FLUCTUATIONS

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Summary

Fluctuations are ubiquitous in nature and their understanding is of crucial importance in several domains including physics, mathematics, and biology. It is also recognized that fluctuations play the role of a unifying theme for diverse disciplines from cosmology to the design of sophisticated electronic devices, medicine and economics. Initially, we discuss the role of fluctuations in cosmological models, DNA proofreading mechanisms and recognition processes in macromolecular structures, motor protein engines, and stochastic resonance. The relationship of fluctuations with physical properties is reviewed through the discussion of Brownian motion, Langevin stochastic differential equation and time correlation functions. Special emphasis has been placed on quantum fluctuations. They are understood in operational terms, not as well in conceptual ones. But our control of quantum fluctuations may lead to new technological developments of unpredictable impact.

1. Introduction

Spontaneous fluctuations (random noise) are a fundamental and ubiquitous manifestation intrinsically associated with the specific nature of physical and biological systems. The study of fluctuations is a unifying theme for diverse disciplines from cosmology to electronic devices, biology, medicine and economics. Therefore,

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physicists working with stochastic processes and chaos as well as mathematicians, biologists and economists are involved in the analysis of noise and fluctuations.

In 1828, the botanist Robert Brown observed the random paths of tiny particles in a fluid. Brownian motion was qualitatively explained by Einstein in 1905 then mathematically by Wiener in 1923. Einstein's formula for the mean squared displacement of Brownian motion was verified experimentally by Perrin in 1908 who, based on Einstein's formula, estimated a value of the Avogadro's number in good agreement with the accepted value, providing a convincing evidence on the atomic nature of matter.

Density fluctuations can be related to the range of the interactions between the particles. Long-range density fluctuations of unexpected magnitude were observed in fluids under confinement. Aggregates of strongly correlated particles, reflecting significant and local density fluctuations are also characteristic of long-range interacting systems.

Density fluctuations are of fundamental importance for understanding critical phenomena and phase transitions. When a system approaches a critical point, long range correlations between the particles induce strong fluctuations on every scale, from the particles to the entire system. Important examples include critical opalescence at the critical point of carbon dioxide reflecting density fluctuations due to light scattering, and nanometer-scale domain organization in lipid-bilayer component of biological membranes.

Density fluctuations are also quite sensitive to specific interactions in quantum systems. Strong density fluctuations are observed in an ideal gas with Coulomb interactions (Hartree model). They are however, significantly reduced when exchange interactions (Fermi model) are considered. Another relevant aspect concerns the dynamics of density fluctuations in many body interacting systems. Recent investigations indicate that different fluids with very different interatomic potentials might have similar density fluctuations if they have similar static correlation functions, which leads to the possibility of a general scaling principle for the dynamics of fluctuations in atomic liquids.

Fluctuations are also of fundamental interest in cosmologic models, where they may be responsible for seeding specific cosmic structures. Therefore, different models of structure formation of the universe are based on the primordial density fluctuations of the universe on spatial scales, which may range three orders of magnitude. The seeds of large-scale structure were possibly related to infinitesimal density perturbations induced by gravitational instability leading to the formation of massive structures such as galaxies and agglomerates. The rate of growth of density fluctuations is dependent on the specific cosmological model. An important issue concerns the origin of the density fluctuations. Density fluctuations associated with vacuum quantum fluctuations were invoked to explain how the current large scale structure of the universe evolved from primordial conditions. However, some recent investigations pointed out the possibility that thermal (i.e. classical) fluctuations provided seeds for currently observed cosmic structures.

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The role of fluctuations for understanding DNA proofreading mechanisms and recognition processes in macromolecular structures is an actual subject of research.

Some authors pointed out the importance of protein structural and energetic fluctuations for explaining high-fidelity DNA sensing and transcription mechanisms. Therefore, enhanced bio-molecular precision induced by fluctuations is presented as a natural design principle in the noisy realm of the living cell. On the other hand, structural fluctuations of macromolecular structures were associated with their ability to bind a variety of guests. Another fundamental issue concerns the importance of the correlation between structural and electronic density fluctuations in DNA. The reorganization of the electronic density induced by conformational/structural modifications are essential for understanding intermolecular interactions, recognition and the binding ability of complex molecular structures. Thermal fluctuations may also induce fluctuations of ionic densities in biological cells creating random electric fields which may affect transport dynamics across biological membranes. Moreover, thermal fluctuations can drive chemical reactions, including those taking place in biological systems.

The statistical nature of price fluctuations in different stock markets has been the subject of numerous investigations since L. Bachelier who, together with A. Einstein, was the first to apply Brownian motion to real phenomena. One basic issue concerns the probability distribution of price fluctuations. Some studies indicate that they follow a Markovian process and can be described by a normal (Gaussian) distribution. On the other hand, universal power law behavior was also proposed for describing the stock market evolution. The study of market fluctuations are of fundamental importance for understanding economics dynamics and stability.

Actual and unsolved problems of noise and fluctuations include Brownian ratchets, noise-induced transitions and stochastic resonance.

Brownian ratchets can model motor protein engines that can convert the energy of chemical reactions into mechanical motion. They involve a net current of particles that can be driven by noise. This particular phenomenon may underlie the transport of macromolecules within biological cells. Man-made Brownian ratchets are microscopic devices which can drive colloidal particles by ratcheting their Brownian motion.

Noise induced transitions involve the state of a nonlinear system which can be utterly changed by the introduction of a noise above a critical intensity. Noise induced transitions were found to be of importance for understanding the complex behavior of excitable neuron models and the diffusion of culture on a global scale.

Stochastic resonance is being currently applied to model the evolution of populations in globally coupled biological systems. Initial works on stochastic resonance focused on climate evolution, but this phenomenon is now regarded as far more common, occurring in lasers, electronic devices and sensory neurons.

2. Fluctuations and Physical Properties

General definition of fluctuations

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The statistical analysis of a system with a large number (N>>1) of particles is characterized by fluctuations. Fluctuations reflect deviations from the mean values of statistical properties. For a random variable x, the mathematical expectation or mean value of x is defined by:

$$\langle x \rangle = \int x p(x) dx \qquad (1)$$

where $p(x)$ is the probability distribution (density) function of x. A first measure of fluctuations is the variance of x, given by

$$\sigma_x = <(x - <x>)^2> \qquad (2)$$

Another useful quantity is the standard deviation of x, $\Delta x \equiv \sqrt{\sigma_x}$. One interesting aspect of fluctuations concerns the behavior with the number N of particles, which is given by:

$$\frac{\Delta x}{<x>} = \frac{C}{\sqrt{N}} \qquad (3)$$

C is a constant which is usually independent on N. In general, fluctuations are negligible in a macroscopic system, where N is comparable to Avogadro's number. However, fluctuations can be significant for a mesoscopic subsystem of a macroscopic system in thermodynamic equilibrium. The classical example is the Brownian motion of suspended colloidal particles.

Several important properties of many-body interacting systems are related to fluctuations. The general interest is in the fluctuation of properties including, for example, the density, the charge density in electrolytes, the concentrations of various species within a mixture, and energy fluctuations. For an ideal gas, with a fixed number of particles N and pressure P, the Boltzmann probability distribution for the fluctuating volume V, leads to the following expression, which is a particular case of (3):

$$\frac{\Delta V}{<V>} = \frac{1}{\sqrt{N}} \qquad (4)$$

Fluctuations, phase transitions and critical properties

Fluctuations are also of fundamental interest for investigating phase transitions and critical properties. Defining the density of a system with a fixed number of particles N as $\rho \equiv \frac{N}{V}$, density fluctuations at a temperature T are given by:

$$\frac{\Delta \rho}{<\rho>} = \frac{\Delta V}{<V>} = \left[-\frac{k_{\mathrm{B}}T}{V^2} \left(\frac{\partial V}{\partial P} \right)_{T,N} \right]^{1/2} = \left[-\frac{k_{\mathrm{B}}T}{V} \chi_{T,N} \right]^{1/2} \qquad (5)$$

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k_B the Boltzmann's constant and $\chi_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,N}$ is the isothermal compressibility, which is a measure of how the volume of a system changes when the pressure is modified at constant temperature.

Consequently, at the critical point of the liquid-gas transition, which is characterized by $\left(\frac{\partial P}{\partial V}\right)_{T,N} = 0$, or by a diverging compressibility χ_T, we observe that $\frac{\Delta\rho}{<\rho>} \to \infty$. The behavior of density fluctuations at the critical point illustrates that the density is not described by a Gaussian distribution. Therefore, the standard deviation is not sufficient anymore to describe the fluctuations close to the critical point of a fluid.

Another useful expression involving fluctuations is

$$\Delta H = \left[k_B T^2 \left(\frac{\partial H}{\partial T}\right)_{N,P}\right]^{1/2} = \left[k_B T^2 C_P\right]^{1/2} \qquad (6)$$

$H = E + PV$ is the enthalpy of the system and $C_P = \left(\frac{\partial H}{\partial T}\right)_{N,P}$ is the specific heat at constant pressure *P*. Expressions (5) and (6) illustrate how fluctuations can be related to macroscopic properties.

Correlation between fluctuations and the structure of fluids

A particularly important aspect relating fluctuations and the structural properties of fluids concerns the correlation between local density fluctuations and macroscopic properties. The correlation between local density fluctuations of $\rho(r')$ and $\rho(r'')$ can be written as:

$$h(r', r'') = <\rho(r')\rho(r'')> - \rho^2 \qquad (7)$$

where $\rho = <\rho(r)>$. For an isotropic fluid, translational and rotational invariance leads to $h(r', r'') = h(r' - r'') = h(r)$, which is defined as the pair correlation function. When local density fluctuations are uncorrelated $h(r) \to 0$. The relationship between pair correlations of local fluctuations in the microscopic scale and macroscopic properties is illustrated by the expression:

$$1 + \rho\int h(r)dr = 1 + \rho\int\left[g(r) - 1\right]dr = \rho k_B T \chi_{T,N} \qquad (8)$$

$g(r) = h(r) + 1$ and $\chi_{T,N}$ is the isothermal compressibility.

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Biographical Sketches

Benedito José Costa Cabral, was born in Belém (Brazil) 1951. His main scientific interests are structural, dynamics and electronic properties of liquids and chemical reactivity in solution. Other interests include statistical physics and density functional theory methodology and applications.
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