



Getting a stochastic process from a conservative Lagrangian: A first approach



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HIGHLIGHTS

- A stochastic process is generated through the path integral with a classical action.
- The transition probability per step is expressed as a perturbation series.
- Moment-generating function is expressed as a perturbation series.

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ABSTRACT

The transition probability P_V for a stochastic process generated by a conservative Lagrangian $\mathcal{L} = \mathcal{L}_0 - \varepsilon V$ is obtained at first order from a perturbation series found using a path integral. This P_V corresponds to the transition probability for a random walk with a probability density given by the sum of a normal distribution and a perturbation which may be understood as the contribution of the interaction of the random walk with the external field. It is also found that the moment-generating function for P_V can be expressed as the generating function of a normal distribution modified by a perturbation. Applications of these results to a linear potential, a harmonic oscillator potential, and an exponentially decaying potential are shown.

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1. Introduction

In 1827, the Scottish botanist Robert Brown discovered under his microscope an irregular and vigorous movement of small particles (originally pollen) floating in water. Additionally, he observed that small mineral particles were also subjected to incessant motion, as if they were living organisms. This amazing behavior is now known as Brownian motion, after its discoverer.

The stochastic fluctuations observed in the Brownian motion of a colloidal particle suspended in a liquid medium arise from the fact that molecules in a fluid have random positions and momenta [1,2]. One way the probabilistic motion of a colloidal particle can be modeled is by direct calculations at the particle level to account for thermal fluctuations, or even using coarse-grained approximations [3–5]. The price one has to pay is the excessive computational time since the dynamics of each molecule is faster than the hydrodynamic scale times [6]. Alternatively, thermal fluctuations may be included in the Navier–Stokes equation by introducing stochastic terms in the force, as proposed by Landau and Lifshitz [7]. The basic idea for the treatment of fluctuations in hydrodynamics is that they may be generated by the addition of a stochastic stress tensor

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to the usual viscosity stress tensor [8]. It has been shown that this model provides good enough results down to, essentially, the molecular scale [5,9–13].

Another stochastic model of Brownian motion builds the colloidal particle path from random independent jumps according to a local transition probability. In the general case, some type of classical chaotic evolution is assumed so that the transition probability is calculated as the average of all possible paths [14].

On the other hand, the path integral formalism for quantum mechanics was introduced by Feynman in 1948 [15]. It is widely used in theoretical physics since it provides an alternative approach to existing treatments and it is useful in the development of new ideas and approximations in the description of physical phenomena [16]. This formalism provides a standard quantization procedure based on the existence of a Hamiltonian or Lagrangian for the system under consideration. Since the path integral is defined by a stationary action integral, this procedure yields the classical equations of motion when \hbar tends to zero [17]. In this sense, it is possible to obtain a theory involving dissipative equations for a quantum system; in particular such theory reproduces the classical equations of Brownian motion in the appropriate limit [18,19].

On the other hand, Langevin equation has been used as a basis for the theory of Brownian motion. However, as it happens for any other phenomenological equation, Langevin equation has a limited validity range. It is then reasonable to use Langevin equations when we are interested in the long-time behavior of the system (long times compared to the relaxation time of the reservoir coupled to the system in question). In this case, a quantum level description is not needed because the effects on macroscopic particles in a viscous fluid can be explained by the classical theory [18]. In the path integral approach, the classical action corresponding to a simple random walk happens to be the action of a free particle in the classical mechanics context [16,20,21,17].

In this work, we use precisely the aforementioned fact, *i.e.*, that the action associated to a random walk under a path integral corresponds to the action of a free particle in a classical mechanics context [16,20,21,17]. We introduce a perturbation due to a conservative force generated by a potential $V(\mathbf{x})$. The Lagrangian for this new system is $\mathcal{L} = \mathcal{L}_0 - \epsilon V$ [17,22,23], where ϵ is the perturbation coupling constant and \mathcal{L}_0 is the Lagrangian for a free particle, *i.e.*, the kinetic energy. Then, using path integral methods, we obtain an approximation of the transition probability for a biased stochastic process. The problem is stated in a general fashion for d dimensions. The result can be applied to get a first approximation of the transition probability and of the moments for a biased random walk.

This paper is organized as follows: in Section 2 the transition probability of a stochastic process is obtained by means of a Green function for an action consisting of a free particle part plus a perturbation potential. In Section 3 the normalization constant is written as a perturbation series and determined to first order. In Section 4 the moment-generating function is calculated. In Section 5 the formalism developed in the previous sections is applied to a linear, a quadratic, and an exponentially-decaying potential. Finally we write our conclusions in Section 6.

2. The Green function and the path integral

In the theory of discrete time Markov chains, the Green function $G(\mathbf{x}, \mathbf{x}_0)$ gives the expected number of total sites visited before arriving at \mathbf{x} when starting at \mathbf{x}_0 . For the Brownian motion, there exists an analogue of the Green function. If the transition probability per step is $P(\mathbf{x}, t; \mathbf{x}_0, t_0)$, the Green function is then defined as [24–28]:

$$G(\mathbf{x}, \mathbf{x}_0) = \int_{t_0}^{\infty} dt P(\mathbf{x}, t; \mathbf{x}_0, t_0). \quad (1)$$

If, in particular, the process corresponds to a free, simple random walk, then the transition probability is

$$P(\mathbf{x}, t; \mathbf{x}_0, t_0) = \frac{1}{[4D\pi(t-t_0)]^{d/2}} \exp\left[-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{4D(t-t_0)}\right]. \quad (2)$$

If we consider random walks as Markov processes, we can write the transition probability, according to the Kolmogorov–Chapman equation, as a convolution [16,20,21]:

$$P(\mathbf{x}, t; \mathbf{x}_0, t_0) = \int_{V'} d\mathbf{x}' P(\mathbf{x}, t; \mathbf{x}', t') P(\mathbf{x}', t'; \mathbf{x}_0, t_0). \quad (3)$$

Using this property for n intermediate steps, we have

$$P(\mathbf{x}, t; \mathbf{x}_0, t_0) = \int \left(\prod_{j=1}^{n-1} d\mathbf{x}_j \right) \left(\prod_{j=0}^{n-1} \frac{1}{[4D\pi(t_{j+1}-t_j)]^{d/2}} \right) \exp\left[-\frac{1}{4D} \sum_{j=0}^{n-1} \frac{(\mathbf{x}_{j+1}-\mathbf{x}_j)^2}{t_{j+1}-t_j}\right], \quad (4)$$

where $\mathbf{x}_n = \mathbf{x}$ and $t_n = t$. For $n \rightarrow \infty$, the Green function takes the form of a path integral:

$$G(\mathbf{x}, \mathbf{x}_0) = \int_{t_0}^{\infty} dt \int \mathcal{D}\mathbf{x}(t) \exp\left[-\int_{t_0}^t d\tau \frac{\dot{\mathbf{x}}^2(\tau)}{4D}\right], \quad (5)$$

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