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Richard F. Voss and John Clarke

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Fluctuation Spectra for Systems Obeying a Diffusion Equation*

Richard F. Voss† and John Clarke††

Department of Physics, University of California
and
Inorganic Materials Research Division,
Lawrence Berkeley Laboratory,
Berkeley, California 94720

ABSTRACT

By considering the specific problem of Brownian motion, we derive the frequency spectrum of fluctuations in the spatial integral of a quantity obeying a diffusion equation. The spectra are 1/f-like over large ranges of frequency for 1-, 2-, and 3-dimensional systems. Spectra from computer simulations confirm our calculations.

The problem of independent particles undergoing Brownian motion has been extensively studied.[1] It is well known that for a small subvolume in a large reservoir the mean square fluctuation, $\langle (\Delta N)^2 \rangle$, in the number of particles is $\langle N \rangle$, the average number in that volume. To our knowledge, however, the frequency spectrum, $S(\omega) \equiv \langle N(\omega)N^*(\omega) \rangle$, of this quantity has not been explicitly calculated. We calculate $S(\omega)$ under the assumptions that the particle density obeys a diffusion equation and that the particles are subject to a random force which gives rise to their motion. $S(\omega)$ is shown to be 1/f-like over many decades in frequency. The theory, which is applicable to any quantity obeying a diffusion equation, suggests a plausible explanation for the occurrence of 1/f noise in many different systems, and yields quantitative predictions of its magnitude that are in good agreement with experiment.[2]

Specifically, we consider the problem of particles undergoing Brownian motion due to their interaction with the surrounding medium. The statistical nature of the system is described by a random force, $\vec{F}(\vec{x},t)$, which is the force acting on a particle at $\vec{x}$ at time t. $\vec{F}$ is assumed to have zero average, to be uniformly distributed in direction, and to be uncorrelated in space and time. As we are interested in time scales long compared to the viscous damping time, the velocity of each particle is the product of a generalized mobility, μ, and the instantaneous force. The particle current density is then given by $\vec{j} = n\mu\vec{F}$ where $n(\vec{x},t)$ is the particle density. If $\delta n(\vec{x},t)$ is the fluctuation in n about its average, n_o, $\vec{j}(\vec{x},t) = \mu n_o \vec{F} + \mu\delta n\vec{F}$.
If we average over an ensemble of such systems with equal initial densities, the first term vanishes since $\langle \vec{F} \rangle = 0$, and the second term must give the diffusion current, $-D\vec{\nabla}n(\vec{x},t)$. We assume, therefore, that each system is adequately described by:

$$\vec{j} = \mu n_o \vec{F}(\vec{x},t) - D\vec{\nabla} n(\vec{x},t) \tag{1}$$

for small fluctuations. Conservation of particles requires that $\vec{\nabla} \cdot \vec{j} + \partial n/\partial t = 0$, and we obtain

$$D\nabla^2 n - \partial n/\partial t = \mu n_o \vec{\nabla} \cdot \vec{F} . \tag{2}$$

To find the frequency spectrum of fluctuations in the number of particles in a given volume out of an infinite system, we limit ourselves initially to a 1-dimensional diffusion process and let

$$n(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} d\omega e^{ikx} e^{-i\omega t} n(k,\omega), \tag{3}$$

where from Eq. (2)

$$n(k,\omega) = ikn_o \mu F(k,\omega) / (-Dk^2 + i\omega). \tag{4}$$

Since the number of particles in the region between $-\ell$ and ℓ at time t is given by $N(t) = \int_{-\ell}^{\ell} n(x,t)dx$, $N(\omega) = \int_{-\ell}^{\ell} n(x,\omega)dx$ or

$$N(\omega) = (2/\pi)^{1/2} \int_{-\infty}^{\infty} k^{-1}\, n(k,\omega) \sin k\ell \; dk. \tag{5}$$

The frequency spectrum is defined by $S(\omega) \equiv \langle N(\omega)\, N^*(\omega) \rangle$. The uncorrelated nature of F in space and time implies that it has a white spectrum in ω space and k space. Thus we set $\langle F(k,\omega)F^*(k',\omega) \rangle = F_o{}^2\delta(k-k')/\mu^2 n_o{}^2$ so that $S(\omega)$ reduces to

$$S(\omega) = \frac{2F_o{}^2}{\pi}\int_{-\infty}^{\infty} \frac{\sin^2 k\ell}{k^2}\, \frac{k^2 dk}{D^2k^4+\omega^2}\ . \tag{6}$$

$F_o{}^2$ is a measure of the average amplitude of the random driving force. Its value may be determined from the requirement that $\int_{-\infty}^{\infty} S(\omega)\, d\omega = \langle (\Delta N)^2 \rangle = \langle N \rangle = 2n_o\ell$, from which we find $F_o{}^2 = Dn_o/\pi$. $S(\omega)$ may now be explicitly integrated to give

$$S(\omega) = \frac{n_o D^{1/2}}{\sqrt{2}\pi\omega^{3/2}}\ [1 - e^{-\theta}(\sin\theta + \cos\theta)], \tag{7}$$

where $\theta \equiv (\omega/\omega_o)^{1/2}$. The natural frequency defined by the problem is $\omega_o = D/2\ell^2$. $S(\omega) \rightarrow 2^{-1/2}\pi^{-1}\, D^{1/2} n_o \omega^{-3/2}$ for $\omega \gg \omega_o$, and $S(\omega) \rightarrow 2^{1/2}\pi^{-1}D^{-1/2}n_o\ell^2\omega^{-1/2}$ for $\omega \ll \omega_o$. $S(\omega)$ is plotted in Fig. 1(a).

As a check on the formalism one may obtain from Eq. (4) the space-time correlation function, $c(s,\tau) \equiv \langle n(x+s,t+\tau)n(x,t) \rangle$,

$$c(s,\tau) = n_o(4\pi D\tau)^{-1/2}\ \exp(-s^2/4D\tau), \tag{8}$$

which is the familiar result for a 1-dimensional diffusion process.[1] The physical insight into the connection between 1/f-like fluctuations and diffusion, however, comes from a calculation of the frequency-dependent correlation function, $c(s,\omega) \equiv \langle n(x+s,\omega)n^*(x,\omega) \rangle$. For the 1-dimensional case, we obtain from Eq. (4)

$$c_1(s,\omega) = \frac{n_o \cos[(\pi/4)+|s|/\lambda]}{2\pi D^{1/2}\omega^{1/2}} e^{-|s|/\lambda} , \tag{9}$$

where $\lambda(\omega) \equiv (2D/\omega)^{1/2}$ is the ω-dependent correlation length and is a measure of the average spatial extent of a fluctuation at frequency ω. A low ω fluctuation effectively samples F over a large coherent volume giving a large amplitude.

The low ω behavior of $S(\omega)$ is easily understood in terms of $c_1(s,\omega)$. When $\omega \ll \omega_o$, $\lambda(\omega) \gg 2\ell$ and the fluctuations become correlated across the entire length. Now $S(\omega)$ can also be expressed as

$$S(\omega) = \int dx_1 \int dx_2 c_1(x_1 - x_2,\omega). \tag{10}$$

Since $c_1(s,\omega)$ is independent of s as $\omega \to 0$, $S(\omega) \to (2\ell)^2 c_1(0,\omega)$ as $\omega \to 0$, which is exactly the result obtained above.

In the high ω region $\lambda \ll 2\ell$, and, although 2ℓ may be divided into many correlated regions of length λ, only the two end regions can fluctuate independently of the others. The behavior is then best understood in terms of one dimensional flow across the boundaries. From Eqs. (1) and (4) we find $j(k,\omega) = i\omega n_o \mu F(k,\omega)/(-Dk^2+i\omega)$. If $N_1(t)$ represents the number of particles on one side of a boundary at $x = \ell$, we have that $\partial N_1/\partial t = j(\ell,t)$, and $N_1(\omega) = (2\pi)^{-1/2}\omega^{-1}\int_{-\infty}^{\infty}\exp(ik\ell)\, j(k,\omega)dk$. Thus

$$\langle N_1^2(\omega) \rangle = \frac{F_o^2}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{D^2k^4+\omega^2} = \frac{D^{1/2}n_o}{2^{3/2}\pi\,\omega^{3/2}} \tag{11}$$

for fluctuations due to flow across a single boundary. For $\omega \gg \omega_o$ the flows across the two ends are independent, and $S(\omega) \to 2\langle N_1^2(\omega)\rangle = 2^{-1/2}\pi^{-1}D^{1/2}n_o\omega^{-3/2}$, as before.

The formalism can be readily generalized to m dimensions. If $N(t)$ is the number of particles in a box of volume $2^m \ell_1 \ldots \ell_m$, then

$$S(\omega) = \left(\frac{2}{\pi}\right)^m F_o{}^2 \int_{-\infty}^{\infty} \frac{d^m k\, k^2}{D^2 k^4 + \omega^2} \prod_{i=1}^{m} \frac{\sin^2 k_i \ell_i}{k_i{}^2} . \tag{12}$$

The requirement that $\langle (\Delta N)^2 \rangle = \int S(\omega) d\omega$ gives $F_o{}^2 = n_o D/\pi$. Although we have been unable to determine a general analytic expression for $S(\omega)$, we can determine many of its characteristics from the behavior of the appropriate ω-dependent correlation function, which retains its dependence on $\exp(-|s|/\lambda)$ in all dimensions. Thus, in 2 dimensions

$$c_2(s,\omega) = n_o \ker(\sqrt{2}|s|/\lambda)/2\pi^2 D, \tag{13}$$

where $c_2(s,\omega) \to (n_o/2\pi^2 D)\ln(\sqrt{2}\,\lambda/|s|)$ for $s \ll \lambda$ and $c_2(s,\omega) \propto |s|^{-1/2} \exp(-\sqrt{2}\,|s|/\lambda)$ for $s \gg \lambda$. In 3 dimensions

$$c_3(s,\omega) = \frac{n_o}{4\pi^2 D|s|} \cos(|s|/\lambda) e^{-|s|/\lambda} . \tag{14}$$

In m dimensions there are m characteristic lengths, $2\ell_i$. As in 1 dimension one expects changes in the spectrum when $\lambda(\omega) = 2\ell_i$. This defines the m natural frequencies as $\omega_i \equiv D/2\ell_i{}^2$. The simplest spectra are those in which all the ω_i are equal. In 2-dimensions, for a circle of radius a, $S(\omega) = 2Dn_o a^2 \int_0^\infty k dk J_1{}^2(ak)/(D^2k^4+\omega^2)$. For $\omega \gg \omega_o \equiv D/2a^2$, $S(\omega) \to 2^{-1/2} n_o a D^{1/2} \omega^{-3/2}$. There is no simple limit for $\omega \ll \omega_o$. The simplest 3-dimensional case is a sphere of radius a, for which $S(\omega)$ may be calculated exactly:

$$S(\omega) = 8n_o a^5[e^{-\theta}(1+2\theta+\theta^2/2)\cos\theta + (1+e^{-\theta}\sin\theta)(\theta^2/2-1)]/D\theta^5 \quad (15)$$

where $\theta \equiv (\omega/\omega_o)^{1/2}$ with $\omega_o \equiv D/2a^2$. $S(\omega) \to 2^{1/2} n_o a^2 D^{1/2} \omega^{-3/2}$ for $\omega \gg \omega_o$ $\to 2n_o a^5/3D$ for $\omega \ll \omega_o$, and is shown in Fig. 1(f).

For 2 and 3 dimensions, the high ω behavior is again best understood in terms of flow across a boundary. When $\lambda \ll$ any length, $2\ell_i$, only the outer shell of the volume can fluctuate independently of the remainder and then only by 1-dimensional flow across the boundary. Eq. (11) may be immediately generalized. If we divide a multidimensional surface into independent areas, dA, the number of particles per unit length in the direction perpendicular to the surface is $n_o dA$, and the total mean square fluctuation across the boundary is the sum of those for each dA. Thus the high ω behavior of an arbitrary volume of surface area A is

$$S(\omega) \to D^{1/2} n_o A / 2^{3/2} \pi \omega^{3/2}. \quad (16)$$

Eq. (16) leads to the same high frequency behavior for 2 and 3 dimensions as before.

The low ω behavior, on the other hand, is characteristic of $c_m(s,\omega)$ in the limit $\lambda \gg s$. Thus in 2 dimensions we expect $S(\omega) \propto \ell n(1/\omega)$, while in 3 dimensions we expect $S(\omega) \to$ constant, as $\omega \to 0$.

Although both low and high ω limiting behavior is readily understood in all dimensions, the intermediate behavior of Eq. (12) in which $\omega_i < \omega < \omega_j$ is complicated both physically and mathematically. In this region λ is smaller than some ℓ_i and greater than others. $S(\omega)$ is a monotonically decreasing function of ω. We expect a relatively smooth transition from low to high ω behavior with changes in slope generally occurring only at ω_i. In 2 dimensions, for a box $2\ell_1 \times 2\ell_2$ with $\ell_1 \gg \ell_2$, both an exact series calculation for a finite lattice [Fig. 1(b)] and approximate integration techniques [Fig. 1(c)] give essentially an ω^{-1} spectrum for $\omega_1 < \omega < \omega_2$.

As a test of the theory and in an attempt to determine the slope in the intermediate region, we simulated Brownian motion on a computer. A random walk model was used in 2 and 3 dimensions with electrical noise determining the direction of each step. After each particle had been moved, the number in a given subvolume was counted. This quantity was used as the driving force for a series of tuned circuits modeled in the computer whose output was squared and averaged to give the spectra. We have used the same method to measure low frequency noise spectra of actual electrical devices.[2] Several of the simulations are shown in Figs. 1(d), (e), (g), and (h). The results confirm our expectation that there is a smooth transition from high frequency behavior ($\omega^{-3/2}$) to low frequency behavior, and that the intermediate region is well approximated by $\omega^{-\gamma}$, where $\gamma \approx 1$.

The procedure for determining $S(\omega)$ developed here is not limited to Brownian motion but is applicable to any diffusion mechanism. In general, the fluctuating variable, $N(t)$, corresponds to a spatial integral of the quantity obeying the diffusion equation, Eq. (2), while the magnitude of the spectrum, or F_o^2, is determined from $\int S(\omega)d\omega = \langle (\Delta N)^2 \rangle$. Both the spectrum, with its dimensionality-dependent low frequency behavior, 1/f-like intermediate region, and $\omega^{-3/2}$ high frequency limit, and the frequency-dependent correlation length are characteristic of the diffusion process.

REFERENCES AND FOOTNOTES

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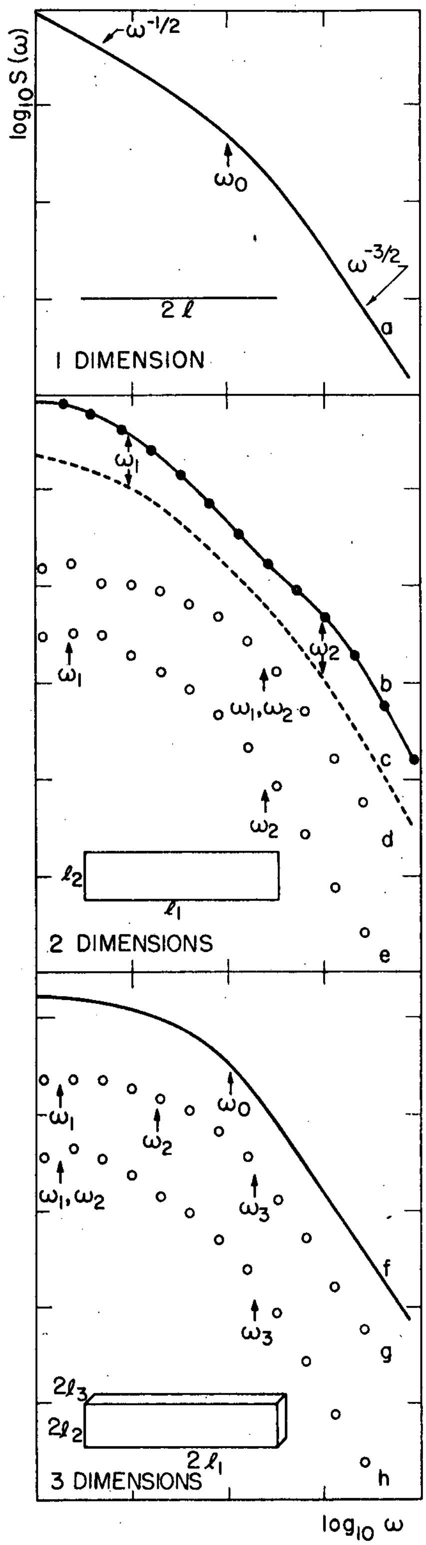
1. S. Chandrasekhar, Rev. Mod. Phys. 15, 1 (1943).

2. See following letter.

FIGURE CAPTION

Fig. 1 Fluctuation spectra: (a) and (f) are exact calculations, (b) and (c) are approximations, and (d), (e), (g), and (h) are computer simulations. Each scale division represents one decade.



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TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720