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Random walks on hyperspheres of arbitrary dimensions

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Abstract

We consider random walks on the surface of the sphere S_{n-1} ($n \geq 2$) of the n -dimensional Euclidean space E_n , in short a hypersphere. By solving the diffusion equation in S_{n-1} we show that the usual law $\langle r^2 \rangle \propto t$ valid in E_{n-1} should be replaced in S_{n-1} by the generic law $\langle \cos \theta \rangle \propto \exp(-t/\tau)$, where θ denotes the angular displacement of the walker. More generally one has $\langle C_L^{n/2-1}(\cos \theta) \rangle \propto \exp(-t/\tau(L, n))$ where $C_L^{n/2-1}$ is a Gegenbauer polynomial. Conjectures concerning random walks on a fractal inscribed in S_{n-1} are given tentatively.

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1. Introduction

We consider a random walk (RW) on the surface of a sphere S_{n-1} of the real Euclidean space E_n of dimension n , a hypersphere for short. Let O be the centre of the hypersphere and R its radius, S_{n-1} is thus defined as the set of points $M \equiv (x_1, \dots, x_n)$ of E_n such that $\sum_{i=1}^n x_i^2 = R^2$. If the legs of the walker are much smaller than the radius R of the sphere, then the diffusion process can be described by a continuous diffusion equation, i.e.

$$\mathcal{D}\rho(M, t) \equiv \left(\frac{\partial}{\partial t} - D\Delta^{S_{n-1}} \right) \rho(M, t) = 0 \quad (1.1)$$

where $\rho(M, t)$ is the density probability for the walker to be at point M at time t . $D (> 0)$ is the diffusion coefficient and $\Delta^{S_{n-1}}$ denotes the Laplace–Beltrami operator in space S_{n-1} . Explicit initial conditions will be specified later. Note that for imaginary times equation (1.1) identifies with the Schrödinger equation of a free particle of S_{n-1} , alternatively this equation can be considered as describing the diffusive rotational motion of a n -dimensional linear polar molecule.

The solution of equation (1.1) in the case $n = 3$ has been known since the work of Debye on Brownian rotors [1, 2]. In this paper we extend Debye's proof to arbitrary dimensions n and show that a salient feature of a RW on a hypersphere is the validity of the generic law

$$\langle \xi(0) \cdot \xi(t) \rangle \equiv \langle \cos \theta(t) \rangle = \exp(-D(n-1)t/R^2) \quad (1.2)$$

where the unit vector $\xi = OM/R$ denotes the orientation of vector OM in E_n . With the north pole of S_{n-1} chosen to be $M(t=0)$ the angle θ in equation (1.2) is thus the colatitude of point M in spherical coordinates. The brackets $\langle \dots \rangle$ denote a spatial average with weight $\rho(M, t)$, and the dot in the LHS is the usual scalar product in E_n . Result (1.2), given without proof in [3], is not surprising; indeed as noted by Jund *et al* when $Dt/R^2 \ll 1$ one can expand both sides of equation (1.2) yielding for the projection x of vector OM in the Euclidean plane E_{n-1} tangent to S_{n-1} at point M_0 to the behaviour $\langle x^2 \rangle \sim R^2 \langle \theta^2 \rangle \sim 2t(n-1)D$ characteristic of a random walk in an Euclidean space of $(n-1)$ dimensions.

Recently Nissfolk *et al* have given a solution of (1.1) in the special case $n = 4$ [4]. Their expression for $\rho(M, t)$ is different from that which we derive in section 3 and, in particular, does not allow us to recover easily equation (1.2). The equivalence of the two solutions is established in the last section of this paper.

Our paper is organized as follows. In section 2 we give an elementary proof of equation (1.2). The expression of the Green function of equation (1.1) is derived in section 3 from which equation (1.2) can be deduced. The solution, inspired by the seminal paper of Debye on 3D rotors [1, 2], requires the whole machinery of hyperspherical harmonics and the use of some properties of the rotation group $SO(n)$ [5]. Finally in section 4 we consider in more detail the case $n = 4$. Our solution of (1.1) for $n = 4$ and that proposed by Nissfolk *et al* [4] are shown to be identical. A preliminary account of the present work, however devoted to the special case $n = 4$, can be found in [7].

2. An elementary proof of $\langle \cos \theta \rangle \propto \exp(-T/\tau)$

We suppose that the walker is standing at some point $OM_0 = R\xi_0$ of S_{n-1} at time $t = 0$. At subsequent times its dynamics is governed by equation (1.1) and we study the time behaviour of the random variable $\cos \theta \equiv \xi_0 \cdot \xi$. We choose the north pole of S_{n-1} to be M_0 and θ is thus the colatitude of point M in spherical coordinates. We define

$$\langle \cos \theta \rangle(t) = \int_{S_{n-1}} \rho(M, t) \cos \theta \, d\tau(M) \quad (2.1)$$

where $d\tau(M)$ is the infinitesimal volume element in S_{n-1} . It follows from equation (1.1) that

$$\begin{aligned} \frac{\partial}{\partial t} \langle \cos \theta \rangle &= \int_{S_{n-1}} D \cos \theta \Delta^{S_{n-1}} \rho(M, t) \, d\tau(M) \\ &= \int_{S_{n-1}} D \rho(M, t) \Delta^{S_{n-1}} \cos \theta \, d\tau(M) \end{aligned} \quad (2.2)$$

where we have made use of Green's theorem in S_{n-1} [6]. At this point we recall that the Laplacian Δ^{E_n} in E_n may be decomposed as the sum [5]

$$\begin{aligned} \Delta^{E_n} &= \Delta^R + \Delta^{S_{n-1}} \\ \Delta^R &= \frac{1}{R^{n-1}} \frac{\partial}{\partial R} R^{n-1} \frac{\partial}{\partial R} \end{aligned} \quad (2.3)$$

where Δ^R acts only on the variable R and $\Delta^{S_{n-1}}$, which acts only on angular variables, is called the angular part of the Laplacian or, alternatively, the Laplace–Beltrami operator [5].

From these remarks, the action of $\Delta^{S_{n-1}}$ on $\cos \theta$ will easily be obtained. On one hand we have obviously $\Delta^{E_n}(OM \cdot \xi_0) = 0$; however, on the other hand, it follows from equations (2.3) that $\Delta^{E_n}(OM \cdot \xi_0) \equiv \Delta^{E_n}(R \cos \theta) = (n - 1) \cos \theta / R + R \Delta^{S_{n-1}} \cos \theta$ whence $\Delta^{S_{n-1}} \cos \theta = -(n - 1) \cos \theta / R^2$ yielding, when inserted in equation (2.2), the simple equation

$$\frac{\partial}{\partial t} \langle \cos \theta \rangle + (n - 1) \frac{D}{R^2} \langle \cos \theta \rangle = 0 \tag{2.4}$$

the solution of which being of course given by equation (1.2).

3. The general solution

We shall make extensive use of the properties of the hyperspherical harmonics to solve equation (1.1). A short résumé on these functions might prove useful for the reader. We will adopt the definitions and notation of the chapter IX of the classical textbook by Vilenkin [5]. In the case $n = 4$ this yields a definition of the harmonics which is slightly different from that which we used previously [8–10].

To avoid confusion we shall denote by S_{n-1} the hypersphere of radius $R = 1$. (When, incidentally, we talk about the volumes of the spaces S_{n-1} or \mathcal{S}_{n-1} we mean in fact the areas of these spheres considered as manifolds of E_n .) The spherical coordinates of the unit vector $\xi = OM \equiv (\xi_1, \dots, \xi_n)$ of S_{n-1} are defined by the relations

$$\begin{aligned} \xi_1 &= \sin \theta_{n-1} \dots \sin \theta_2 \sin \theta_1 \\ \xi_2 &= \sin \theta_{n-1} \dots \sin \theta_2 \cos \theta_1, \dots \\ \xi_{n-1} &= \sin \theta_{n-1} \cos \theta_{n-2} \\ \xi_n &= \cos \theta_{n-1} \end{aligned} \tag{3.1}$$

where $0 \leq \theta_1 < 2\pi$ and $0 \leq \theta_k < \pi$ for $k \neq 1$. Note that θ_{n-1} is the colatitude of point M and was denoted by θ in section 2. The integration measure in S_{n-1} will be defined as

$$d\xi \equiv \frac{1}{A_{n-1}} \sin^{n-2} \theta_{n-1} \dots \sin \theta_2 d\theta_1 \dots d\theta_{n-1} \tag{3.2}$$

where $A_{n-1} = 2\pi^{n/2} / \Gamma(n/2)$ is the surface of the sphere S_{n-1} . With this normalization

$$\int_{S_{n-1}} d\xi = 1 \tag{3.3}$$

and the infinitesimal volume element in S_{n-1} is given by $d\tau = R^{n-1} A_{n-1} d\xi$. The expression of the Laplacian $\Delta^{S_{n-1}} \equiv R^2 \Delta^{E_n}$ in spherical coordinates reads as

$$\begin{aligned} \Delta^{S_{n-1}} &= \frac{1}{\sin^{n-2} \theta_{n-1}} \frac{\partial}{\partial \theta_{n-1}} \sin^{n-2} \theta_{n-1} \frac{\partial}{\partial \theta_{n-1}} + \frac{1}{\sin^2 \theta_{n-1} \sin^{n-3} \theta_{n-2}} \frac{\partial}{\partial \theta_{n-2}} \sin^{n-3} \theta_{n-2} \frac{\partial}{\partial \theta_{n-2}} \\ &+ \dots + \frac{1}{\sin^2 \theta_{n-1} \dots \sin^2 \theta_2} \frac{\partial^2}{\partial \theta_1^2}. \end{aligned} \tag{3.4}$$

The (hyper)spherical harmonics $\Xi_{L,K}(\xi)$ are defined to be the eigenvectors of the operator $\Delta^{S_{n-1}}$. The spectrum of $\Delta^{S_{n-1}}$ is given by the integers $\lambda(n, L) = -L(L + n - 2)$ where $L = 0, 1, \dots$ is a positive integer. One can show that $K \equiv (k_1, \dots, \pm k_{n-2})$ with $L \geq k_1 \geq k_2 \geq k_{n-2} \geq 0$. Therefore, there are exactly $h(n, L) = (2L + n - 2)(n + L - 3)! / (n - 2)! L!$ distinct harmonics $\Xi_{L,K}(\xi)$ corresponding to the eigenvalue $\lambda(n, L)$. The $\Xi_{L,K}(\xi)$ constitute a complete basis set for expanding any square integrable function $f \in \mathcal{L}^2[S_{n-1}]$ defined on S_{n-1} . An explicit expression of $\Xi_{L,K}(\xi)$ will be of little use and can be found

in Vilenkin [5]. As the usual spherical harmonics the $\Xi_{L,K}(\xi)$ satisfy the following properties [5]

- (i) orthogonality

$$\int_{S_{n-1}} \Xi_{L,K}^*(\xi) \Xi_{L',K'}(\xi) d\xi = \delta_{L,L'} \delta_{K,K'} \tag{3.5}$$

- (ii) completeness

$$\sum_{L,K} \Xi_{L,K}^*(\xi) \Xi_{L,K}(\xi') = \delta^{S_{n-1}}(\xi, \xi') \tag{3.6}$$

where $\delta^{S_{n-1}}$ is the Dirac distribution for the unit hypersphere defined as

$$\int_{S_{n-1}} f(\xi) \delta^{S_{n-1}}(\xi, \xi') d\xi = f(\xi') \tag{3.7}$$

- (iii) addition theorem

$$\sum_K \Xi_{L,K}^*(\xi) \Xi_{L,K}(\xi') = \frac{2L+n-2}{n-2} C_L^{n/2-1}(\xi \cdot \xi') \tag{3.8}$$

where the dot on the RHS denotes the usual scalar product in E_n , i.e. $\xi \cdot \xi' = \cos \psi$ where ψ is the angle between the two unit vectors ξ and ξ' , and $C_L^{n/2-1}$ is a Gegenbauer polynomial. The Gegenbauer polynomials C_L^p are a generalization of Legendre polynomials. C_L^p is defined as the coefficient of h^L in the power-series expansion of the function

$$(1 - 2th + h^2)^{-p} = \sum_{L=0}^{\infty} C_L^p(t) h^L. \tag{3.9}$$

We have now in hand all the tools to solve equation (1.1). We first expand $\rho(M, T)$ in terms of the $\Xi_{L,K}$,

$$\rho(M, t) = \sum_{L=0}^{\infty} \sum_K \rho_{L,K}(t) \Xi_{L,K}(\xi) \tag{3.10}$$

and then insert expansion (3.10) in equation (1.1). Making use of the orthogonal properties of the $\Xi_{L,K}$ yields an infinite system of non-coupled equations

$$\left(\frac{\partial}{\partial t} + D \frac{L(L+n-2)}{R^2} \right) \rho_{L,K}(t) = 0 \tag{3.11}$$

the solution of which reads obviously as

$$\rho_{L,K}(t) = \rho_{L,K}(0) \exp(-DL(L+n-2)t/R^2). \tag{3.12}$$

We shall denote by $\rho(M, t|M_0, 0)$ the solution of (1.1) corresponding to the initial condition $\rho(M, 0) = \delta^{S_{n-1}}(M, M_0) \equiv \delta^{S_{n-1}}(\xi, \xi_0)/R^{n-1} A_{n-1}$, i.e. the solution of

$$\mathcal{D}\rho(M, t|M_0, 0) = \delta(t) \frac{1}{R^{n-1} A_{n-1}} \delta^{S_{n-1}}(\xi, \xi_0). \tag{3.13}$$

It follows readily from equations (3.12) and (3.6) that the Green function $\rho(M, t|M_0, 0)$ can be expressed as

$$\begin{aligned} \rho(M, t|M_0, 0) &= 0 && (t < 0) \\ \rho(M, t|M_0, 0) &= \frac{1}{R^{n-1} A_{n-1}} \sum_{L=0}^{\infty} \sum_K \Xi_{L,K}^*(\xi_0) \Xi_{L,K}(\xi) \\ &\quad \times \exp(-DL(L+n-2)t/R^2) && (t > 0). \end{aligned} \tag{3.14}$$

Equation (3.14) can be further simplified with the help of the addition theorem (3.8) yielding our final result

$$\rho(M, t|M_0, 0) = \frac{1}{R^{n-1}A_{n-1}} \sum_{L=0}^{\infty} \frac{2L+n-2}{n-2} C_L^{n/2-1}(\xi_0 \cdot \xi) \times \exp(-DL(L+n-2)t/R^2) \quad (t > 0). \tag{3.15}$$

Some comments on equation (3.15) are in order.

- (i) Solution (3.15) is invariant under rotation about the axis ξ_0 as expected. Equation (3.15) is a generalization for all n of Debye's result which corresponds to the case $n = 3$ [1, 2]. In this case the Gegenbauer polynomials reduce to the Legendre polynomials P_L . In the case $n = 4$ we recover the result of [7] where the Gegenbauer polynomials reduce to Tchebycheff polynomials of second kind. To be more precise, we recall that [5]

$$C_L^{1/2}(\cos \theta) = P_L(\cos \theta) \quad (n = 3) \tag{3.16}$$

$$C_L^1(\cos \theta) = \frac{\sin(L+1)\theta}{\sin \theta} \quad (n = 4). \tag{3.17}$$

- (ii) Note that $\int_{S_{n-1}} \rho(M, t|M_0, 0) d\tau = \rho_{0,0} = 1$, i.e. the probability is conserved, and that we also have $\lim_{t \rightarrow +\infty} \rho(M, t|M_0, 0) = 1/\Omega_{n-1}$, where $\Omega_{n-1} = R^{n-1}A_{n-1}$ is the volume of the space S_{n-1} , i.e. the solution of the diffusive process is uniform after infinite time.
- (iii) Let us define the time correlation functions

$$\begin{aligned} \mathcal{F}_L^{n/2-1}(t) &\equiv \langle C_L^{n/2-1}(\xi_0 \cdot \xi) \rangle \quad (L \geq 1) \\ &= \int_{S_{n-1}} d\xi_0 \int_{S_{n-1}} d\xi C_L^{n/2-1}(\xi_0 \cdot \xi) \hat{\rho}(M, t|M_0, 0) \end{aligned} \tag{3.18}$$

where we have introduced the reduced Green function $\hat{\rho} \equiv R^{n-1}A_{n-1}\rho$. As a consequence of the orthogonality properties (3.5) we find that

$$\mathcal{F}_L^{n/2-1}(t) = \frac{(n-3+L)!}{L!(n-3)!} \exp(-DL(L+n-2)t/R^2). \tag{3.19}$$

Special cases are of interest. Firstly, since for $L = 1$ we have $C_1^{n/2-1}(u) = (n-2)u$, equation (3.19) indeed gives back equation (1.2). For $n = 3$ and 4 we recover the results for the 3D and 4D rotors [1, 2, 7]

$$\langle P_L(\cos \theta) \rangle = \exp(-DL(L+1)t/R^2) \quad (n = 3) \tag{3.20}$$

$$\left\langle \frac{\sin(L+1)\theta}{\sin \theta} \right\rangle = (L+1) \exp(-DL(L+2)t/R^2) \quad (n = 4). \tag{3.21}$$

Defining now the reorientational time $\tau_L^{n/2-1}$ as

$$\tau_L^{n/2-1} = \int_0^\infty \frac{\mathcal{F}_L^{n/2-1}(t)}{\mathcal{F}_L^{n/2-1}(0)} dt = \frac{R^2}{DL(L+n-2)} \tag{3.22}$$

we have now at our disposal a Kubo formula for the diffusion coefficient D . Note the aesthetic relation $\tau_L^{n/2-1}/\tau_{L'}^{n/2-1} = L'(L'+n-2)/L(L+n-2)$ which generalizes Debye's result to arbitrary dimensions [1, 2]. Since simulations of real 3D liquids or plasmas are feasible (moreover efficient) in S_3 [8–10] equation (3.22) is of prime importance since it should allow the computation of the self-diffusion coefficient of such systems in the course of equilibrium molecular dynamics simulations.

- (iv) Simulations of random walks on fractals inscribed in S_{n-1} were reported recently [3]. While it is known that for random walks on fractal clusters in Euclidean spaces the anomalous diffusion law $\langle r^2(t) \rangle \propto t^\beta$ holds [11, 12] (where β is some exponent depending on the fractal dimensions of the cluster) the numerical results of [3] give evidence of the law $\langle \cos \theta \rangle \propto \exp(-(t/\tau)^\beta)$, i.e. a stretched exponential relaxation, on the hypersphere. As suggested by Jund *et al* [3] the anomalous diffusion law for a RW on a fractal can be understood by replacing the time t by a fractal time t^β in the diffusion equation (1.1) and thus in the solution (3.15). With this assumption we now have the ansatz

$$\left(\tau_L^{n/2-1} / \tau_{L'}^{n/2-1}\right)^{1/\beta} = L'(L' + n - 2) / L(L + n - 2) \quad (3.23)$$

which could be checked in numerical simulations.

4. Random walks in S_3

We specialize to the case $n = 3$ and want to show that expression (3.15) of $\rho(M, t | M_0, 0)$ is equivalent to that of [4]. This can be done as follows. Let us rewrite the reduced $\hat{\rho} = 2\pi^2 R^3 \rho(M, t | M_0, 0)$ as

$$\hat{\rho} = \sum_{L=0}^{\infty} (L+1) \frac{\sin(L+1)\psi}{\sin \psi} \exp(-KL(L+2)) \quad (4.1)$$

where $K = Dt/R^2$. *A priori* the angle ψ is in the range $(0, \pi)$, however, since the function is formally even in ψ we define $\hat{\rho}(-\psi) = \hat{\rho}(\psi)$ for negative angles. This gives us a periodic function of period 2π defined for all $\psi \in \mathbb{R}$. We introduce now the periodic function

$$F(\psi) = \int_0^\psi d\psi' \hat{\rho}(\psi') \sin(\psi') \quad (4.2)$$

which can be rewritten after some algebra as

$$F(\psi) = F_0 - \frac{\exp K}{2} \sum_{p=-\infty}^{+\infty} \exp(-Kp^2) \exp(-ip\psi) \quad (4.3)$$

where F_0 is some unessential constant independent of angle ψ . At this point we recall the Poisson summation theorem which states that for any function $\varphi(x)$ holomorphic in the strip $-a < \text{Im } z < a$ one has

$$\sum_{n=-\infty}^{+\infty} \varphi(x + 2n\pi) = \frac{1}{2\pi} \sum_{p=-\infty}^{+\infty} e^{-ipx} \int_{-\infty}^{+\infty} \varphi(y) e^{ipy} dy. \quad (4.4)$$

Applying the Poisson theorem for the Gaussian we get

$$F(\psi) = F_0 - \frac{\sqrt{\pi} \exp K}{2\sqrt{K}} \sum_{n=-\infty}^{+\infty} \exp\left(-\frac{(\psi + 2n\pi)^2}{4K}\right) \quad (4.5)$$

which after differentiation yields for $\hat{\rho}$

$$\hat{\rho}(\psi, t) = \frac{\sqrt{\pi} \exp K}{4K^{3/2} \sin \psi} \sum_{n=-\infty}^{+\infty} (\psi + 2n\pi) \exp\left(-\frac{(\psi + 2n\pi)^2}{4K}\right) \quad (4.6)$$

which coincides with the result of [4], apart from the prefactor which is not specified. Relations similar to equation (4.6) can be obtained for *even* values of n (other than 4) but we failed to get anything similar for odd n .

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References

- [1] Debye P 1929 *Polar Molecules* (London: Dover)
- [2] Berne B J and Pecora P 1976 *Dynamic Light Scattering* (New York: Wiley)
- [3] Jund P, Jullien R and Campbell I 2001 *Phys. Rev. E* **63** 036131
- [4] Nissfolk J, Ekholm T and Elvingson C 2002 *J. Chem. Phys.* **119** 6423
- [5] Vilenkin N Ja 1969 *Fonctions Spéciales et Théorie de la Représentation des Groupes* (Paris: Dunod)
- [6] Rosenberg S 1997 *Laplacian on a Riemannian Manifold* (Cambridge: Cambridge University Press)
- [7] Caillol J-M 2003 *Preprint cond-mat/0309706* (unpublished)
- [8] Caillol J-M and Levesque D 1991 *J. Chem. Phys.* **94** 597
- [9] Caillol J-M 1993 *J. Chem. Phys.* **99** 8953
- [10] Caillol J-M and Gilles D 2000 *J. Stat. Phys.* **100** 905
- [11] Alexander S and Orbach R 1982 *J. Phys. (France) Lett.* **43** L625
- [12] Gefen Y, Aharony A and Alexander S 1983 *Phys. Rev. Lett.* **50** 77