The Diffusion Equation on a Hypersphere

Jean-Michel Caillol

Laboratoire de Physique Théorique
UMR 8267, Bât. 210
Université de Paris-Sud
91405 Orsay Cedex, France

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Abstract

We study the diffusion equation on the surface of a 4D sphere and obtain a Kubo formula for the diffusion coefficient.
Since numerical simulations of fluids or plasmas within hyperspherical boundary conditions are appealing, it is not without interest to dispose of an explicit expression for the diffusion coefficient $D$ in terms of time averages of microscopic quantities. Our starting point will be the diffusion equation

$$D \rho(M, t) \equiv \left( \frac{\partial}{\partial t} - D \Delta_{S^3} \right) \rho(M, t) = 0,$$

(1)

where the point $M$ lives on the surface of the four dimensional (4D) sphere $S^3$ of center $O$ and radius $R$ (a hypersphere for short). $D(>0)$ is the diffusion coefficient and $\Delta_{S^3}$ is the Laplacian appropriate to the geometry. Eq. (1) was solved recently by Nissfolk et al.; their expression for $\rho(M, t)$ is however awkward and does not allow to obtain an explicit expression for $D$. A more convenient expression for $\rho(M, t)$ is obtained in this paper which yields an explicit expression for $D$.

We first note that the Brownian motion of a particle in $S^3$ may also be viewed as the Brownian rotation of a linear 4D molecule. As the expression of the rotational diffusion coefficient of a 3D rotator is known since the work of Debye it should be easy to extend this old result to the 4D case. Following Berne and Pecora we first expand $\rho(M, t)$ on the complete basis set of hyperspherical harmonics

$$\rho(M, t) = \sum_{L=0}^{\infty} \sum_{\alpha} \rho_{L, \alpha}(t) Y_{L, \alpha}(\xi),$$

(2)

where the unit vector $\xi = OM/R$ denotes the orientation of vector $OM$ in $\mathbb{R}^4$ and $Y_{L, \alpha}(\xi)$ is a 4D hyperspherical harmonics. We recall that the quantum number $L$ is a positive integer and that $\alpha = (m_1, m_2)$ where $m_i$ ($i = 1, 2$) takes the $L + 1$ values $m_i = -L/2, -L/2 + 1, \ldots, L/2$. The 4D harmonics $Y_{L, \alpha}(\xi)$ satisfy the following properties:

- (i) orthogonality

$$\int d\Omega(\xi) Y_{L, \alpha}^*(\xi) Y_{L', \alpha'}(\xi) = \delta_{L, L'} \delta_{\alpha, \alpha'},$$

(3)

where $d\Omega(\xi)$ denotes the infinitesimal volume element (or 4D infinitesimal solid angle) on the hypersphere of unit radius.

- (ii) completeness

$$\sum_{L, \alpha} Y_{L, \alpha}^*(\xi) Y_{L, \alpha}(\xi') = \delta^{S^3}(\xi, \xi'),$$

(4)
where $\delta^{S_3}$ is the Dirac distribution for the unit hypersphere defined as
\[
\int d\Omega(\xi) \ f(\xi)\delta^{S_3}(\xi, \xi') = f(\xi').
\] (5)

• (iii) addition theorem
\[
\sum_{\alpha} Y_{L,\alpha}^*(\xi) Y_{L,\alpha}(\xi') = P_L(\xi \cdot \xi'),
\] (6)
where the dot denotes the usual 4D scalar product, i.e $\xi \cdot \xi' = \cos(\psi)$ where $\psi$ is the angle between the two unit vectors $\xi$ and $\xi'$ and
\[
P_L(\cos(\psi)) = \frac{L + 1}{2} \frac{\sin(L + 1) \psi}{\pi}.
\] (7)

Note that $R\psi$ is the geodesic length between the points $M$ and $M'$ of $S_3$.

Moreover the $Y_{L,\alpha}(\xi)$ are the eigenvectors of the Laplace-Beltrami operator $\Delta^{S_3}$ with eigenvalues $-L(L + 2)/R^2$. It follows from this important property that eq. (11) is equivalent to the set of equations
\[
\left( \frac{\partial}{\partial t} + D \frac{L(L + 2)}{R^2} \right) \rho_{L,\alpha}(t) = 0,
\] (8)
the solution of which reads obviously as
\[
\rho_{L,\alpha}(t) = \rho_{L,\alpha}(0) \exp \left( -DL(L + 2) t/R^2 \right).
\] (9)

We shall denote by $\rho(M, t|M_0, 0)$ the solution of (11) corresponding to the initial condition $\rho(M, 0) = \delta^{S_3}(M, M_0) \equiv R^{-3} \delta^{S_3}(\xi, \xi_0)$, i.e. the solution of
\[
\mathcal{D} \rho(M, t|M_0, 0) = \delta(t) R^{-3} \delta^{S_3}(\xi, \xi_0).
\] (10)

It follows readily from eqs. (9) and (4) that the Green function $\rho(M, t|M_0, 0)$ can be expressed as
\[
\rho(M, t|M_0, 0) = 0 \quad (t < 0)
\]
\[
\rho(M, t|M_0, 0) = \frac{1}{R^3} \sum_{L,\alpha} Y_{L,\alpha}^*(\xi_0) Y_{L,\alpha}(\xi) \exp \left( -DL(L + 2) t/R^2 \right) \quad (t > 0).
\] (11)

Eq. (11) can be further simplified with the help of the addition theorem (6) which yields our final result
\[
\rho(M, t|M_0, 0) = \frac{1}{R^3} \sum_{L} P_L(\xi_0 \cdot \xi) \exp \left( -DL(L + 2) t/R^2 \right) \quad (t > 0).
\] (12)
Some comments are in order.

(i) The solution (12) is invariant upon rotations about the axis \( \xi_0 \) as expected. Eq. (12) is a trivial generalization of Debye’s result\(^4,5,6\) (for the 3D rotor the Tchebychev polynomial \( P_L \) in eq. (12) has to be replaced by a Legendre polynomial, up to a multiplicative constant)

(ii) Note that
\[
\int R^3 d\Omega(\xi) \rho(M,t|M_0,0) = 1 \quad (t > 0),
\] i.e. the probability is conserved, the particle does not evaporate.

(iii) We have also
\[
\lim_{t \to +\infty} \rho(M,t|M_0,0) = \frac{1}{2\pi^2R^3},
\] i.e. the solution of the diffusive process is uniform after infinite time (the volume of \( S_3 \) is equal precisely to \( 2\pi^2R^3 \))

(iv) Let us define, following Berne and Pecora\(^5\), the time correlation function
\[
C_L(t) \equiv \langle P_L(\xi(0) \cdot \xi(t)) \rangle
= \frac{d\Omega(\xi_0)}{2\pi^2} \int R^3 d\Omega(\xi) P_L(\xi_0 \cdot \xi) \rho(M,t|M_0,0),
\] where we have averaged the initial position uniformly on \( S_3 \). As a consequence of the orthogonality properties of the \( P_L \) we find that
\[
C_L(t) = \frac{(L+1)^2}{2\pi^2} \exp(-DL(L+2)t/R^2).
\] Defining now the reorientational time \( \tau_L \) of our 4D rotor as
\[
\tau_L = \int_0^\infty dt \frac{C_L(t)}{C_L(0)}
= \frac{R^2}{DL(L+2)},
\] we have now at our disposal an explicit expression of the diffusion coefficient \( D \). Note the aesthetic relation \( \tau_L/\tau_{L'} = L'(L'+2)/L(L+2) \) which generalizes Debye’s relation to the 4D rotor.

(v) It does not seem possible to obtain from eqs. (16) an expression for \( D \) in term of the time autocorrelation function of the velocity of the particle. Moreover one can deduce from eq. (12) that the mean square displacement of the stereographic projection of point \( M \) vanishes for \( t \to \infty \).
It remains now to show that the expression (12) of $\rho(M,t|M_0,0)$ is equivalent to that of ref.2. This can be done as follows. Let us rewrite the reduced $\hat{\rho} = 2\pi R^3 \rho(M,t|M_0,0)$ as

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

(18)

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 $\hat{\rho}(-\psi) = \hat{\rho}(\psi)$ 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

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

(19)

which can be rewritten after some algebra as

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

(20)

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

$$\sum_{n=-\infty}^{+\infty} \varphi(x + 2n\pi) = \frac{1}{2\pi} \sum_{p=-\infty}^{+\infty} \exp(-ipx) \tilde{\varphi}(p) ,$$

(21)

where

$$\tilde{\varphi}(p) = \int_{-\infty}^{+\infty} dx \varphi(x) \exp(ipx) .$$

(22)

Applying Poisson theorem for the Gaussian we get

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

(23)

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

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

(24)

which coincides with the result of ref.2 apart the prefactor which is not specified.

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