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 $\theta$ 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 $C_{L}^{n/2-1}$ a Gegenbauer polynomial. Conjectures concerning random walks on a fractal inscribed in $S_{n-1}$ are given tentatively.

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I. 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 center of the hypersphere and $R$ its radius, $S_{n-1}$ is thus defined as the set of points $M \equiv (x_1, \ldots, x_n)$ 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.

$$D \rho(M, t) \equiv \left( \frac{\partial}{\partial t} - D \Delta_{S_{n-1}} \right) \rho(M, t) = 0,$$

(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 eq. (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 eq. (1.1) in the case $n = 3$ is known since the work of Debye on Brownian rotors. 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

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

(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 $\theta$ in eq. (1.2) is thus the colatitude of point $M$ in spherical coordinates. The brackets $\langle \ldots \rangle$ denote a spatial average with weight $\rho(M, t)$, and the dot in the LHS is the usual scalar product in $E_n$. The result (1.2), given without proof in ref. 3, is not surprising; indeed as noted by Jund et al. when $Dt/R^2 \ll 1$ one can expand both sides of eq. (1.2) yielding for the projection $\mathbf{x}$ of vector $OM$ in the euclidean plane $E_{n-1}$ tangent to $S_{n-1}$ at point $M_0$ to the behavior $\langle x^2 \rangle \sim R^2 \langle \theta^2 \rangle \sim 2t(n-1)D$ 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 $n = 4$. Their expression for $\rho(M, t)$ is different from that which we derive in sec. III and, in particular, does not allow to recover easily eq. (1.2). The equivalence of the two solutions is established in the last section of this paper.
Our paper is organized as follows. In next section II we give an elementary proof of eq. (1.2). The expression of the Green’s function of eq. (1.1) is derived in section III from which eq. (1.2) can deduced. The solution, inspired from the seminal paper of Debye on 3D rotors, requires the whole machinery of hyperspherical harmonics and the use of some properties of the rotation group $SO(n)$. Finally in section IV we consider in more details the case $n = 4$. Our solution of (1.1) for $n = 4$ and that proposed by Nissfolk et al. are shown to be identical. A preliminary account of the present work, however devoted to the special case $n = 4$, can be found in ref. 7.

II. AN ELEMENTARY PROOF OF \( \langle \cos \theta \rangle \propto \exp(-t/\tau) \)

We suppose that the walker it 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 eq. (1.1) and we study the time behavior 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 $\theta$ is thus the colatitude of point $M$ in spherical coordinates. We define

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

(2.1)

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

\[
\frac{\partial}{\partial t} \langle \cos \theta \rangle = \int_{S_{n-1}} D \cos \theta \, \Delta^{S_{n-1}} \rho(M,t) \, d\tau(M)
\]

\[
= \int_{S_{n-1}} D\rho(M,t) \, \Delta^{S_{n-1}} \cos \theta \, d\tau(M),
\]

(2.2)

where we have made use of Green’s theorem in $S_{n-1}$. At this point we recall that the Laplacian $\Delta^E$ in $E_n$ may be decomposed as the sum $\Delta^S$

\[
\Delta^E = \Delta^R + \Delta^{S_{n-1}},
\]

\[
\Delta^R = \frac{1}{R^{n-1}} \frac{\partial}{\partial R} R^{n-1} \frac{\partial}{\partial R},
\]

(2.3)

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

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

(2.4)

the solution of which being of course given by eq. (2.2).

III. THE GENERAL SOLUTION

We shall make extensive use of the properties of the hyperspherical harmonics to solve eq. (1.1). A short résumé on these functions might prove useful for the reader. We will adopt the definitions and notations of the chapter IX of the classical textbook by Vilenkin.\textsuperscript{5}

In the case $n = 4$ this yields to a definition of the harmonics which is slightly different from that which we used previously.\textsuperscript{8,9,10}

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 $S_{n-1}$ we will mean in fact the areas of these spheres considered as manifolds of $E_n$). The spherical coordinates of the unit vector $\xi = OM \equiv (\xi_1, \ldots, \xi_n)$ of $S_{n-1}$ are defined by the relations

$$\xi_1 = \sin \theta_{n-1} \ldots \sin \theta_2 \sin \theta_1 ,$$

$$\xi_2 = \sin \theta_{n-1} \ldots \sin \theta_2 \cos \theta_1 , \ldots ,$$

$$\xi_{n-1} = \sin \theta_{n-1} \cos \theta_{n-2} ,$$

$$\xi_n = \cos \theta_{n-1} ,$$

(3.1)

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

$$d\xi \equiv \frac{1}{A_{n-1}} \sin^{n-2} \theta_{n-1} \ldots \sin \theta_2 \, d\theta_1 \ldots d\theta_{n-1} ,$$

(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

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

(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 $\Delta^{S_{n-1}} \equiv R^2 \Delta^{S_{n-1}}$ in spherical coordinates reads as

$$
\Delta^{S_{n-1}} = \frac{1}{\sin^{n-2} \theta_{n-1}} \frac{\partial}{\partial \theta_{n-1}} \sin^{n-2} \theta_{n-1} \frac{\partial}{\partial \theta_{n-1}} + \frac{1}{\sin^2 \theta_{n-1} \sin^{n-3} \theta_{n-2}} \frac{\partial}{\partial \theta_{n-2}} \sin^{n-3} \theta_{n-2} \frac{\partial}{\partial \theta_{n-2}} + \ldots + \frac{1}{\sin^2 \theta_{n-1} \ldots \sin^2 \theta_2} \frac{\partial^2}{\partial \theta_1^2}.
$$

(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 $L = 0, 1, \ldots$ is a positive integer. One can show that $K \equiv (k_1, \ldots, \pm k_{n-2})$ 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 $f \in L^2[S_{n-1}]$ defined on $S_{n-1}$. An explicit expression of $\Xi_L, K(\xi)$ will be of little use and can be found in the Vilenkin.\textsuperscript{5}

As the usual spherical harmonics the $\Xi_L, K(\xi)$ satisfy to the following properties:

- (i) orthogonality

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

(3.5)

- (ii) completeness

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

(3.6)

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

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

(3.7)

- (iii) addition theorem

$$
\sum_{K} \Xi_L^*, K(\xi) \Xi_L, K(\xi') = \frac{2L + n - 2}{n - 2} C_{L/2-1}^n(\xi \cdot \xi'),
$$

(3.8)

where the dot in the RHS denotes the usual scalar product in $E_n$, i.e $\xi \cdot \xi' = \cos \psi$ where $\psi$ is the angle between the two unit vectors $\xi$ and $\xi'$, and $C_{L/2-1}^n$ 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

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

(3.9)
We have now in hand all the tools to solve eq. (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 the expansion (3.10) in eq. (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

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

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 eqs. (3.12) and (3.16) that the Green function \( \rho(M,t|M_0,0) \) can be expressed as

\[
\rho(M,t|M_0,0) = 0 \quad (t < 0) \\
\rho(M,t|M_0,0) = \frac{1}{R^{n-1}A_{n-1}} \sum_{L=0}^{\infty} \sum_{K} \Xi^*_{L,K}(\xi_0) \Xi_{L,K}(\xi) \\
\times \exp \left( -DL(L + n - 2)t/R^2 \right) \quad (t > 0) . \tag{3.14}
\]

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

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

Some comments on eq. (3.15) are in order.

(i) The solution (3.15) is invariant under rotation about the axis \( \xi_0 \) as expected. Eq. (3.15) is a generalization for all \( n \) of Debye’s result which corresponds to the case \( n = 3 \). 

In this case the Gegenbauer polynomials reduce to the Legendre polynomials \( P_L \). In the
case $n = 4$ we recover the result of ref. 7, where the Gegenbauer polynomials reduce to Tchebycheff polynomials of second kind. To be more precise, recall that

\begin{align*}
C_{1}^{1/2}(\cos \theta) &= P_{L}(\cos \theta) \quad (n = 3) \\
C_{L}^{1}(\cos \theta) &= \frac{\sin(L + 1)\theta}{\sin \theta} \quad (n = 4)
\end{align*}

(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 $\lim_{t \to +\infty} \rho(M, t|M_{0}, 0) = 1/\Omega_{n-1}$, 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{align*}
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{align*}

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

\begin{align*}
F_{L}^{n/2-1}(t) &= \frac{(n - 3 + L)!}{L!(n - 3)!} \exp \left( -DL(L + n - 2)t/R^{2} \right)
\end{align*}

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 eq. (1.2). For $n = 3$ and 4 we recover the results for the 3D and 4D rotors 1, 2, 7.

\begin{align*}
\langle P_{L}(\cos \theta) \rangle &= \exp \left( -DL(L + 1)t/R^{2} \right) \quad (n = 3) \\
\langle \frac{\sin(L + 1)\theta}{\sin \theta} \rangle &= (L + 1) \exp \left( -DL(L + 2)t/R^{2} \right) \quad (n = 4)
\end{align*}

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

\begin{align*}
\tau_{L}^{n/2-1} &= \int_{0}^{\infty} \frac{F_{L}^{n/2-1}(t)}{F_{L}^{n/2-1}(0)} dt = \frac{R^{2}}{DL(L + n - 2)},
\end{align*}

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, 7. Since simulations of real 3D liquids or plasmas are feasible (moreover efficient) in $S_{3}$, 8, 9, 10, eq. (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.
Simulations of random walks on fractals inscribed in $S_{n-1}$ were reported recently. 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 (where $\beta$ is some exponent depending on the fractal dimensions of the cluster) the numerical results of ref. 3 give evidence of the law $\langle \cos \theta \rangle \propto \exp \left( -\frac{t}{\tau} \right)^{\beta}$, i.e. a stretched exponential relaxation, on the hypersphere. As suggested by Jund et al. the anomalous diffusion law for a RW on a fractal can be understood by replacing the time $t$ by a fractal time $t^\beta$ in the diffusion equation (1.1) and thus in the solution (3.15). With this assumption we now have the ansatz

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

which could be checked in numerical simulations.

**IV. RANDOM WALKS IN $S_3$**

We specialize to the case $n = 3$ and want to show that the expression (3.15) of $\rho(M, t|M_0, 0)$ is equivalent to that of ref. 4. This can be done as follows. Let us rewrite the reduced $\widehat{\rho} = 2\pi^2 R_3^3 \rho(M, t|M_0, 0)$ as

$$\widehat{\rho} = \sum_{L=0}^{\infty} (L + 1) \frac{\sin(L + 1)\psi}{\sin \psi} \exp(-K \ L(L + 2)) ,$$

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

$$F(\psi) = \int_{0}^{\psi} d\psi' \ \widehat{\rho}(\psi') \sin(\psi')$$

which can be rewritten after some algebra as

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

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

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

(4.4)
Applying Poisson theorem for the Gaussian we get

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

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

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

which coincides with the result of ref. 4, apart the prefactor which is not specified. Relations similar to eq. (4.6) can be obtained for even values of $n$ (other than 4) but we failed to get anything similar for odd $n$’s.

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