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Diffusion Equations in Lie Group Manifold *

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Abstract To describe the random motion in the symmetric space, the diffusion equations in a group manifold have been developed. A concrete formula of the diffusion equation on the compact Riemannian space was presented. Furthermore, the corresponding quantum diffusion motion in the space was also discussed.

Key words diffusion equation, Brownian motion, group manifold

Random walks(RW) and their continuous counterparts, Brownian motions(BM), describe perhaps the simplest stochastic process pervading statistical physics, probability theory, and even biology, The most of the theories have been expressed in general d-dimensional space. However, it was found that some random walks relate to the symmetric properties of space, for example, the nuclear spin relaxation, the random motion of a complex molecule. In this letter a general formulation of the problem based on group theory is presented in a symmetric space.

Let us consider a molecule which may have different configurations. For instance, let a rigid molecule be of different orientations in a symmetric space, i. e., a molecule can have "internal motion". It will be described by using $\gamma_1, \gamma_2, \cdots\cdots, \gamma_r$, real parameters(angles, lengths, and so on) Assuming that G is a group manifold spanned by parameters $\{\gamma\}$, a given configuration of the molecule is then represented by a point on G and the eventual Brownian motion of the molecule can be described by a Brownian motion of the point on G.

Let $G \times R$ be the manifold with coordinate $t \in R$, denoted as a time variable and $p(\alpha;t)\mathrm{d}\alpha$ be the probability of the system being in the infinitesimal volume $\mathrm{d}\alpha$ round the point α on G at time t; $\mathrm{d}\alpha$, the usual invariant differential volume and we normalize it so that $\int_G \mathrm{d}\mu(\alpha) = 1$, $\mathrm{d}\mu(\alpha)$ is the measure on the manifold G. For any two points $\alpha_0, \alpha \in \omega$, we may write, according to transformation properties of group[1],

$$p(\alpha_0;t) = \exp\{-\alpha_0^l \hat{I}_l(\alpha)\} p(\alpha;t) \tag{1}$$

and $\hat{I}_l(\alpha)$ are generators of the Lie group at the point α. Here we used the summing convention.

Using the so-called Gain-Loss equation(Master Equation)[2] and Eq. (1) one derives the diffusion equation on the group manifold

$$\partial_t p(\alpha;t) = D^{ll'} \hat{I}_l(\alpha) \hat{I}_{l'}(\alpha) p(\alpha;t) - v^l \hat{I}_l(\alpha) p(\alpha;t) \tag{2}$$

in which the diffusion vector on the manifold G is defined as

$$v^l \equiv \lim_{\Delta t \to 0} \frac{\langle \delta\alpha_0^l \rangle}{\Delta t} \tag{3}$$

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and the diffusion tensor

$$D^{ll'} = \lim_{\Delta t \to 0} \frac{1}{2\Delta t} \langle \delta\alpha_0^l \delta\alpha_0^{l'} \rangle. \tag{4}$$

Futhermore, let G be a compact semi-simple group manifold. In the case of free motion, $v^l = 0$ and the Cartan metric tensor can be defined by the structure constant C_{lk}^i as

$$\gamma_{ll'} = C_{lk}^i C_{il'}^k. \tag{5}$$

We can rewrite the diffusion tensor[3] as follows

$$\lim_{\Delta t \to 0} \frac{1}{2\Delta t} \langle \delta\alpha_0^l \delta\alpha_0^{l'} \rangle = D_0 \gamma^{ll'} \tag{6}$$

where the diffusion coefficient D_0 is a constant. From the discussion above the diffusion equation on Lie group manifold can be easily deduced

$$\partial_t p(\alpha;t) = D_0 \gamma^{ll'} \hat{I}_l(\alpha) \hat{I}_{l'}(\alpha) p(\alpha;t). \tag{7}$$

Now we introduce a symbol

$$\hat{C} = \gamma^{ll'} \hat{I}_l(\alpha) \hat{I}_{l'}(\alpha). \tag{8}$$

It is just the Casimir operator. Then the diffusion equation has a compact form

$$\partial_t p(\alpha;t) = D_0 \hat{C} p(\alpha, t). \tag{9}$$

The existence of the limits in Eq. (3) and Eq. (4) is precisely the main hypothesis of the Brownian motion. In addition, remenber that in writing Eq. (6) we have assumed the diffusion coefficient to be independent of the point α.

Random walks on Riemannian surfaces are common phenomena in the nature. To describe Browian motions and their quantum actions in terms of the Riemannian manifold, we go ahead another step to discuss the concrete formula of the diffusion equation in a compact Riemannian space.

The $\hat{I}_l(\alpha)$ in Eq. (7), generators of the Lie group at the point α, are defined as

$$\hat{I}_l = S_{lk}^{L}(\alpha) \frac{\partial}{\partial \alpha^k} \tag{10}$$

in which S_{lk}^{L} is the auxiliary function[4], it has form like

$$S_{ij}^{L}(\alpha) = \frac{\partial}{\partial \alpha'^j} f_i(\alpha', \alpha)\,|_{\alpha'=0}, S_{ij}^{R}(\alpha) = \frac{\partial}{\partial \alpha'^j} f_i(\alpha, \alpha')\,|_{\alpha'=0},$$

where, $f_i(\alpha', \alpha)$ is the composition functions of Lie group.

For the manifold G, the Riemannian metric can be expressed by[4]

$$g_{nm} = \gamma_{ll'} (S_{nl}^{L})^{-1} (S_{ml'}^{L})^{-1}. \tag{12}$$

So the line element on the manifold G is

$$\Delta s^2 = g_{nm}(\alpha) \mathrm{d}\alpha^n \mathrm{d}\alpha^m \tag{13}$$

From Eq. (5) it is easy to obtain the relation

$$g^{ll'} = S_{lk}^{L} \gamma^{km} S_{ml}^{L}, \tag{14}$$

where $g_{lk} g^{kl'} = \delta_l^{l'}$, $\gamma_{lk} \gamma^{kl'} = \delta_l^{l'}$. Considering the determinant of $g_{ll'}$

$$g = \det| g_{ll'} | = ((\det S^{L})^{-1})^2 \gamma^{-1},$$

where $\gamma = \det| \gamma^{ll'} |$. For the compact Lie group, using $\det A^{-1} \det A = 1$, one gets

$$\det S^{L} = \sqrt{\gamma g} = \det S^{R}$$

On the other hand, according to the composition of Lie group it is not difficult to derive

$$\frac{\partial}{\partial \alpha_i} S_{ik}^{L}(\alpha) = \frac{\partial}{\partial \alpha^n} [\ln(\det S^{R}(\alpha))] S_{nk}^{L}(\alpha).$$

Substituting Eqs. (10) and (16) into Eq. (7), we finally reach

$$\partial_t p(\alpha;t) = D_0 \Delta p(\alpha;t),$$

where

$$\Delta = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \alpha_i} \left(\sqrt{g} g^{ij} \frac{\partial}{\partial \alpha_j} \right) \tag{18}$$

is the general Laplace-Beltrami operator on Riemannian manifold G. This is a concrete form of diffusion equations on compact Riemann manifold.

Eq. (17) looks like a Schrödinger equation. without interaction potentioal. But it is different from the Schrödinger equation. The Δ on the ringht side of Eq. (17) is general variance Laplace-Beltrami operator. We can assume that its sulotion has an exponential time-dependence, $p(\alpha;t) = \exp\{tD_0\Delta\}\varphi(\alpha)$. The probability of the transition from α at 0 to α' at τ can be given by[5]

$$p(\alpha,\alpha';\tau) = \exp\{tD_0\Delta\} \sum_m \phi_m(\alpha')\phi_m(\alpha) = \sum_m \phi_m(\alpha')\exp\{-tD_0\lambda_m\}\phi_m(\alpha), \tag{19}$$

where

$$\Delta\phi_m(\alpha) = -\lambda_m\phi_m(\alpha). \tag{20}$$

On the other hand, if the diffusion coefficient D_0 takes the value $\hbar/2m$ given by Ref. [6], Eq. (17) then becomes the follows

$$\partial_t\psi(\alpha,t) = \frac{\hbar}{2m}\Delta\psi(\alpha,t). \tag{21}$$

We may use this Eq. (21) to describe the quantum random walks.

Here we mainly study the diffusion equations on the symmerty space. It may be a useful tool to describe the internal random walks in a complex molecule.

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李群流形中的扩散方程*

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摘要 为了描述对称空间中的无规运动,建立了群流形中的扩散方程,给出了紧致黎曼空间中扩散方程的一种具体形式,并进一步讨论了紧致黎曼空间中量子扩散运动.

关键词 扩散方程 布朗运动 李群流形

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