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Anomalous paths in quantum mechanical path-integrals

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ABSTRACT

We investigate modifications of the discrete-time lattice action, for a quantum mechanical particle in one spatial dimension, that vanish in the naïve continuum limit but which, nevertheless, induce non-trivial effects due to quantum fluctuations. These effects are seen to modify the geometry of the paths contributing to the path-integral describing the time evolution of the particle, which we investigate through numerical simulations. In particular, we demonstrate the existence of a modified lattice action resulting in paths with any fractal dimension, d_f, between one and two. We argue that $d_f = 2$ is a critical value, and we exhibit a type of lattice modification where the fluctuations in the position of the particle becomes independent of the time step, in which case the paths are interpreted as superdiffusive Lévy flights. We also consider the jaggedness of the paths, and show that this gives an independent classification of lattice theories.

1. Introduction

The path-integral representation of the amplitude $\langle x', t'|x, t\rangle$ for a quantum mechanical particle of mass m moving in a local potential $V(x)$ is usually written as a limit of a multi-dimensional integral [1]:

$$Z \equiv \langle x', t'|x, t\rangle = \lim_{N\to\infty} \mathcal{N} \int dx_1 \ldots dx_{N-1}\, e^{-S_N}, \tag{1}$$

where we have changed to imaginary time ($t \to -it$) and set $\hbar = 1$. Here $\mathcal{N} = (m/2\pi a)^{N/2}$ and S_N is the discrete-time action which should approach the classical continuum action S as the lattice constant $a \equiv (t_f - t_i)/N$ goes to zero, *i.e.*,

$$\lim_{N\to\infty} S_N = S = \int_{t_i}^{t_f} dt \left[\frac{1}{2}\dot{x}^2 + V(x)\right]. \tag{2}$$

We have chosen units such that the mass m of the particle is one. The particular choice

$$S_N \equiv \sum_{k=0}^{N-1} S_k = \sum_{k=0}^{N-1} a\left[\frac{1}{2}\left(\frac{\Delta x_k}{a}\right)^2 + V(x_k)\right], \tag{3}$$

where $\Delta x_k \equiv x_{k+1} - x_k$, with a time-step $dt \to \Delta t \equiv a$, is referred to as the naïve discretization of the classical action S, and has, for example, been used in modeling time as a discrete and dynamical variable [2]. The choice of Eq. (3) is, however, by no means unique and the ambiguity of the discretization has been investigated previously by, *e.g.*, Klauder et al. in Ref. [3]. As an interesting example, it has also been shown that adding terms proportional to $a\Delta x_k^{2n}$, as $a \to 0$ ($n = 1, 2, \ldots$), to each term S_k in the sum in Eq. (3) permits a radical speedup of the convergence in Monte Carlo simulations [5]. Classically, one expects $\Delta x_k/a \to \dot{x}$ to be well-defined as $a \to 0$ and thus $S_k = \mathcal{O}(a)$, and, as was noted in Ref. [5], one would have $a\Delta x_k^{2n} \to a^{2n+1}\dot{x}^{2n} = \mathcal{O}(a^{2n+1})$, which clearly vanish in the $a \to 0$ limit. We will refer to these considerations as the "naïve continuum limit" in the following.

As was pointed out in Ref. [3], and in a related framework in Ref. [4], the argumentation above is, however, not true for quantum mechanical paths, as one expects $\Delta x_k = \mathcal{O}(\sqrt{a})$ in accordance with the Itô calculus for a Wiener process, and thus the action then contains terms S_k of order one. Modifications as those considered in Ref. [5] still vanish, but only as fast as $\mathcal{O}(a^{n+1})$. This implies no difficulty for the numerical speedup procedure, but in general, it is clear that one must take care when modifying the action in the presence of quantum fluctuations.

We now wish to expand on the work from Ref. [3] and proceed to study precisely those modifications to the discrete action that vanish in the naïve limit, but might induce non-trivial effects when quantum fluctuations are taken into account. We will

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show that not only can non-vanishing local potentials be induced by such alterations, as was shown in Ref. [3], but the situation is further complicated in that the size of quantum fluctuations can be changed under the modified lattice theory, such that no naïve assumptions on the continuum limit can be made. This can be seen to manifest itself in the geometrical properties of the paths contributing to the path-integral, and as we will see shortly, can generate both sub- and super-diffusive behaviour.

2. Geometry of path-integral trajectories

We now quickly review two useful measures that will be used to quantify the geometry of relevant paths in the path-integral. The geometry of path-integral trajectories has been investigated previously, in particular by Kröger et al. in Ref. [6], where a fractal dimension was defined and found both analytically and numerically for local and velocity-dependent potentials. More recently a complementary property termed "jaggedness" was identified by Bogojevic et al. in Ref. [7]. Both of these measures signify the relevance of different paths as to what degree they contribute to the total path-integral.

To define the fractal dimension, d_f, for path-integral trajectories, we recall that the fractal dimension for a classical path can be defined in the following way: We first define a length of the path, $L(\epsilon)$, as obtained with some fundamental resolution ϵ. This can, for example, be done by making use of a minimal covering of the path with "balls" of diameter ϵ such that $L(\epsilon) = N(\epsilon) \times \epsilon$, where $N(\epsilon)$ is the number of balls. A fractal dimension can then be defined as the unique number d_f such that $L(\epsilon) \sim \epsilon^{1-d_f}$ as $\epsilon \to 0$ [12]. For path-integral trajectories, a total length can be defined as $\langle L\rangle = \langle \sum_k |\Delta x_k|\rangle$, and the role of ϵ will be played by the expected absolute change in position, $\langle|\Delta x_k|\rangle$, over one small time step $\Delta t \simeq a$. Here $\langle\cdot\rangle$ denotes the quantum-mechanical average using the probability distribution obtained from Eq. (1). For a typical value, $|\Delta x|$, of $\langle|\Delta x_k|\rangle$, say $|\Delta x| \simeq (\Delta t)^{1/\gamma}$, we then have that $\langle L\rangle \simeq N|\Delta x| \simeq T|\Delta x|^{1-\gamma}$ since $N \simeq T/\Delta t$, with $T = t_f - t_i$. We then conclude that $d_f = \gamma$. The fractal dimension can therefore be obtained through a scaling with the number of lattice sites N, as $N \to \infty$, with $T = N\Delta t \simeq Na$ held fixed, *i.e.*,

$$\langle L\rangle \sim N^{1-1/d_f}, \tag{4}$$

for sufficiently large N. This is also the definition made use of in Ref. [6], and is a measure of how the increments $\langle|\Delta x_k|\rangle$ scale with the time step $\Delta t \simeq a$. In the spirit of anomalous-diffusion considerations (see *e.g.* Ref. [13]), we will refer to those paths with a fractal dimension $d_f < 2$, as defined above, as sub-diffusive, reflecting that they spread in space at a slower than normal rate. Similarly those paths with $d_f > 2$ are referred to as super-diffusive, which then corresponds to Lévy flights (see *e.g.* Ref. [14]).

A remark on the physical interpretation of d_f is in order before we proceed. The length $\langle L\rangle$ defined above is not necessarily an experimentally observable length. It gives us, however, an insight into the nature of how the geometry of those paths with a non-zero measure change under modification of the lattice action. The definition of a fractal dimension for the *physical* path of a quantum mechanical particle must necessarily involve considerations of a measuring apparatus, as was done by Abbott and Wise [8]. Inclusion of quantum measurements in a path-integral framework has been discussed in the literature (see *e.g.* Ref. [9]), but will not be considered in this work.

It is well known that the paths contributing to the path-integral, Eq. (1), are continuous but non-differentiable. Indeed, using a partial integration, Feynman and Hibbs [1] showed that for any observable F the identity

$$\left\langle \frac{\delta F}{\delta x_k}\right\rangle = \left\langle F\frac{\delta S}{\delta x_k}\right\rangle \tag{5}$$

holds. In the case $F = x_k$ this leads to

$$\langle \Delta x_k^2\rangle = \mathcal{O}(a), \tag{6}$$

for the lattice action Eq. (3) and for sufficiently small a, and where we from now on assume that expressions like $\langle x_k\, dV(x_k)/dx_k\rangle$ are finite. Hence, we expect $\langle|\Delta x_k|\rangle \propto 1/\sqrt{N}$ and $\langle L\rangle \propto \sqrt{N}$ corresponding to a fractal dimension of $d_f = 2$, which has been confirmed numerically in Ref. [6].

The second measure we will use to describe the relevant paths in the path-integral, is the "jaggedness", J, defined in Ref. [7], which counts the number of maxima and minima of a given path:

$$J = \frac{1}{N-1}\sum_{k=0}^{N-2}\frac{1}{2}\left[1 - \left\langle \operatorname{sgn}(\Delta x_k \Delta x_{k+1})\right\rangle\right], \tag{7}$$

with $J \in [0,1]$. It is a measure of the correlation between Δx_k and Δx_{k+1} with $J = 1/2 + \mathcal{O}(a)$ for completely uncorrelated increments. We therefore expect the jaggedness to be invariant under modifications only altering nearest neighbor interactions on the lattice. Below we will consider the average value of J for sub- and super-diffusive paths.

3. Sub-diffusive paths

Sub-diffusive paths, as defined here, were discovered to be the contributing paths in the presence of a velocity dependent potential, $V_0|v|^\alpha$, in Ref. [6]. We will here consider a similar modification, that in fact *vanish* in the naïve continuum limit, yet changes the geometry of the paths when quantum fluctuations are taken into account:

$$S_k \to S_k + g a^\xi \left|\frac{\Delta x_k}{a}\right|^\alpha, \tag{8}$$

where g is a coupling constant, $\xi \geqslant 1$ and $\alpha \geqslant 0$. The last term is identical to the modification considered in Ref. [6] for $\xi = 1$, but naïvely vanishes for any $\xi > 1$. Due to quantum fluctuations, however, Eq. (6) must be replaced by

$$\frac{1}{a}\langle \Delta x_k^2\rangle + g\alpha a^{\xi-\alpha}\langle|\Delta x_k|^\alpha\rangle = \mathcal{O}(1), \tag{9}$$

showing that for $\alpha > 2\xi$ the last term dominates, and we expect $\langle|\Delta x_k|\rangle \propto a^{(\alpha-\xi)/\alpha}$, corresponding to a fractal dimension of $d_f = \alpha/(\alpha-\xi)$. For $\alpha \leqslant 2\xi$ we still have $d_f = 2$ showing that 2ξ is a critical point for the fractal dimension as a function of α. For $\xi = 1$ this reproduces the results from [6]. In Fig. 1 we show how the length $\langle L\rangle$ scales with the number of lattice sites N for various α and $\xi = 2$. The results are produced numerically by standard Monte Carlo methods [6,10,11]. From this scaling one can find the fractal dimension according to Eq. (4). In Fig. 2 we have extracted the fractal dimension as a function of α numerically for $\xi = 1$, 2 and 3. We see that the numerical results fit well to the expected values of $d_f = 2$ for $\alpha \leqslant 2\xi$ and $d_f = \alpha/(\alpha-\xi)$ for $\alpha > 2\xi$, shown as solid lines in the figure.

4. Super-diffusive paths

Consider now modifications of the form

$$S_k \to f(S_k), \tag{10}$$

for some analytical function, $f(x)$, with the constraint $f(x) = x$ as $x \to 0$, in order to reproduce the classical limit. This constitutes