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Fractal Brownian motion and nuclear spin echoes

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Abstract. It is well known that spin echo experiments can measure the diffusion coefficient D of classical Brownian motion for which $\langle \Delta x(t)^2 \rangle = 2D|t|$. There has been considerable recent interest in fractal Brownian motion in which case $\langle \Delta x(t)^2 \rangle = 2D_\nu |t|^{(1-\nu)}$, where $-1 < \nu < 1$ is the fractal exponent. The spin echo damping implications of fractal diffusion are derived.

1. Introduction

It has long been known that the microscopic Brownian diffusion coefficient D of a 'particle' in a fluid can be measured via the amplitude of the magnetic echo signal from nuclear spins subject to an appropriate sequence of magnetic field pulses [1]. Here the diffusion coefficient is defined via the mean-square displacement of the Brownian particle x-coordinate in a time period t, i.e.

$$\Delta x(t) = x(t) - x(0) = \int_0^t v_x(s)\,\mathrm{d}s \tag{1}$$

$$\langle \Delta x(t)^2 \rangle = 2D|t|\,. \tag{2}$$

The classical Brownian motion is an independent random process in which the correlation between past and future movements is zero. If there are longer time correlations among the individual movements, then the motion becomes the fractal Brownian process [2]. Investigations concerning the nature of noise and fractal geometry have led to a generalization of (2). In fractal Brownian motion one may introduce a fractional spectral exponent ν, and then define fractal Brownian motion as a Gaussian random process [3] with

$$\langle \Delta x(t)^2 \rangle_\nu = 2D_\nu |t|^{(1-\nu)} \qquad (-1 < \nu < 1)\,. \tag{3}$$

Exploring laboratory systems in which fractal Brownian motion for microscopic particles exists is a fruitful area [4] of materials research. The fractal diffusion also gives a better modelling of chemical reaction kinetics [5, 6]. Fluid particles embedded in porous media, or fluid films absorbed on rough surfaces [7] also appear to be natural candidates for exhibiting fractal Brownian motion effects.

Our purpose is to point out that field gradient spin echo experiments are a natural tool with which to experimentally probe for the possible existence of fractal Brownian motion. Here we provide the fractal generalization of the conventional spin diffusion theory which has proved so successful in measuring Brownian diffusion coefficients.

In section 2 the spectral functions for velocity fluctuations are discussed. In section 3 these spectral functions are employed to evaluate the spin echo damping due to fractal Brownian motion in a magnetic field gradient. In the concluding section 4, our central results are compared with the conventional spin diffusion approach.

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2. Velocity spectral functions

The spectral function $S(\omega)$ for thermal Brownian velocity fluctuations is defined by

$$\langle v_x(t)v_x(t')\rangle = \int_{-\infty}^{\infty} \mathrm{d}\omega\, S(\omega)\cos[\omega(t-t')]\,. \tag{4}$$

Equations (1) and (4) imply a mean-square Brownian motion displacement

$$\langle \Delta x(t)^2\rangle = 4\int_0^{\infty} \frac{\mathrm{d}\omega}{\omega^2} S(\omega)[1-\cos(\omega t)]\,. \tag{5}$$

The spectral function for fractal Brownian motion may be defined as

$$S_\nu(\omega) = \frac{D}{\pi}(\omega\tau)^\nu\,. \tag{6}$$

Equations (5) and (6) imply

$$\langle \Delta x(t)^2\rangle_\nu = \frac{4D\tau^\nu |t|^{(1-\nu)}}{\pi}\int_0^{\infty} \frac{\mathrm{d}x}{x^2} x^\nu[1-\cos x]\,. \tag{7}$$

Equivalently

$$\langle \Delta x(t)^2\rangle_\nu = 2D_\nu |t|^{(1-\nu)} \qquad (-1<\nu<1) \tag{8}$$

where

$$D_\nu = \frac{2\sin(\pi\nu/2)\Gamma(1+\nu)D\tau^\nu}{(\pi\nu)(1-\nu)} \tag{9}$$

and where the gamma function is defined as

$$\Gamma(z) = \int_0^{\infty} \frac{\mathrm{d}x}{x} x^z \mathrm{e}^{-x} \qquad (\mathrm{Re}\; z>0)\,. \tag{10}$$

The above definitions of fractal Brownian motion have been extensively discussed in the literature [8].

3. Spin echo damping

Suppose that a nuclear spin moves in an inhomogeneous magnetic field $H_z(x)$ and thereby has a Larmor frequency $\omega(x) = \gamma H_z(x)$ which varies in space as

$$\omega(x) = \omega(0) + gx \tag{11}$$

where $g = \gamma\, \mathrm{d}H_z(x)/\mathrm{d}x$ is considered to be constant. As the particle undergoes random motion, the Larmor frequency will be randomly modulated in time according to

$$\omega(t) = \omega_0 + g\int_0^t \mathrm{d}s\, v_x(s)\,. \tag{12}$$

The random velocity then leads to a random rotation angle $\Delta\theta$ for the spin components in the plane normal to the applied magnetic field;

$$\Delta\theta(t) = \int_0^t \mathrm{d}s[\omega(s) - \omega_0] = g \int_0^t \mathrm{d}s \int_0^s \mathrm{d}s'\, v_x(s'). \tag{13}$$

The resulting random loss of phase information leads to the damping factor

$$A(t) = \langle \exp[-\mathrm{i}\Delta\theta(t)] \rangle = \exp\left[-\tfrac{1}{2}\langle \Delta\theta(t)^2 \rangle\right] \tag{14}$$

where Gaussian averaging [9] has been invoked. Equations (4), (13) and (14) imply

$$A(t) = \exp[-g^2\chi(t)] \tag{15}$$

where

$$\chi(t) = \tfrac{1}{2} \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_1' \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_2' \langle v_x(s_1') v_x(s_2') \rangle \tag{16}$$

or equivalently

$$\chi(t) = \int_0^\infty \mathrm{d}\omega\, S(\omega) \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_1' \int_0^t \mathrm{d}s_2 \int_0^{s_2} \mathrm{d}s_2' \cos[\omega(s_1' - s_2')]. \tag{17}$$

Equation (17) simplifies to

$$\chi(t) = \int_0^\infty \frac{\mathrm{d}\omega}{\omega^4} S(\omega) \left\{ 2[1 - \cos(\omega t) - (\omega t)\sin(\omega t)] + (\omega t)^2 \right\}. \tag{18}$$

For fractal Brownian motion, (6) and (18) yield

$$\chi_\nu(t) = \frac{D\tau^\nu |t|^{(3-\nu)}}{\pi} \int_0^\infty \frac{\mathrm{d}x}{x^4} x^\nu \left\{ 2[1 - \cos x - x \sin x] + x^2 \right\}. \tag{19}$$

Explicitly calculating the integral in (19) yields

$$\chi_\nu(t) = \frac{2 \sin(\pi\nu/2) \Gamma(1+\nu) D\tau^\nu |t|^{(3-\nu)}}{(\pi\nu)(3-\nu)(1-\nu)}. \tag{20}$$

Finally, the central result of this work follows from (9), (15) and (20). It is the expression

$$A_\nu(t) = \exp\left[-\frac{g^2 D_\nu t^{(3-\nu)}}{(3-\nu)} \right] \tag{21}$$

for the spin damping amplitude in a magnetic field gradient corresponding to the fractal Brownian motion equation (3). For classical Brownian motion with fractal exponent $\nu = 0$, the conventional spin diffusion result

$$A_0(t) = \exp\left[-\tfrac{1}{3} g^2 D t^3\right] \tag{22}$$

is recovered.

In spin echo experiments (21) is invoked to describe spin motions between RF pulses. Suppose a 90° pulse at time zero. If we apply (21) in the time interval $0 < t < (\tau_e/2)$, then at the 180° pulse at time $(\tau_e/2)$

$$A_{\nu,180}(\tau_e/2) = \exp\left[-\frac{g^2 D_\nu (\tau_e/2)^{(3-\nu)}}{(3-\nu)}\right]. \tag{23}$$

Now we apply (21) in the time interval $(\tau_e/2) < t < \tau_e$. The spin echo occurs at time τ_e, and

$$A_\nu^{\text{echo}}(\tau_e) = A_{\nu,180}^2(\tau_e/2)\,. \tag{24}$$

Combining (23) and (24) yields

$$A_\nu^{\text{echo}}(\tau_e) = \exp\left[-\frac{g^2 D_\nu \tau_e^{(3-\nu)}}{2^{(2-\nu)}(3-\nu)}\right] = \exp\left[-(\Omega_\nu \tau_e)^{(3-\nu)}\right] \tag{25a}$$

where

$$\Omega_\nu = \left(2^{(\nu-2)} g^2 D_\nu\right)^{[1/(3-\nu)]}. \tag{25b}$$

Some spin echo decay curves are shown in figure 1. For the $\nu = 0$ case,

$$A_0^{\text{echo}}(\tau_e) = \exp\left[-\tfrac{1}{12} D g^2 \tau_e^3\right] \tag{26}$$

becomes the well known result for classical Brownian motion. Within present nuclear magnetic resonant pulse technology fractal exponents $\nu \neq 0$ exponents can be probed.

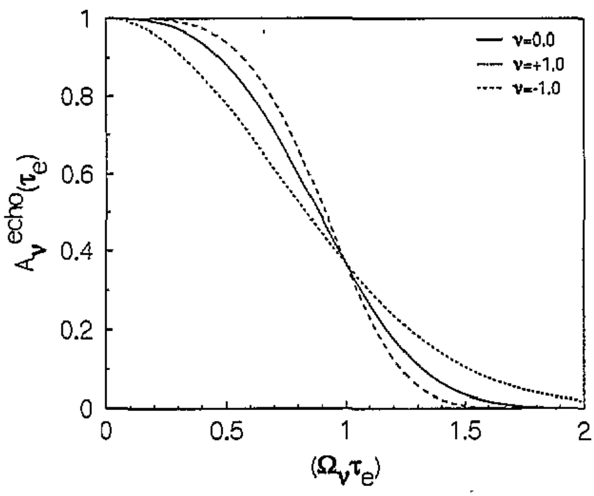

Figure 1. Exhibited are the spin echo decay amplitude for the extreme cases (broken curves) of $\nu = -1$ and $\nu = 1$. The classical Brownian motion value $\nu = 0$ (full curve) is also shown.

4. Conclusion

For completeness of presentation, let us recall the usual treatment of spin diffusion based on classical Brownian motion. If $\boldsymbol{g} = \gamma \boldsymbol{\nabla} H_z(\boldsymbol{r})$ describes the magnetic field gradient, and if the (complex) nuclear magnetic moment per unit volume for components of magnetization normal to the field z-direction is described by

$$M(\boldsymbol{r}, t) = M_x(\boldsymbol{r}, t) + \mathrm{i}M_y(\boldsymbol{r}, t) \tag{27}$$

then (in conventional nuclear magnetic resonance literature) the magnetization is thought to obey [10]

$$\frac{\partial M(\boldsymbol{r}, t)}{\partial t} = -\left\{\mathrm{i}(\omega_o + \boldsymbol{g}\cdot\boldsymbol{r}) + \frac{1}{T_2}\right\} M(\boldsymbol{r}, t) + D\nabla^2 M(\boldsymbol{r}, t) \tag{28}$$

where T_2 is the transverse magnetic relaxation time. If one looks for a solution of (27) and (28) of the form

$$M(\boldsymbol{r}, t) = A_0(t)\exp\left[-\mathrm{i}(\omega_o + \boldsymbol{g}\cdot\boldsymbol{r})t - \frac{t}{T_2}\right] \tag{29}$$

then one finds

$$\frac{\mathrm{d}A_0(t)}{\mathrm{d}t} = -Dg^2t^2A_0(t)\,. \tag{30}$$

This presents an alternative derivation of (22) for describing the damping due to a field gradient. Equations (22) and (30) correspond to classical Brownian motion exponent $\nu = 0$.

Our central result concerns the predication for fractal Brownian motion. From (21) we find

$$\frac{\mathrm{d}A_\nu(t)}{\mathrm{d}t} = -D_\nu g^2 t^{(2-\nu)} A_\nu(t) \tag{31}$$

where the fractional exponent ν is defined by

$$\langle \Delta x(t)^2 \rangle_\nu = 2D_\nu |t|^{(1-\nu)} \qquad (-1 < \nu < 1)\,. \tag{32}$$

To the authors knowledge there have not been spin echo measurements performed where fractal exponents $\nu \neq 0$ have been probed, so that our central equations (25) are presently only theoretical. However, if fractal Brownian motion is a reality in some materials, then spin echo experiments seem to be an appropriate tool for laboratory studies.

References

[1] Hahn E 1957 *Phys. Rev.* **106** 918
[2] Mandelbrot B B and van Ness J W 1968 *SIAM Rev.* **10** 422–37
[3] Gefen Y, Aharony A and Alexander S S 1983 *Phys. Rev. Lett.* **50** 77–80
[4] Ihle T and Muller-Krumbhaur H 1994 *Phys. Rev.* E **49** 2972
[5] Barzykin A V and Tachiya M 1993 *J. Chem. Phys.* **99** 9591
[6] Seri-Levy A and Avnir D 1993 *J. Phys. Chem.* **97** 10380
[7] Panella P V and Krim J 1994 *Phys. Rev.* E **49** 4179
[8] Mandelbrot B B 1983 *J. Stat. Phys.* **34** 895
[9] Feder J 1988 *Fractals* (New York: Plenum) pp 149–92
[10] Abragam A 1961 *The Principles of Nuclear Magnetism* (Oxford: Oxford University Press) pp 59–62