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Johan Carlström,[1] Nikolay Prokof'ev,[1,2,3] and Boris Svistunov[1,3,4]
[1] *Department of Physics, University of Massachusetts, Amherst MA 01003 USA*
[2] *Department of Theoretical Physics, The Royal Institute of Technology, Stockholm SE-10691 Sweden*
[3] *National Research Center "Kurchatov Institute," 123182 Moscow, Russia and*
[4] *Wilczek Quantum Center, Zhejiang University of Technology, Hangzhou 310014, China*
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We study the propagation of a hole in degenerate (paramagnetic) spin environments. This canonical problem has important connections to a number of physical systems, and is perfectly suited for experimental realization with ultra-cold atoms in an optical lattice. At the short-to-intermediate timescale that we can access using a stochastic-series-type numeric scheme, the propagation turns out to be distinctly non-diffusive with the probability distribution featuring minima in both space and time due to quantum interference, yet the motion is not ballistic, except at the beginning. We discuss possible scenarios for long-term evolution that could be explored with an unprecedented degree of detail in experiments with single-atom resolved imaging.

While classical random walks are well-understood as a diffusive process realized in a wide range of physical systems, their quantum-mechanical counterparts are far more subtle [1]. To be more specific, consider vacancy motion in the paramagnetic phase of solid ^{3}He, or, equivalently, hole propagation in the strongly correlated Mott-insulator (MI) state of electrons. Even though the dynamics of holes/vacancies are governed by standard quantum mechanics, the probability amplitudes for various trajectories do not interfere the same way as they do for ballistic motion in a perfect (or spin polarized) lattice because propagating holes often leave behind a trace in the spin environment that effectively "records" where they have been (see Fig. 1). This disrupts quantum interference between different paths, which, otherwise, would lead to a much larger mean-square displacement than in the classical case for the same path arc-length. However, some trajectories and even whole classes of trajectories (see panel (d) in Fig. 1) do interfere. This leads to a highly nontrivial propagation intermediate between the quantum-ballistic and classical-diffusive limits. Interference between trajectories (leading to one and the same final state) may also depend on whether the lattice is bipartite or not, as well as on the statistics of particles behind the spin components (see below).

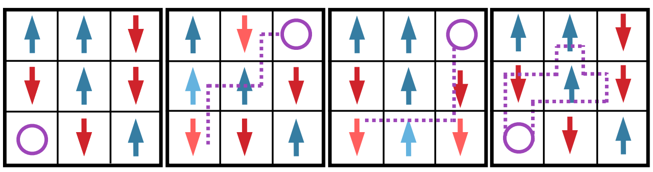

Figure 1. Hole propagation in a spin environment. (a) The hole starts at the lower left corner. As it moves, it leaves behind a trace of altered spins. In (b,c), the final destination is the upper right corner, yet the paths taken differ (purple dashed lines), and so do the resulting spin states. In (d), we show a self-retracing trajectory described as a necklace of zero-area loops; all such trajectories interfere because at the end the hole returns to the origin, and the spin environment is inherently preserved.

In condensed matter systems that are too complicated/strongly interacting to allow for exact solution, accurate analytic treatment, or viable numerical computations in the thermodynamic limit, the study of hole propagation in model systems where lattice sites carry an additional "flavor" index offers a means of gaining insight into density of states, transport properties, formation of magnetic polarons, and the nature of ferromagnetic instability in MI [2]. Characteristic examples include the Fermi Hubbard and $t-J$ models [2–5], the Kitaev-Heisenberg model [6], as well as vacancy motion in solid ^{3}He crystals [7–9]. In quantum computing and information processing, relevant problems and algorithms are also frequently formulated as quantum walks on a network [10–12]. Finally, hole propagation in a degenerate spin environment provides an important physical realization of a system experiencing so-called dissipation-less decoherence when the environment "records" particle trajectories with negligible energy transfer [13, 14].

To the best of our knowledge, the problem of hole propagation in degenerate magnetic environments is still far from being understood even at the conceptual level despite a considerable long-standing interest in a variety of contexts. On the one hand, such basic questions as the probability of return, dynamic formation of magnetic domains, the value of the diffusion constant (if any) and its dependence on the initial conditions, remain unanswered theoretically. On the other hand, it is virtually impossible to obtain accurate experimental information about hole dynamics and changes in its local spin environment as it moves along for realistic condensed matter systems. However, an experimental realization of relevant model systems in a controlled setup with full access to all lattice sites is now possible using cold atoms/ions trapped in an optical lattice and imaged with single-site resolution [15–20]. These techniques have previously been applied to study quantum walks, and yield a resolution in the time domain that is much finer than the inverse hopping, allowing observation of interference patterns at extremely short timescales [16]. Recently, it has also become clear that N-component fermions with $N > 2$ can be realised in optical traps by exploiting nuclear spin [21–23]. Remarkably, the most interesting regime of a near-degenerate spin environment also happens to be the least demanding in terms of lattice parameters and system temperature, and is easily implementable with existing technology. In fact, the fermionic MI phase corresponding to large U/J (where J is the hopping matrix element and U is on-site repulsion) at temperature $T > 4J^2/U$ (above the onset of strong anti-ferromagnetic correlations) was already created some years ago [24, 25].

In this Letter, we address the topic of a quantum walk undertaken by the hole in degenerate spin environments on a square lattice with the goal of establishing precise data for hole dynamics over short-to-intermediate time-scales, testing existing analytical predictions, discussing open questions and possible scenarios concerning long-time dynamics, and motivating (apart from providing benchmarks) future experimental studies.

Physically, our system corresponds to the N-component Hubbard model

$$H = -J \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_i^2 \quad (\sigma = 1, 2, \ldots, N), \quad (1)$$

deep into the MI phase, $U/J \gg 1$, at high temperature $T \gg J^2/U$, i.e. in the absence of antiferromagnetic correlations (which is also the parameter regime where direct single-site resolved imaging techniques work best). All components are assumed to have one and the same—either bosonic, or fermionic—statistics. For brevity we will refer to σ as the spin index. Then, $c^\dagger_{i,\sigma}$ is the creation operator of a σ-particle on site i, $n_{i\sigma} = c^\dagger_{i,\sigma} c_{i\sigma}$, and $\langle i, j\rangle$ stands for pairs of n.n. sites. To obtain the time-dependent wave function $\psi(t)$, we expand the evolution operator in the Taylor series:

$$U(t) = e^{-iHt} = \sum_n (-i)^n \frac{t^n}{n!} H^n \,. \quad (2)$$

In the $U/J \to \infty$ limit at unit filling factor when doubly occupied sites are forbidden, the only allowed dynamic process in (1) is hole-propagation which can be viewed as a quantum walk that alters the configuration of lattice spins. Then, on a square lattice with coordination number $z = 4$, one can describe H^n as a sum of z^n possible trajectories. Using Monte Carlo simulation techniques, we sample all sums stochastically [26] and classify trajectories according to their distinguishable final states. This allows us to study the evolution of the spatial distribution function for the hole over some time interval, limited by the available memory resources. The specific protocol is as follows:

• We start by proposing n from the Poisson distribution

$$p(n) = \frac{(zt)^n}{n!}\, e^{-zt} \,, \quad (3)$$

where time is given in units of $1/J$;

• Then, a random walk of the hole with n steps is conducted (at each step the hole is moved randomly to one of the n.n. sites);

• The final displacement of the hole, $\mathbf{r}$, and the resulting configuration of the spin environment, γ, are registered, and $(-i)^n$ is added to a bin corresponding to the $|\mathbf{r}, \gamma\rangle$ state. This contribution is real or imaginary depending on the parity of n;

• The procedure is repeated, and the set of generated states is used to construct the wave function

$$\psi(t) = \sum_{\mathbf{r},\gamma} A_\gamma(\mathbf{r}, t) |\mathbf{r}, \gamma\rangle \,, \quad (4)$$

where amplitudes $A_\gamma(\mathbf{r}, t)$ are normalized to unity, $\sum_{\mathbf{r},\gamma} |A_\gamma(\mathbf{r}, t)|^2 = 1$. The spatial probability distribution for the hole position is then given by

$$\rho(\mathbf{r}, t) = \sum_\gamma |A_\gamma(\mathbf{r}, t)|^2 \,; \quad (5)$$

• Finally, the entire procedure is repeated for multiple (256) randomly generated initial states $|\mathbf{r} = 0, \gamma_{\rm in}\rangle$ to obtain averaged results for $\rho(\mathbf{r}, t)$.

There is no extra sign associated with fermionic exchange cycles in our case because closed trajectories on bipartite lattice always result in an even number of exchanges. Moreover, since real and imaginary parts of $\psi(t)$ are based on trajectories with different parity of n, the probability distribution $\rho(\mathbf{r}, t)$ remains insensitive to particle statistics even if the lattice is not bipartite. However, if one considers hole propagation in a bose-fermi mixture, then the fermionic sign does matter. Also, if the initial state is a superposition $\psi(0) = \sum_{\mathbf{r}',\beta} C_{\mathbf{r}',\beta} |\mathbf{r}', \beta\rangle$, then particle statistics become important on non-bipartite lattices. On bipartite lattices it is always possible to map between the ferminic and bosonic problems, even if the initial state is a superposition.

In Fig. 2, we show the "survival" probability $\rho(0, t)$ for systems with different number of spin components $N = 2$, 3, 4 and ∞. For comparison, we also include analytic results for ballistic propagation in a perfect spin-polarized lattice as well as the Brinkman-Rice (BR) approximation [3]. [The latter approximates $\bar{A}(0, t) = \langle r = 0, \gamma_{\rm in} | \psi(t)\rangle$ by considering only self-retracing closed paths (see panel (d) in Fig. 1) that by construction preserve the original spin configuration $\gamma_{\rm in}$; then the spacial probability distribution is obtained through a second approximation given by $\rho(0, t) \approx |\bar{A}(0, t)|^2$.] Up to the first minimum, taking place at $t_{\rm min} \approx 0.9$, the different scenarios are very similar, suggesting that the underlying spin degrees of freedom have little effect on the early evolution, because it is dominated by the self-retracing paths that inherently preserve the spin environment. Indeed, $n = 0$, four $n = 2$, and thirty two out of forty $n = 4$ closed loop trajectories are from the self-retracing set. Still, by excluding certain trajectories from interference, the BR approximation predicts $t_{\rm min}$ much more accurately than ballistic propagation, indicating that dissipation-less decoherence starts playing a role at this time scale. From Fig. 2 (b) it is clear that all spin systems exhibit near-complete destructive interference at the first minimum with survival probabilities dropping below half a percent.

After the first minimum, the evolution is clearly dependent on the environment. Since the BR approximation only takes into account trajectories that preserve the spin configuration,

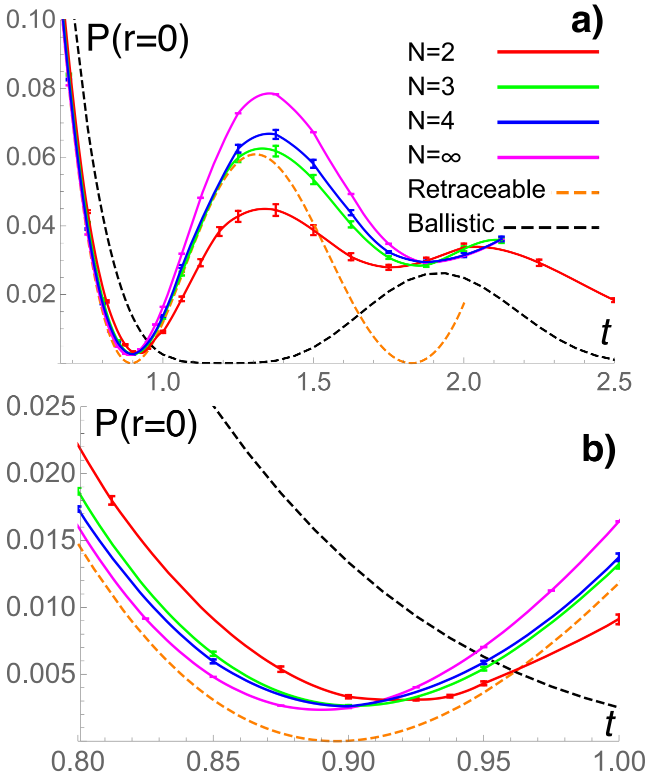

Figure 2. Probability of finding the hole at the origin as a function of time (in units of inverse hopping, $1/J$). The two panels show the same data for different time intervals. The curves correspond to different spin values $N = 2,\ 3,\ 4$ and ∞, the Brinkman & Rice self-retracing approximation, and ballistic propagation (see legend). All curves, except that for ballistic motion, follow each other closely up to the first minimum at $t \approx 0.9$, but beyond that point, the details of the spin environment becomes important to the hole propagation. The BR approximation is very accurate up to the first minimum, but quickly fails at longer t.

it goes completely wrong by predicting instances of perfect destructive interference occurring at a later time [an impossible effect due to the large number of $|\gamma\rangle$ states contributing to $\rho(0)$, see Eq. (5)]. The survival probability does show oscillations in time but they are strongly damped, and, presumably, go away at longer time scales (determining whether interference ceases to be relevant, and if so than at what time scales, requires access to longer time scales). Unexpectedly, the first oscillation is much weaker for $N = 2$ than for $N > 2$. Intuitively, the probablity of finding the hole at the origin should be higher in systems with larger value of N due to stronger decoherence effects; what comes as a surprise is the crossing of the curves at $t \approx 1.9$.

Minima and maxima in the survival probability are correlated with minima and maxima in the spatial probability distributions, see Fig. 3. The random walk in a degenerate spin environment is thus strikingly different from the case of ballistic motion in a spin-polarized system that features perfect destructive interference events at arbitrary long times (see

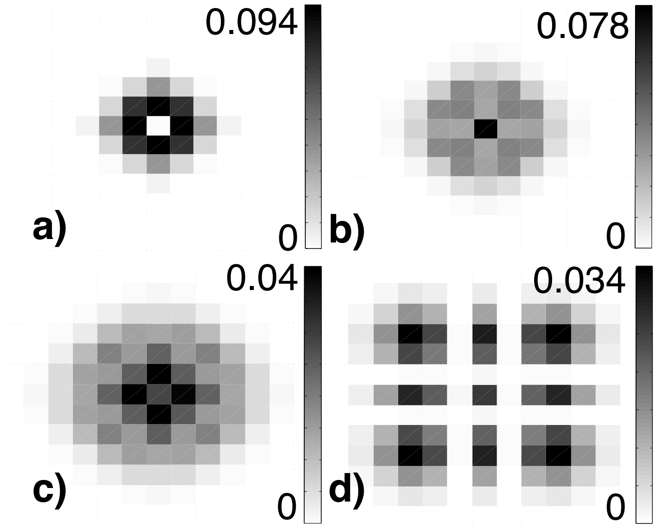

Figure 3. Spatial probability distributions $\rho(\mathbf{r}, t)$ (Eq. 5). Images (a-c) correspond to $N = \infty$ at $t = 0.9,\ t = 1.375$ and $t = 1.875$, while (d) shows the case of ballistic motion in a polarised lattice at $t = 2$. In (a), $\rho(0)$ is close to zero due to destructive interference, changing to maximum in (b) only to become a local minimum again in (c) at $t = 1.875$, which also corresponds to a shallow local minimum in the survival probability, see Fig. 2. In the ballistic case, strong destructive interference is possible at arbitrary long times.

Fig. 3d). Yet the distribution function is not that of a classical random walk either, which is just a gaussian without local minima in time or space.

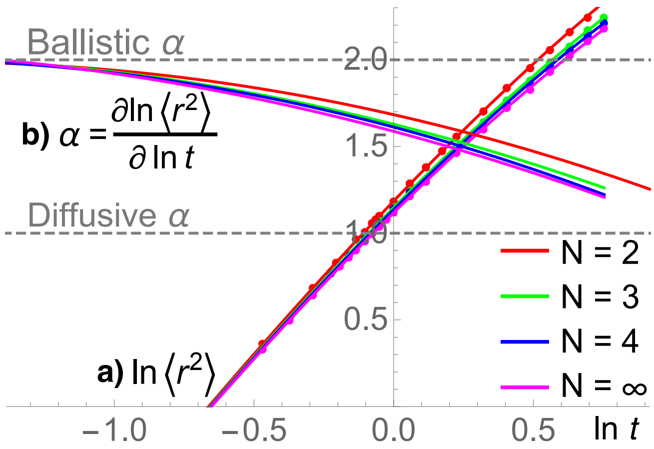

Figure 4. (a) Logarithmic plot of the mean-square displacement as a function of time. The lines correspond to cubic polynomial fits to data. (b) MSD exponent α. At small t it is close to 2, as expected for coherent propagation in a perfect lattice. Within the timescale of these simulations, α does not converge to a constant value, so the precise nature of the propagation at large t (specifically if the motion is diffusive) remains an open question.

The most natural assumption is that in the long-time limit decoherence effects ultimately lead to diffusive propagation characterized by linear dependence of the mean-square displacement (MSD) on time. To see if our simulations have reached this asymptotic behavior, we introduce the time-dependent MSD exponent α as the logarithmic derivative

$$\alpha = \frac{\partial \ln \langle r^2 \rangle}{\partial \ln t}\,. \tag{6}$$

Then, α can be deduced from the slope of the MSD curve on the log-log plot, see Fig. 4a. Fitting a cubic polynomial to the data we can take the required logarithmic derivative. The result is shown in Fig. 4b. Clearly, the diffusive regime was not yet reached within the timescale of our simulations and we are still in the crossover region (assuming that diffusion does take place, see below). For $t \to 0$ the motion is nearly ballistic and $\alpha(t \to 0) \to 2$, as expected.

Even though diffusion seems to be the most natural outcome of long time evolution, this quantum walk has several features that make it fundamentally different from what takes place in more conventional dissipative environments where external degrees of freedom have dynamics of their own. In our case, *any* change in the spin environment is completely "slaved" to the hole dynamics. It is also different from coherent propagation in static random media, because the spin environment does change under evolution. The combination of these two circumstances leads to long-term memory effects because previously created trajectory "records" can only be erased or scrambled by the subsequent hole motion. These (and further) considerations make the problem of long-time evolution in our system highly nontrivial.

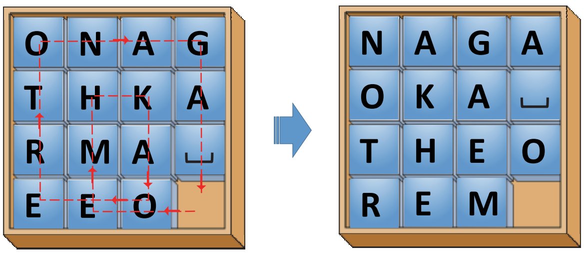

Figure 5. Hole propagation in a dynamically passive environment amounts to a quantum mechanical realisation of the N-puzzle game [27], where a particular order is sought with as few tile movements as possible. While the classical problem is NP-hard, in the quantum mechanical system, all possible trajectories are realized in superposition.

In the limit $U/J \to \infty$, the ground state of the Fermi-Hubbard model with one hole added to the MI phase is a ferromagnet (Nagaoka theorem) [2] with a delocalized hole and a kinetic energy of $-zJ$. The maximum energy is $+zJ$, and also corresponds to a hole delocalised on a ferromagnetic background, differing from the ground state only by having the hole momentum shifted by $\{\pi, \pi\}$. States with energies slightly above minimum or below maximum can be realised in the form of a hole delocalised in a finite sized ferromagnetic "bubble," i.e. they constitute a type of low and high energy polarons [28, 29].

The fact that the energy is bound so that $-zJ \le \epsilon \le zJ$ has important implications for experimental realisations with optically trapped atoms. These are generally implemented with a harmonic trap, and so the hole is effectively subject to an inverted harmonic trap—it attains a potential energy that is maximal in the center of the trap; $U(\bar{r}) \approx \alpha r^2$, $\alpha < 0$. The maximum energy that the hole can absorb is $\Delta E_{\text{max}} = 2z|J|$ implying that if the hole originates in the center of the trap, then it is bound to a region $|\alpha| r^2 \le \Delta E_{\text{max}} \to |\bar{r}| \le r_{\text{max}} = \sqrt{\Delta E_{\text{max}}/|\alpha|}$. In addition, any hole found sufficiently close to $|\bar{r}| = r_{\text{max}}$ has absorbed enough energy to necessarily form a high energy polaron. While it is possible to find ferromagnetic regions in a degenerate system by sheer accident, these can also be assembled by hole motion; compare to the N-puzzle game in Fig. 5. In this sense, the most energetic states can be viewed as a particular class of (ferromagnetic) solutions to the N-puzzle game that are strongly correlated with large hole displacement.

The presence of polarons in this model also raises questions about hole mobility in the absence of a harmonic trap (or in the interior of the trap where the potential energy changes slowly). Specifically, such objects should move slowly, suggesting that the edges of the energy spectrum are associated with reduced hole mobility.

In conclusion, we find that at the early stages, the quantum walk of a hole in a degenerate spin environment is profoundly different from both the classical diffusive case and the quantum ballistic propagation in a polarized environment. Whether the motion is diffusive in the long-time limit remains an open question. We point out mechanisms that give rise to long-term memory effects, making interference and thus mobility highly nontrivial. We also propose that polarons at the edges of the energy spectrum may be associated with impaired hole mobility. Such effects are however outside of the capacity of our simulation software, which is limited in terms of accessible time scales. Unitary evolution of the entire system further complicates the observation of polarons because holes in random local spin configurations and holes in "bubbles" are in a superposition state. One possible solution is to study dynamics of initial states with holes delocalized in "bubbles."

We argue that real progress in understanding this long-standing problem is possible by performing experiments with ultra-cold atoms in optical lattices and studying the hole dynamics using single-site resolution imaging. The most interesting parameter regime ($U/J \gg 1, T \gg J^2/U$, deep in the MI phase at relatively high temperature) is already widely accessible. In this limit, single-site imaging techniques work best and can provide an unprecedented amount of detail about hole-evolution as well as the state of the environment that is left behind. Moreover, experimentally, one can reach timescales orders of magnitude longer than in our simulations, which can be used to benchmark experimental data at intermediate times.

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