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Exactly solvable models of evolution processes in random environments

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Точно-решаемые модели эволюционных процессов в неупорядоченных средах:Препринт ИТЭФ 16-01/

Ф.С.Джепаров, В.Е.Шестопал – М., 2001 – 7 с.

Доклад, представленный на Международную Конференцию по Математической Физике, посвященную 75-летию проф. Р.Минлоса. Работа содержит краткий обзор современных исследований по построению асимптотически (при больших временах) точно решаемых моделей случайных блужданий в неупорядоченных средах.

Exactly solvable models of evolution processes in random environments:

F.S.Dzheparov, V.E.Shestopal [1]

A talk presented at the Int. Conference on Mathematical Physics, devoted to 75 years jubilee of Prof. R.Minlos. It contains a short review of modern studies on construction of asympthtically (for long times) exactly silvable models of random walks in disordered media.

Список лит. - 14 наим.

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The probability $\tilde{P}_{xy}(t)$ (propagator) to find a walker (excitation) at site x at moment t, if it was initially localized at y, for random walk in disordered media (RWDM) is described by the law

$$\frac{d}{dt}\tilde{P}_{xy} = -(\tilde{A}\tilde{P})_{xy} = -\sum_z (\tilde{W}_{zx}\tilde{P}_{xy} - \tilde{W}_{xz}\tilde{P}_{zy}),$$

$$\tilde{P}_{xy}(t=0) = \delta_{xy}. \tag{1}$$

The symbols x, y, z are assumed here to be sites of some regular d-dimensional lattice (simple cubic for example) with prime cell parameter a. A transition to continuous media corresponds to limit, when lattice parameter $a \to 0$, but distance $|x-y|$ and time t are finite.

The disorder of media is reflected in the transition rates $\tilde{W}_{zx}$ and in the set of positions, allowed for the walker.

One of the most important problems consists in calculation of the propagator, averaged over distribution of transition rates, assumed as translational invariant:

$$P_{x,y}(t) = \langle \tilde{P}_{x,y}(t) \rangle = P_{x-y,0}(t).$$

The problem belongs to most important in modern statistical physics due to wide applications in physics, chemistry and engineering, and due to important connections with the quantum field theory. Prof. Robert Minlos is one of outstanding researchers, who gave their remarkable pioneering contributions here (see for example [1,2]). Nevertheless the problem of long-time asymptotics is unsolved up to now for many important systems with **large fluctuations**, and, particularly, for such simplest realistic models as **random sites problem** and **random bounds problem**.

The disorder in **random sites problem** is created by random positions of sites allowed to carry the excitation, when transition rate has simple dependence

on distance. It is useful to rewrite the problem in the representation of occupation numbers as

$$\frac{d}{dt}\tilde{P}_{xy} = -\sum_z n_x n_z \nu(x-z)(\tilde{P}_{xy}-\tilde{P}_{zy}) = -\sum_z \nu(x-z)(n_z\tilde{P}_{xy}-n_x\tilde{P}_{zy}), \quad (2)$$

$$\tilde{P}_{xy}(t=0) = \frac{n_x}{c}\delta_{xy}, \quad \langle n_x\rangle = c, \quad \langle n_x n_z\rangle = c\delta_{xz} + c^2(1-\delta_{xz}), \quad \cdots.$$

Here $\nu(x)$ is a regular function, and random sites are produced by occupation numbers n_x: $n_x = 1$ if site x is allowed for excitation and $n_x = 0$ in opposite case. One of representative properties is given by the decay law

$$\langle e^{-\sum_z n_z \nu(z-x)t}\rangle = e^{-(bt)^{d/s}},$$

w here $\nu(x) \propto 1/|x|^s$, and continuum media approximation is assumed.

The **random bonds problem:**

$$\frac{d}{dt}\tilde{P}_{xy} = -\sum_{\alpha=1}^{Z} w_\alpha(x)(\tilde{P}_{xy} - \tilde{P}_{x+e_\alpha,y}), \quad (3)$$

where e_α is $\alpha-$th basic lattice vectors, $w_\alpha(x)$ is a random variable, and Z is the coordination number.

Only 1d random bonds problem is soluble now (see for example [1] - first correct definition of the diffusion coefficient; [2] - discovery of anomalous diffusion, [3] - a review of more recent progress).

Simple (asymptotically) exactly solvable model.

Random jumps model (RJM):

$$\frac{d}{dt}\tilde{P}_{xy} = -\sum_z w(x-z)(\xi_x\tilde{P}_{xy} - \xi_z\tilde{P}_{zy}), \quad \tilde{P}_{xy}(t=0) = \delta_{xy}. \quad (4)$$

Here $w(z)$ is a regular function and ξ_x is random variable.

The 1d RJM is isomorphic to the 1d random bonds problem [6]. Basic works:
1) Transport to nearest neighbors, $w(z) = w_0\vartheta(|z| = a)$:
a) Haus, Kehr, Lyklema [7]:

$$D = D_0 \cdot \varkappa, \quad D_0 = \frac{Z}{2d}w_0, \quad \frac{1}{\varkappa} = \langle\frac{1}{\xi_x}\rangle.$$

The diffusion coefficient D here is connected with D_0, corresponding to the transport on regular lattice with transition rate $w(x-z)$.
b) Refs. 6,8 - a way to formal long time expansion.
2) general (long range) interactions and correct construction of asymptotic long time expansion - Ref.9.

The method

Next transformations are basic for our construction:

$$\tilde{P}(\lambda) = \int_0^\infty dt\tilde{P}(t) = (\lambda + \tilde{A})^{-1}, \quad \tilde{A} = A_0\xi,$$

$$(A_0)_{xz} = \delta_{xz}\sum_y w(x-y) - w(x-z), \quad \xi_{xz} = \delta_{xz}\xi_x,$$

$$\tilde{P} = (\lambda + A_0\xi)^{-1} = \frac{1}{\lambda}(1 - A_0\xi\frac{1}{\lambda + A_0\xi}) = \frac{1}{\lambda}(1 - A_0\frac{1}{\frac{\lambda}{\xi} + A_0}). \tag{5}$$

It is an important representation, because

1) due to general properties of random walks and Laplace transformation the long time asymptotics is connected with small λ expansion of $P(\lambda)$, and

2) random ξ and small λ are collected together in λ/ξ.

Our next step is expansion in terms of fluctuations

$$\eta_x = \frac{1}{\varkappa} - \frac{1}{\xi_x}, \quad \frac{1}{\varkappa} = \langle\frac{1}{\xi_x}\rangle. \tag{6}$$

Starting with identity

$$Q = (\lambda/\xi + A_0)^{-1} = (\lambda/\varkappa + A_0 - \lambda\eta)^{-1} = G(1 - \lambda\eta G)^{-1} =$$

$$= G[\sum_{m=0}^{M}(\lambda\eta G)^m + (\lambda\eta G)^M\lambda\eta Q], \quad G = (\lambda/\varkappa + A_0)^{-1}, \tag{7}$$

the (small λ) asymptotic expansion can be obtained if

1) $\langle(1/\xi^m\rangle < \infty, \quad 1 \le m \le M$;

2) correlation radius for random η_x is finite;

and taking into account that

3) $\|P\| \le 2\bar{D}/\lambda^2 \leftrightarrow l_1$-norm, $\quad \bar{D} = \sup_x \sum_z \tilde{W}_{xz}, \quad \lambda \to +0$,

4) $|\langle F\tilde{P}\rangle_{xy}|^2 \le \langle FF^\dagger\rangle_{xx}\langle\tilde{P}^\dagger\tilde{P}\rangle_{yy}$, - Schwarz inequality;

5) representation

$$G_{x0}(\lambda) = \int \frac{d^dk}{V_B}\cdot\frac{\exp(ikx)}{\frac{\lambda}{\varkappa} + A_0(k)}, \quad A_0|k\rangle = A_0(k)|k\rangle \tag{8}$$

gives direct way to obtain small λ expansion of G, here V_B as a volume of Brillouin zone.

How small parameter is produced?
In first terms

$$Q = G + G\lambda\eta G + G(\lambda\eta G)^2 + \cdots. \tag{9}$$

There is no small parameter here, because $\lambda G \propto \lambda^0 = 1$; but

$$\langle Q\rangle = G + G^2\lambda^2\langle\eta_0^2\rangle G_{00} + \cdots = G(1 + \lambda G \cdot \lambda G_{00}\langle\eta_0^2\rangle + \cdots), \tag{10}$$

and λG_{00} is small in any dimension d.

Applications

1) Checking of numerical studies. For example physically important 3d random site problem with dipole transport ($w(x-z) \propto |x-z|^{-6}$) was studied numerically, and the program was shown as correct in computing for corresponding RJM with similar scale of fluctuations [10].

2) Construction of new solvable models, having more realistic properties [11,12]. Simple estimation: random bonds model on cubic lattice has d (or $Z/2$) random parameters per lattice site, when RJM has one parameter per site only.

Generalizations

If the generator $-\tilde{A}$ is of the form

$$\tilde{A} = B\xi C, \tag{11}$$

where B and C are translational invariant operators, then using the identity

$$\tilde{P} = (\lambda + \tilde{A})^{-1} = (\lambda + B\xi C)^{-1} =$$
$$= \frac{1}{\lambda}(1 - B\xi\frac{1}{\lambda + CB\xi}C) = \frac{1}{\lambda}(1 - B\frac{1}{\frac{\lambda}{\xi} + CB}C), \tag{12}$$

we again came to expansion in terms of

$$\lambda\eta = \lambda(\frac{1}{\varkappa} - \frac{1}{\xi}), \quad \frac{1}{\varkappa} = \langle\frac{1}{\xi}\rangle.$$

Examples

a) 1d.

If 1d lattice is separated into elementary cells with length N, then a coordinate x can be presented as

$$x = nN + \nu, \quad 1 \le \nu \le N.$$

Next model gives a generalization of simplest 1d random bonds problem, introducing a correlation between hopping rates in different points:

$$B = \nabla \leftrightarrow (Bf)_x = f_{x+1} - f_x, \quad C = B^\dagger;$$
$$\xi^{\mu\nu}_{mn} = \delta_{mn}\xi^{\mu\nu}_n, \quad \xi^{\mu\nu}_n = \phi^\mu_n \delta^{\mu\nu} + \chi_n, \tag{13}$$

Combining the Eq.12 with

$$(\xi^{-1})^{\mu\nu}_n = \frac{\delta^{\mu\nu}}{\phi^\mu_n} - \frac{\chi_n}{\phi^\mu_n \phi^\nu_n}(1 + \chi_n \sum_\sigma \frac{1}{\phi^\sigma_n}),$$

we obtain, that

$$P(t \to \infty) = \exp(-\nabla \varkappa \nabla^\dagger t) \quad , \varkappa = \langle \frac{1}{\xi} \rangle^{-1}. \tag{14}$$

The example has evident generalization to any effectively invertible ξ.

b) Arbitrary dimension d.

Let us consider a lattice with prime cell consisting of two sites, 1 and 2, and a generator of the form

$$\tilde{A} = A\xi; \quad \xi^{\mu\nu}_{xz} = \delta_{xz}\xi^{\mu\nu}_x = \delta_{xz} \begin{pmatrix} \alpha_x & \beta_x \\ \beta_x & \alpha_x \end{pmatrix}, \tag{15}$$

$$A^{\mu\nu}_{xz} = \begin{pmatrix} \sum_q (a_{qx} + b_{qx})\delta_{xq} - a_{xz} & -b_{xz} \\ -b_{xz} & \sum_q (b_{qx} + c_{qx})\delta_{xq} - c_{xz} \end{pmatrix},$$

The methods works here directly and

$$P(t \to \infty) = \exp(-A_{eff} t), \quad A_{eff} = A\varkappa, \quad \varkappa = \langle \frac{1}{\xi} \rangle^{-1}. \tag{16}$$

Other details see in Ref.12. The model has 3 random parameters per 2 lattice sites instead 1 per 1 for standard RJM.

Primary RJM was asymmetrical, therefore construction of symmetrical multidimensional model is of special interest. It is realized in similar way for lattice, defined in preceding example using

$$\tilde{A} = \zeta B \zeta^\dagger \tag{17}$$

with regular B and random $\zeta^{\mu\nu}_{xz} = \delta_{xz}\zeta^{\mu\nu}_x$. Necessary limitation on parameters are described in Ref.12.

If $\tilde{A} = \zeta B \eta$, and again $\eta^{\mu\nu}_{xz} = \delta_{xz}\eta^{\mu\nu}_x$, then up to 8 parameters per 2 sites are admitted.

Example of ergodic theorem

In the final part of our report we would like to attract the attention to a Hamiltonian system [13], which gives a model of the system of impurity spins, placed in the crystal, having other spins with strong interaction. The Hamiltonian is of the form

$$H = \frac{1}{2}\sum_{i,j} b_{ij} I_i^+ I_j^- + \sum_j \omega_j(t) I_j^z. \tag{18}$$

Here coefficient $b_{ij}(\propto |r_i - r_j|^{-3}$ for dipole-dipole interaction) defines a strength of interaction between spins, placed at r_i and r_j; I_i^α $(\alpha = x, y, z)$ is standard spin operator, $I_j^+ = I_j^x + iI_j^y$, $I_j^- = (I_j^+)^\dagger$, and c-number functions $\omega_j(t)$ gives realizations of a normal delta-correlated process:

$$\langle \omega_i(t)\omega_j(t_1)\rangle = \frac{2}{T}\delta_{ij}\delta(t - t_1). \tag{19}$$

In the natural limit of small interaction (for $\epsilon = \max_{ij} b_{ij}^2 T^2 \ll 1$, and $wt = \epsilon t/T \sim \epsilon^0$) the evolution of the system with $I_j = 1/2$ is described by a set of master equation, and simplest of them coincides with random site problem for one walker. Other equations describe many walkers evolution.

The model (18),(19) produce a mathematical basis for description of some real transport processes in modern physics (see for example [14]).

The system has simple but rich in context ergodic properties, some of them are studied for arbitrary ϵ in Ref.13. It was shown particularly that in leading order in ϵ the set of master equations has Gibbsian distribution ρ_G as a final state ρ_f

$$\rho_f = \rho_G = \exp(-\beta \sum_j I_j^z)$$

if initial state has finite correlations radius, and if correlations are long ranged then ρ_f is not a Gibbsian. The same property is valid for arbitrary ϵ.

The work was supported by RFBR, grants 00-01-00271-a, 99-01-00284, 00-01-00271.

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