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Nikolai Prokof'ev
University of Massachusetts - Amherst, prokofev@physics.umass.edu

P.C.E Stamp

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N.V. Prokof'ev[1,2] and P.C.E. Stamp[3,4]

[1]Department of Physics, University of Massachusetts, Amherst, MA 01003, USA
[2]BEC-INFM, Dipartimento di Fisica, Universita di Trento, Via Sommarive 14, I-38050 Povo, Italy
[3]Department of Physics & Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1
[4]Pacific Institute of Theoretical Physics, University of British Columbia, Vancouver, BC, Canada V6T 1Z1

The common perception is that strong coupling to the environment will always render the evolution of the system density matrix quasi-classical (in fact, diffusive) in the long time limit. We present here a counter-example, in which a particle makes quantum transitions between the sites of a d-dimensional hypercubic lattice whilst strongly coupled to a bath of two-level systems which 'record' the transitions. The long-time evolution of an initial wave packet is found to be most unusual: the mean square displacement n^2 of the particle density matrix shows long-range ballitic behaviour, with $\langle n^2 \rangle \sim t^2$, but simultaneously a kind of weakly-localised behaviour near the origin. This result may have important implications for the design of quantum computing algorithms, since it describes a class of quantum walks.

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One can think of the trajectory of a quantum particle hopping between 2 nodes A and B on some lattice or 'graph', as a 'quantum walk', in which the amplitude to go from A to B is given by summing over all possible paths (or 'walks') between them. Amusingly, such walks can also describe the time evolution of quantum algorithms, including the Grover search algorithm and Shor's algorithm. One can find explicit mappings between the Hamiltonian of a quantum computer built from spin-1/2 'qubits' and gates, and that for a quantum particle moving on some graph[1, 2]. Each graph node represents a state in the system Hilbert space, and the system then walks in 'information space'. This mapping is most transparent for spatial search algorithms with the local structure of the database. Amongst the graphs so far studied are 'decision trees'[1, 3, 4] and hypercubes[5, 6]; quantum walks on other graphs, and their connection to algorithms, were recently reviewed[2].

The quantum dynamics between two sites A and B on a given graph is often much faster (sometimes exponentially faster) than for a classical walk on the same graph [4, 7, 8]. It has been argued that quantum walks may generate new kinds of quantum algorithm, which have proved very hard to find. Several recent papers have also considered experimental implementations of quantum walks for quantum information processing[9, 10]; some involve walks in real space, whereas others are purely computational (eg., a walk in the Hilbert space of a quantum register[10]). Many experiments over the years, particularly in solid-state physics, have also been implicitly testing features of quantum walks.

As always, the main problem confronting any quantum algorithm is environmental decoherence - the gradual entanglement of the system with the 'environment' means that phase interference effects are gradually lost, in measurements performed on the system alone. It is generally assumed that the system dynamics will then show classical diffusion at long times[11], at least if the environment is at or near equilibrium[12]. This 'folk theorem' is supported by results on many models[13] (except for certain very unusual 1-dimensional systems[14]). Recent investigations of decoherence effects on quantum walks[15]-[19] give similar results, although in one investigation of random walks driven by coin-tosses[17], non-classical behavior was found. In these recent investigations, the decoherence mechanism was either (i) an external noise source (ii) a coupling to a set of tossing 'coins'; or (iii) a coupling of the coins to a heat bath. In solid-state and atomic qubits systems, the heat bath is modelled either by a set of oscillators (representing delocalised modes like phonons, photons, or electrons), or by a set of '2-level systems', or 'TLS' (representing localised modes like defects, topological disorder, or nuclear and paramagnetic spins). Both are important in experiment; TLS are particularly important for decoherence in magnetic[20], superconducting[21], and conducting[22] qubit systems, and tend to dominate at low temperature.

In this paper we consider a class of quantum walk models having a very unusual dynamics- not only is the long-time behaviour not classically diffusive, but a part of the single-particle reduced density matrix always continues to show coherent dynamics. These models are very relevant to solid-state quantum information processing systems, since they involve a TLS bath- we couple a quantum particle moving on a graph to a bath described by a set $\{\boldsymbol{\sigma}_k\}$ of TLS, written as spin-1/2 Pauli spins (with $k = 1, 2, ...N$). We first describe the dynamics of these models, and then their physical interpretation.

Quantum Walker: For definiteness we choose a d-dimensional hypercubic graph for the walking particle (our main conclusions do not depend on this assumption), with the 'bare' Hamiltonian

$$\mathcal{H}_o = \Delta_o \sum_{<ij>} (c_i^\dagger c_j + h.c.) \tag{1}$$

Here $c_i^\dagger$ creates the particle on site i, and $< ij >$ restricts the dynamics to nearest neighbor hopping. The particle moves in a Bloch band with dispersion relation $\epsilon_o(\mathbf{k}) = 2\Delta_o \sum_{\mu=1}^{d} \cos(k_\mu a_o)$ and bandwidth $W_o = 4d\Delta_o$. Here a_o is the lattice constant, and $\mathbf{k}$ the d-dimensional momentum. Henceforth we measure all distances in units of a_o, and label lattice sites by a lattice vector $\mathbf{n}$.

For this quantum walker, the solution of Schrödinger's equation is standard. Thus a particle initially localized at the origin, with wave-function $\psi_n(t=0) = \delta_{\mathbf{n0}}$ at $t = 0$, evolves to $\psi_n(t) = L^{-d} \sum_{\mathbf{k}} e^{i[\mathbf{k}\cdot\mathbf{n} - \epsilon_o(\mathbf{k})]t}$ at a later time, where L is the linear system size. The probability distribution $P^o_{n0}(t) = |\psi_n(t)|^2$ is then

$$P^o_{n0}(t) = \prod_{\mu=1}^{d} J^2_{n_\mu}(z)\ ; \quad z = 2\Delta_o t\ , \tag{2}$$

where $J_n(z)$ is the n-th order Bessel function. The continuum-space limit is recovered by considering a broad Gaussian initial wave-packet, initially centred at the origin, of form $\psi_n(t=0) \approx (1/\sqrt{\pi}R)^{d/2}\, e^{-n^2/2R^2}$ with $R \gg 1$. Then for later times

$$P^o_{n0}(t) \approx \left(\frac{R^2}{\pi(R^4+z^2)}\right)^{d/2} e^{-n^2R^2/(R^4+z^2)}\ . \tag{3}$$

As expected, a purely quantum-mechanical evolution gives $P^o_{00}(t) \propto 1/t^d$ and $\langle n^2\rangle \propto t^2$ at long times.

Environmental decoherence: Coupling the quantum walker to an environment is supposed to change the long-time evolution to classical diffusion, characterized at long times by $P^{(cl)}_{00}(t) \propto 1/t^{d/2}$ and $\langle n^2_{cl}\rangle \propto t$. We certainly expect this for models in which the particle coordinate is coupled to an Ohmic oscillator bath, but we now examine the effect of a coupling between the particle and a TLS bath. On its own, this bath has a Hamiltonian $\mathcal{H}_{TLS} = \sum_k \mathbf{h}_k \cdot \boldsymbol{\sigma}_k + \sum_{kk'} V^{\alpha\beta}_{kk'} \sigma^\alpha_k \sigma^\beta_{k'}$, where the $\{\mathbf{h}_k\}$ are fields acting on each TLS, and the $V^{\alpha\beta}_{kk'}$ describe interactions between them. Typically the $V^{\alpha\beta}_{kk'}$ are very small, and lead only to a very slow dynamics of the TLS bath, so we shall drop them[25]. Various couplings of the bath to the walker are possible, but we are interested in those which monitor transitions of the walker, ie., those triggered when the particle hops between nodes. We can then distinguish 2 important limiting cases:

(i) the TLS bath is acted on by only weak external fields, which we then neglect. Now assume that each time the quantum walker hops it can flip the k-th TLS $\boldsymbol{\sigma}_k$ with amplitude α_k. We can write the effective Hamiltonian as

$$\mathcal{H} = \Delta_o \sum_{<ij>} \left\{ c^\dagger_i c_j\ \cos\left(\sum_k \alpha_k \sigma^x_k\right) + H.c.\right\}\ , \tag{4}$$

In what follows we will assume that the individual α_k are small but that the number N of TLS is so large that $\kappa = \sum_k \alpha^2_k \gg 1$, i.e. hopping events are accomplished by simultaneous transitions in a large number of TLS. In other words, we look at the case of *strong decoherence*.

(ii) The TLS bath is polarised by strong external field $\mathbf{h}_k = \mathbf{h}$. Defining the unit vector $\{\hat{z}\}$ along the axis of this field, and the total polarisation $M = \sum_k \sigma^z_k$ of the TLS bath with respect to this axis, we see that in this strong field limit, only bath transitions which conserve M are allowed. In this case one has an effective Hamiltonian

$$\mathcal{H}_M = \Delta_o \sum_{<ij>} \left\{ c^\dagger_i c_j\, [P_{-M}\ e^{i\sum_k \alpha_k \sigma^x_k}\ P_M] + H.c.\right\} \tag{5}$$

where P_M projects the state of the TLS bath onto the subspace with polarization M. We have dropped the large Zeeman term $\sum_k \mathbf{h}\cdot\boldsymbol{\sigma}_k$ from this Hamiltonian, since it is now just an M-dependent constant.

We now proceed with the solution for the probability distribution $P_{n0}(t)$. We shall look in detail at the first model (4) above, and then comment on the second one. The form of (4) is a simple generalisation of a Hamiltonian $\mathcal{H} = \Delta_o\{\hat{\tau}_x \cos[\sum_k \alpha_k \sigma^x_k] + H.c.\}$, which describes one limiting case of the interaction of a single qubit $\boldsymbol{\tau}$ with a spin bath. The density matrix of this model is given exactly as a phase average over the propagator of the 'bare' qubit [23, 24], and one can use precisely the same technique to write the solution for (4). Thus, for the initially localised state $\psi_n(t=0) = \delta_{\mathbf{n0}}$, assuming the strong decoherence limit described above, one finds the solution at time t as

$$P_{n0}(t) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \prod_{\mu=1}^{d} J^2_{n_\mu}(z\cos\varphi)\ , \tag{6}$$

and similarly for the initially broad wave-packet one gets

$$P_{n0}(t) \approx \int_0^{2\pi} \frac{d\varphi}{2\pi}\ \frac{R^d\ e^{-n^2R^2/(R^4+z^2\cos^2\varphi)}}{\left[\pi(R^4+z^2\cos^2\varphi)\right]^{d/2}}\ . \tag{7}$$

We will rederive this result using a rather different method at the end of the paper. Given the strong coupling to the TLS environment, one intuitively expects classical diffusive dynamics at long times. Surprisingly, the actual evolution is radically different. Consider first the probability at long times of finding a particle back at the origin, $P_{00}(z \to \infty)$, in Eq. (6). The asymptotic expansion for the Bessel function $J_0(z\cos\varphi) \approx \sqrt{2/\pi}\cos(z\cos\varphi - \pi/4)/(z\cos\varphi)$ is not possible because $\cos\varphi \to 0$ for $\varphi \to \pm\pi/2$. In fact, in the $t \to \infty$ limit the dominant contribution (for $d > 1$) comes from $\varphi \approx \pm\pi/2$. Then

$$P_{00}(z\to\infty) \approx \frac{1}{\pi}\int_{-\infty}^{\infty} d\varphi J^{2d}_0(z\varphi) = \frac{A_d}{\Delta_o t}\ , \tag{8}$$

where $A_d = (2\pi)^{-1}\int_{-\infty}^{\infty} dx J^{2d}_0(x)$ is a constant (in $d = 1$ there is an additional $\ln(2\Delta_o t)$ factor). This result is already rather peculiar since in $d > 2$ the decay of $P_{00}(t)$ is integrable both in the classical diffusion, $P^{(cl)}_{00} \propto t^{-d/2}$, and in the ideal, or ballistic, quantum propagation, $P^o_{00} \propto$

t^{-d}. We get qualitatively similar answers for the broad initial state (7), where

$$P_{00}(z \to \infty) \approx \frac{A_d R^{2-d}}{\Delta_o t} \ , \tag{9}$$

and $A_d = 2\pi^{-(1+d/2)} \int_0^\infty dx/(1+x^2)^{d/2}$. The dependence on the initial wave-packet spread in the long time-limit is another unusual feature of the solution.

From the divergence of the total time spent at the origin $\tau = \int_0^{t\to\infty} d\tau P_0(\tau) \propto \Delta_o^{-1} \ln(\Delta_o t) \to \infty$ one's first suspicion is that the strong environmental decoherence is causing some kind of quasi-localization of the particle, analogous to weak localisation in solid-state physics. It then comes as an astonishing paradox that a calculation of the mean-square displacement from (6) gives

$$< ((\mathbf{n}(t) - \mathbf{n}(0))^2 >= 12 \sum_n \mathbf{n}^2 P_{\mathbf{n0}}(z) = \frac{d}{2}(\Delta_o t)^2 \ , \tag{10}$$

which is only a factor of two smaller then the coherent quantum evolution! Thus the solution shows quasi-localsation near the origin, coexisting with coherent ballistic dynamics at large distances.

Having both $P_{00}(t) \propto 1/t$ and $\sum_\mathbf{n} \mathbf{n}^2 P_{n0}(t) \propto t^2$ at the same time is obviously inconsistent with the simple scaling form $t^{-d} f(n^2/t^2)$. The solution to the paradox requires a more complex shape for the distribution function, which we show in Fig. 1 and derive here for the Gaussian initial state. We introduce new variables $r = n/R$ and $u = z/R^2$ to simplify the integral in (7) to:

$$P_{r0}(u) = \left(\frac{1}{\pi R^2}\right)^{d/2} \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{e^{-r^2/(1+u^2\cos^2\varphi)}}{[1+u^2\cos^2\varphi)]^{d/2}} \ . \tag{11}$$

It is straightforward at this point, by considering the long-time limit $u \gg 1$, to derive the following relations for the intermediate

$$P_{n0}(t) \approx \frac{\Gamma\left(\frac{d-1}{2}\right)}{2\pi^{d/2+1}} \frac{R}{\Delta_o t \, n^{d-1}} \ , \quad (R \ll n \ll \Delta_o t/R) \ , \tag{12}$$

and large ($n \to \infty$) length scales

$$P_{n0}(t) \approx \frac{1}{\pi^{(d+1)/2} n} \left(\frac{R}{2\Delta_o t}\right)^{d-1} e^{-n^2 (R/2\Delta_o t)^2} \ . \tag{13}$$

As expected from (9), one has an increased probability of finding a walker at the origin. Since the power-law decay $1/n^{d-1}$ is not integrable, the normalization integral and $\langle n^2 \rangle$ are still determined by the parameter z, but the probability of being at the origin is enhanced over that at a distance $\Delta_o t/R$ by a factor $(\Delta_o t/R)^{d-1}$.

Not surprisingly, the thermodynamics of this system is also peculiar. The partition function $Z = \int_0^{2\pi} (d\varphi/2\pi) I_0^d (2\Delta_o \cos\varphi/T)$ is leading to a free energy in the low-temperature limit $T \ll \Delta_o$ given by $F(T) \sim -T(d/2 + 1/2) \ln T + const.$

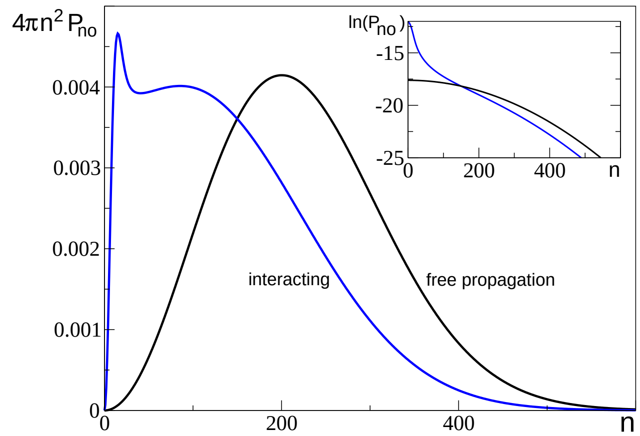

FIG. 1: (Color online). Form of $4\pi n^2 P_{n0}(t)$ after time t such that $z = 2\Delta_o t \gg R^2$, calculated from Eq.(11) with $z = 2000$ and $R = 10$ for the three-dimensional walker. The inset for lnP_{n0} shows the asymptotic decay.

Finally, let us note that the strong-field Hamiltonian (5) gives similar behaviour. For strong decoherence we find that an initially localized state at the origin propagates as

$$P_{n0}(z) = \int_0^\infty dy \, e^{-y} \, P_{n0}^0(z J_M(2\sqrt{\kappa y})) \ . \tag{14}$$

and analysis of this shows the same long-time features as above.

Physical interpretation: A path integral analysis provides some insight here. The anomalous short-distance behaviour arises because the effective interaction between the 2 paths of the density matrix, generated by interactions with the spin bath environment, has long-time memory effects in it - this is because the bath has a degenerate energy spectrum (this is reminiscent of weak localisation[26]). But then how can we explain the long-range ballistic tail? Usually even very weak interaction with a bath gives classical diffusion at long ranges, because the environment 'measures' the position of the particle as it travels along a given path[27]. For this the environment does not have to record *all* possible trajectories of the particle - it only needs to track a 'coarse-grained' trajectory[28]. The same is true if the environment couples to the particle velocity, from measurements of which one can also reconstruct its trajectory.

The answer to the paradox is interesting. Notice that in (4) and (5) the environmental coupling does not distinguish different particle positions in the space of the graph (ie., between different graph nodes), nor the direction of transition between them; it only records that transitions between them have occurred. This leaves room for the constructive interference of many very large paths on the graph.

To gain more insight into the problem we rewrite the Hamiltonian (4) in the momentum representation for the walker and a rotated basis for the TLS spins (rotating $\sigma_k^x \rightarrow \sigma_k^z$). In this basis the Hamiltonian is diagonal; writing $\phi = \sum_k \alpha_k \sigma_k^z$, and given some TLS spin distribution $\{\sigma_k^z\}$ with a given ϕ, then $\mathcal{H}$ acts on the eigenstates $|\mathbf{k}, \{\sigma_k^z\}\rangle$ according to

$$\mathcal{H}\,|\mathbf{k}, \{\sigma_k^z\}\rangle \;=\; \cos\varphi\, \epsilon_o(\mathbf{k})\, |\mathbf{k}, \{\sigma_k^z\}\rangle \;, \qquad (15)$$

If we now start from the initially localized state for the walker and arbitrary $\prod_k |\sigma_k^z\rangle$ state for the environment (in the original, unrotated basis) the system is an equal-weight superposition of all eigenstates. We immediately see that states with the same φ evolve coherently with a renormalized hopping amplitude $\Delta_o \cos\varphi$, and in the strong coupling limit all values of φ on the $[0, 2\pi]$ interval are equally represented (thus we rederive the result given above in eqtns. (6) and (7)). The ballistic long-time behaviour comes from those portions of this mixture with $|\cos\varphi| \sim 1$. The anomalous 'sub-diffusive' long-time behavior at the graph origin, on the other hand, comes from a small fraction $\sim 1/z$ of states having very small effective $\Delta_o \cos\varphi < 1/t$, which cannot propagate anywhere at all!

In quantum information processing systems, where the walk can occur in different kinds of information space, no general principle forces the environmental couplings to distinguish either the different graph nodes, or the direction of transition between them. Thus we see that in the design of quantum computers and certain search algorithms, it becomes of considerable interest to look at quantum walkers for which environmental decoherence may even be strong, provided it is not projecting particle states onto either the 'position' or 'momentum' bases in the information space defined by the graph on which the walk takes place. More generally, we see that there is an interesting class of systems for which the long-time behaviour is very far from diffusive, even in the strong decoherence limit- instead, it combines a short-range 'sub-diffusive' behaviour with long-range coherent dynamics.

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