{43}$$

Let us define the spectral width as $\Omega_0 = \tau_0^{-1}$. Then it is obvious that

$$\Omega_0 = \frac{1}{\pi}\frac{\langle\nu^2\rangle}{S_\nu(0)}. \tag{44}$$

Let the spectrum of fluctuations of frequency is such that: $\pi S_\nu(0) \gg \Omega_0$ (i.e. the spectrum is narrow and tall). In this case with the help of (43), (44) we get that:

$$m \equiv \left\langle\nu^2\right\rangle\tau_0^2 = \frac{\pi S_\nu(0)}{\Omega_0} \gg 1. \tag{45}$$

Let us call the quantity m the modulation index.

The case of $m \gg 1$ is the case of slow (large τ_0) and large (large variance $\langle\nu^2\rangle$) frequency fluctuations. It can be demonstrated, that if the condition (45) is fulfilled the shape of the spectral line is approximately equal to:

$$W_z(\Omega) = \frac{R_0^2}{2}\frac{1}{\sqrt{2\pi\langle\nu^2\rangle}}\exp\left\{-\frac{\Omega^2}{2\langle\nu^2\rangle}\right\},$$

i.e. coincides with the doppler form, which we already obtained above (see (34)) with supposition of as slow as possible $\nu(t)$.

Thus, the first limiting case is approximately realized for $\pi S_\nu(0) \gg \Omega_0$.

Let now the spectrum of frequency fluctuations is such that $\pi S_\nu(0) \ll \Omega_0$. Then

$$m \equiv <\nu^2>\tau_0^2 = \frac{\pi S_\nu(0)}{\Omega_0} \ll 1, \tag{46}$$

and we have the case of fast (small τ_0) and small (small $\langle\nu^2\rangle$) frequency fluctuations. It can be demonstrated that in this case the form of spectral line is approximately equal to (compare with (40)):

$$W_z(\Omega) = \frac{R_0^2}{2\pi}\frac{\langle\nu^2\rangle\tau_0}{(\langle\nu^2\rangle\tau_0)^2+\Omega^2}.$$

Since $\langle \nu^2 \rangle \tau_0 = \pi S_\nu(0)$, then the form of spectral line is approximately equal to:

$$W_z(\Omega) = \frac{R_0^2}{2\pi} \frac{\pi S_\nu(0)}{(\pi S_\nu(0))^2 + \Omega^2}. \tag{47}$$

This is resonant (Lorentzian) shape of line and its width equals:

$$\Delta\Omega = \pi^2 S_\nu(0) = \pi m \Omega_0, \tag{48}$$

i.e. it only depends on the value of spectral density of frequency fluctuations at zero frequency.

Thus, the second limit case leading to resonant form of spectral line is realized approximately for $\pi S_\nu(0) \ll \Omega_0$, i.e. in this case the frequency fluctuations are rather fast. This kind of spectrum of frequency fluctuations is generated either by thermal or shot fluctuations as it will be demonstrated below.

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[1] А.Н. Малахов, Флуктуации в автоколебательных системах - М.: Наука, 1968. - с. 660.