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Dynamics of unvisited sites in presence of mutually repulsive random walkers

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We have considered the persistence of unvisited sites of a lattice, i.e., the probability $S(t)$ that a site remains unvisited till time t in presence of mutually repulsive random walkers. The dynamics of this system has direct correspondence to that of the domain walls in a certain system of Ising spins where the number of domain walls become fixed following a zero termperature quench. Here we get the result that $S(t) \propto \exp(-\alpha t^\beta)$ where β is close to 0.5 and α a function of the density of the walkers ρ. The number of persistent sites in presence of independent walkers of density ρ' is known to be $S'(t) = \exp(-2\sqrt{\frac{2}{\pi}}\rho' t^{1/2})$. We show that a mapping of the interacting walkers' problem to the independent walkers' problem is possible with $\rho' = \rho/(1-\rho)$ provided ρ', ρ are small. We also discuss some other intricate results obtained in the interacting walkers' case.

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I. INTRODUCTION: THE ORIGINAL SPIN PROBLEM

Dynamical evolution of a spin system following a quench to zero temperature from a disordered state may lead to a non-equilibrium state, e.g., as in the one dimensional ANNNI (Axial Next Nearest Neighbor Ising) model [1] which has the Hamiltonian

$$H = -\Sigma S_i S_{i+1} + \kappa \Sigma S_i S_{i+2}, \tag{1}$$

where $S_i = \pm 1$ is the spin at the ith site and $\kappa > 0$ is the ratio of the second neighbour and first neighbour interactions. For $\kappa < 1$, the quench does not lead to the equilibrium configuration which is ferromagnetic for $\kappa < 0.5$ and antiphase for $\kappa > 0.5$. Starting from a random state, there is a short initial time during which the domains of size one die and this eventually results in a configuration with fixed number of domain walls. In this state, the domain walls become "fluid" in the sense that they can move indefinitely (keeping the energy of the system same) [2, 3, 4] but cannot cross each other. In such a system the persistence dynamics shows that the number of persistent spins is neither a power law nor exponential but rather follows a stretched exponential decay,

$$P(t) \sim \exp(-\alpha t^\beta), \tag{2}$$

with $\alpha \approx 1$ and $\beta = 0.45$ [3].

The above dynamical scenario can easily be represented by an equivalent system of mutually avoiding random walkers and the fraction of persistent spins will then be given by the fraction of unvisited sites $S(t)$ till time t in the system [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Representation of the spin dynamics by random walk of domain walls is well-known; in the common examples like the Ising or Potts model, the random walk is accompanied by annihilation of two domain walls if they meet [12, 13, 17].

In the original ANNNI model problem, when there are M domains with each separated by at least two lattice spacings, the probability distribution of the number of domain walls M within a size L is

$$P(L,M) = \binom{L-M}{M} \Big/ \sum_M^{L/2} \binom{L-M}{M}. \tag{3}$$

This equation is easy to derive once it is realised that the problem is identical to the Bose statistics of distributing L particles in M boxes with the number of particles in each box greater than or equal to 2. It has been observed that the ratio $\rho_0 = M/L$ has a mean value quite close to the most probable value $\rho_0 = 0.2764$ [3]. Distribution of the value of ρ_0 can be calculated numerically which shows that its fluctuation decreases with the system size (typically $\Delta\rho_0$ decreases from 0.0645 for $L = 20$ to 0.0225 for $L = 175$ in a power law manner, $\Delta\rho_0 \sim N^{-0.5}$). This indicates that the ANNNI dynamics reflects the behavior of $S(t)$ for a specific value of the density of walkers in the equivalent random wall picture. It is therefore a meaningful exercise to find out $S(t)$ for general density $\rho = N/L$ where N is the number of mutually exclusive walkers and L the chain length. In this paper we have considered $0 < \rho < 1$ and calculated numerically $S(t)$. $S(t)$ shows a stretched exponential behaviour with an exponent close to 1/2.

This problem, as we have shown, can be mapped to that of the independent random walkers with a subtle difference and also for small ρ. The latter problem has been exactly solved [18] and we compare its results with that of the numerical simulation of mutually repulsive walkers to find a good agreement at small values of ρ.

Our results also show a difference when persistence is calculated in terms of a spin system and the system of pure brownian walkers which we have discussed in the paper. Some other dynamical properties have been investigated in this context.

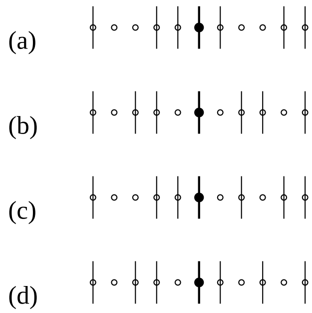

FIG. 1: Possible movement of the tagged walker (highlighted): (a) cannot move. (b) either does not move or can move to the left/right. (c) either does not move or can move to the right. (d) either does not move or can move to the left.

II. PERSISTENCE OF UNVISITED SITES IN PRESENCE OF MUTUALLY EXCLUSIVE WALKERS

To keep correspondence with the original spin dynamics of the ANNNI model, any of the site in the system may be selected for updating. It may or may not contain a random walker. If it does, then the step taken by this random walker is according to the following three situations:
1. If the walker is flanked by two random walkers on both sides; it cannot make any movement and stays there - this corresponds to a locked domain wall (Fig 1a).
2. There are no neighbouring random walker, then the random walker remains at its position with probability 1/2 - this corresponds to the probability that a spin does not flip even at the domain boundary. It can also move to either left or right with equal probability (Fig 1b).
3. There is only one neighbouring walker, say, to the left (right), then it does not move or moves to the right (left) (Fig1 (c) and (d)) with equal probability.
Let us represent this dynamical rule by D_{ANN}, a dynamics which corresponds to the ANNNI model dynamics.

As the walls are reflecting, if the random walker happens to hit the wall, it can only step in-wards or stay there. When L sites are hit, one Monte Carlo step is said to be completed.

It may be noted that in the original ANNNI model, domain walls need to maintain a least distance of two lattice spacings. We have relaxed this condition to one lattice spacing which is equivalent to having on-site repulsion of random walkers. Effectively, this means that the original ratio $\rho_0 = M/L$ in ANNNI corresponds to $\rho = N/L = 2\rho_0$ in the present case.

The starting position of the random walkers may be assumed to be either already visited or not yet visited. The calculation of persistence will depend on it. In what we call the spin picture (SP), they are unvisited and in the random walker picture (RWP) they are assumed to be visited already. This brings in a subtle difference in the two problems. We have discussed the two problems separately in the following two subsections.

A. The spin picture

First, we calculate the survival probability $S(t)$ defined as the probability that a site has not been visited by any of the random walkers till time t. (This corresponds to $P(t)$, the persistence probability of the original ANNNI model with $\rho \simeq 0.54$.)

In Fig. 2, $S(t)$ is plotted against time t for different densities ρ with a fixed lattice size $L = 10000$. In each case, $S(t)$ decays with time following a stretched exponential behavior $\exp(-\alpha t^{\beta})$ where $\beta = 0.50 \pm 0.02$. This value of β compares well with 0.45 obtained for $P(t)$ in the ANNNI model [3]. Increasing the system size does not affect the result, only the variation of $S(t)$ can be observed over a longer duration of time.

Interestingly, the value of α increases with the the increase of the density ρ till the value of $\rho \approx 0.55$. Beyond this value, α decreases gradually as the density increases roughly as $(1-\rho)$ (Fig. 3). The behaviour of α as a function of ρ will be discussed in greater detail in the next section.

The qualitative behaviour of α as a function of ρ is not difficult to explain. For small values of ρ, the probability that a domain wall is hit is small and therefore one gets a slow decay of $S(t)$ with time. On the other hand, for large values of ρ, most of the domain walls will be ‘locked’ such that again the variation of $S(t)$ will be slow.

For very small ρ, we have checked that

$$\alpha(1-\rho) = \sqrt{2}\alpha(\rho) \tag{4}$$

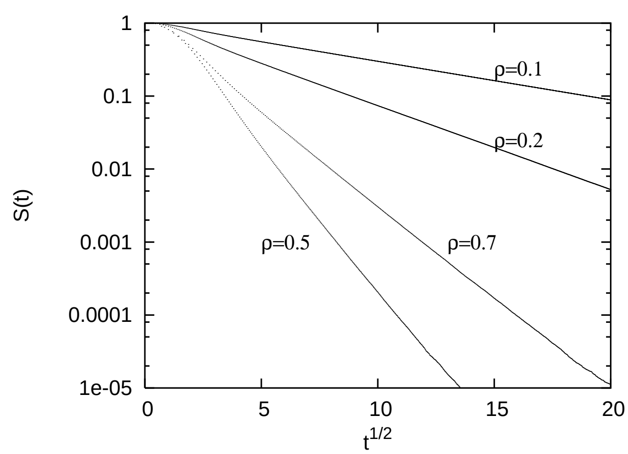

FIG. 2: (a) Survival probability $S(t)$ as a function of time t for different densities of walkers on a lattice of size 10000. Each curve follows a stretched exponential of the form $\exp(-\alpha t^{0.50})$.

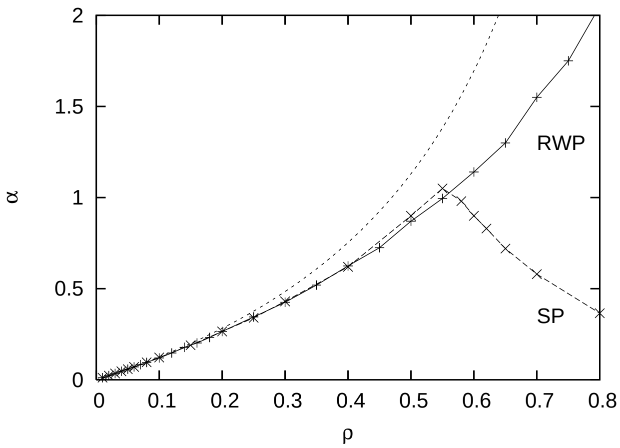

FIG. 3: Slope of the stretched exponential curve α is plotted against the density ρ for both the SP (spin picture) and RWP (random walkers picture) for the dynamical rule D_{ANN} (see section II). Both the curves follow a behaviour $1.13\rho/(1-\rho)$ for small ρ, shown by the dashed line.

holds good to a high degree of accuracy. Effectively this means that the relaxation rate at $\rho \to 1$ is twice as much as that at $\rho \to 0$. This can be explained in the following manner: At $\rho \to 1$, an empty site occurs with a probability $(1-\rho)$ but has both neighbours occupied with a very high probability, almost one. At $\rho \to 0$, an empty site having an occupied neighbour is very rare (probability proportional to ρ). In the former, in one iteration, the empty site can be visited by either of its neighbouring walkers while in the latter, visit to the empty site is possible by one walker only, making the time scale double.

One can now compare the value of α obtained in the present study with that of the ANNNI model where $\rho \simeq 0.27$. In [3], the value of α was found to be equal to 1.06. For $\rho = 2\rho_0 \simeq 0.54$, we find that α is very close to the value 1 (Fig. 3) showing again a good agreement with the ANNNI model dynamics.

B. The Random walker picture

In the RWP everything remains same but the initial sites occupied by the random walkers are assumed to be already visited. Now we find that $S(t)$ again has a stretched exponential behaviour : $S(t) \sim \exp(-\alpha_{RW} t^{\beta_{RW}})$ with $\beta_{RW} = 0.5 \pm 0.01$. Now α_{RW} does not show any non-monotonic behaviour but appears to diverge as $\rho \to 1$. This is again understandable, in the present picture, when ρ is close to one, most of the sites are already non-persistent to begin with and $S(t)$ decays very fast making $\alpha_{RW} \to \infty$.

The exponents β_{RW} and β are apparently equal in the two pictures. In Fig. 3 the behaviour of α_{RW} against ρ is also shown. It is to be noted that upto $\rho \approx 0.5$, α and α_{RW} are equal and behave differently beyond this point. For the SP, the possibility of the domains getting locked increase as ρ increases and this happens with a higher probability beyond $\rho = 0.5$.

III. MAPPING TO A SYSTEM OF NON-INTERACTING WALKERS

In the last section we obtained the result that the fraction of unvisited sites $S(t)$ in presence of mutually repulsive walkers has a stretched exponential decay with exponent 1/2 in both the SP and RWP. This behaviour turns out to be exactly the same as that of $S'(t)$, the number of unvisited sites in the presence of independent or non-interacting walkers. In the latter system it has been shown [18] that when ρ' is the density of independent walkers,

$$S'(t) \sim \exp(-\alpha'\rho'\sqrt{t}), \tag{5}$$

with $\alpha' = 2\sqrt{\frac{2}{\pi}}$.

In this section we show that the interacting system can be mapped to the independent walkers' system with the transformation $\rho' = \rho/(1-\rho)$. To show this, let us consider a configuration C of N interacting walkers of density ρ which follow a dynamics represented by D. For the present discussion, we make the dynamics D simpler than D_{ANN}: the walker will always execute a movement when at least one of the neighbouring site is vacant - if both are vacant, probability to move either to the left or to the right is 1/2. In case only one neighbouring site is occupied, the random walker will move to the empty neighbouring site. (One obtains the same behaviour of $S(t)$ with this rule, including the relation (4), only the numerical value of α increases by a factor of $\sqrt{2}$ compared to D_{ANN} where the time scale is simply double compared to D.)

For the independent walkers, let us consider a configuration C_0 of N walkers of density ρ', who do not "see" each other. The dynamics D_0 here is simply that each walker will move to left or right with equal probability. The world lines in the 1+1 dimension of the walkers are shown in Fig 4a and 4b.

Now let us create a mapping of the original configuration C to C' given by

$$x'_k(t) = x_k(t) - k, \tag{6}$$

where $x_k(t)$ is the position of the kth walker ($k = 1, 2, ...M$ from the left) at time t [19]. Effectively this mapping implies that one spacing between consecutive walkers is being removed. This would remove the constraint in C that two walkers have hard core repulsion and each world line of C' therefore also occurs in C_0. Although all world lines of C' and C_0 have one to one correspondence, in C' one has the constraint that $x_1 < x_2 < x_3..... < x_N$ while in C_0 there is no such constraint. Therefore a particular configuration may occur

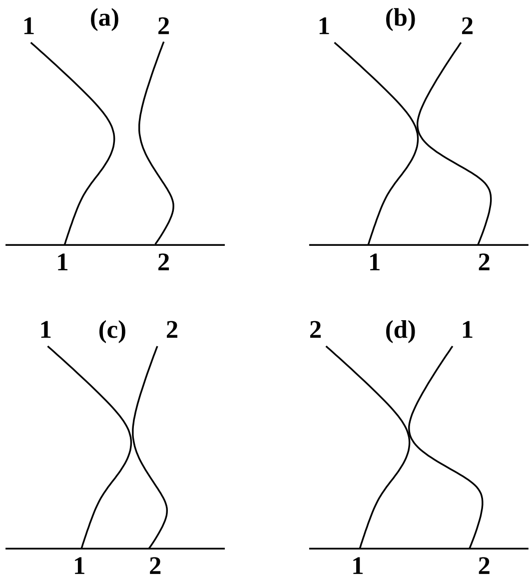

FIG. 4: Typical examples of (a) mutually repulsive walkers (C) and (b) Independent walkers (C_0). (c) The mapped configuration C' following eq. 6. In (d), another realisation for the independent walkers is possible by switching the order of the walkers at the later time. This is not allowed in C'.

with different weight factors in C_0 and C' (Figures 4b,c, and d).

Using the above mapping, the effective chain length in C' is $L-N$ and not L. Thus the density ρ in C is related to the density $\rho\prime$ in C' by the equation

$$\rho' = \frac{\rho}{1-\rho}. \tag{7}$$

Ignoring the weight factor, the mapping is effective in showing the correspondence between the interacting and independent walkers' picture. Exact correspondence will imply that α or α_{RW} (with D) would be equal to $\alpha'(\frac{\rho}{1-\rho})$, where $\alpha' = 2\sqrt{(2/\pi)}$, when dynamics D is used. This can happen if the dynamical rule D applied to C leads to states which when mapped to C' will correspond exactly to the states obtained by applying D_0 on C_0 (with the same weightage). We have verified that this is true for configurations in which either a walker is "alone" (both neighbours are empty) or has at most one walker in a neighbouring site. However, when three walkers occupy consecutive sites (a "three" state), the dynamics D gives rise to states which cannot be obtained from C_0 applying D_0 on it. Since the probability of having "three" states increases with ρ, we expect that the results for independent and interacting walkers will differ at higher ρ. For D_{ANN}, it is expected that α and α_{RW} values would be equal to $\frac{\alpha'}{\sqrt{2}}\rho/(1-\rho) = \frac{1.13\rho}{1-\rho}$ upto small ρ which is exactly what we observe (Fig. 3) (time scales for D_{ANN} being simply twice that of D).

Obviously a "three" state cannot be avoided if $\rho > 2/3$ and this gives an upper bound where the disagreement will occur. In reality, such states occur at values of ρ much below than this, even at about $\rho = 0.2$. We have verified that, if the three-states are forcibly ruled out in the simulation, the correspondence between the independent and interacting walkers remain valid upto $\rho \approx 0.4$.

We would like to comment in this section that while for the interacting walkers' system, α behaves differently in the SP and RWP, no such difference exists for the independent walkers' case. This is because there is no restriction on the movement of the walkers here even as the density becomes high.

A subtle point relevant to the mapping needs to be mentioned here. At small ρ the results for C and C_0 are equivalent indicating that the dynamical evolution of the walkers can be mapped to each other. It may still remain a question whether the persistence probability of C can be mapped to that of C'. The question arises as the N sites removed from the original system may either be persistent or non-persistent. On an average, however, the persistence of the two systems C and C' will be same. This is because the average number of persistent sites removed is $P(t)N$. Thus in the mapped system, persistence probabilty is again $(P(t)L - P(t)N)/(L-N) = P(t)$. This justifies the correspondence of persistence in C and C' and hence C_0. The issue of equivalence of persistence requires special mention as persistence is not related to other dynamical behaviour of a system in general.

IV. NON-MONOTONICITY OF α AND A FEW RELEVANT COMMENTS

The result for persistence probability in the spin picture and random walker picture differ in the interacting walkers' case as in the SP there is a non-monotonicity in α. This non-monotonic behaviour is clearly due to two features (a) presence of interacting walkers and (b) the dynamic quantity under consideration being persistence.

Point (a) is already discussed in the last section. Regarding point (b), it must be noted that the non-monotonicity appears when we assume that the initially occupied points are not visited, a fact which is relevant to persistence dynamics only. In this section we have discussed a few other dynamical phenomena in presence of interacting walkers. However, we find that none of these are accompanied by any non-monotonic behaviour of the relevant quantities appearing in them.

Two dynamic quantities σ_1 and σ_2 representing fluctuations can be defined in the following way: we tag a random walker and calculate the fluctuation of its position $x(t)$ at time t with respect to its initial position $x(0)$ and study its behavior with time (Fig. 5).

Precisely, σ_1 is defined as

$$\sigma_1(t) = \sqrt{\langle (x(t) - x(0))^2 \rangle}. \tag{8}$$

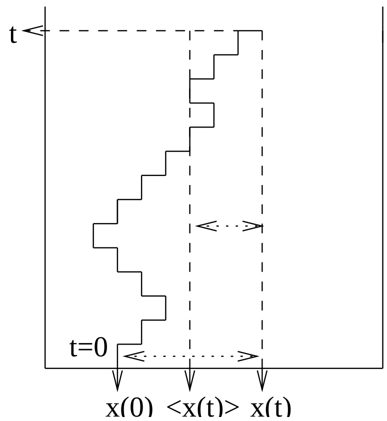

FIG. 5: The movement of a tagged domain wall along time (vertical axis): $x(0)$ is its initial position, $x(t)$ its position at time t and $\langle x(t)\rangle$, the mean position averaged up to time t.

In the second measure, we notice that the path of a walker can be viewed as an interface (with no overhangs) in 1 + 1 dimensions (Fig 5). One can then measure the interface width at any time given by

$$\sigma_2(t) = \sqrt{(\langle x^2(t)\rangle - \langle x(t)\rangle^2)}. \tag{9}$$

where $\langle x(t)\rangle$ is the mean value of the position x at time t. It is known that for a single walker (i.e., $\rho = 0$ in the thermodynamic limit) $\sigma_1(t) = At^\theta$ with $\theta = 0.5$. Here, we find $\sigma_1(t) = t^\theta$ with $\theta \simeq 0.25$ at long times for all values of ρ. This is in agreement with [20] where the result $\theta = 0.25$ has been derived exactly. In the present system, ρ has a finite value and for the smallest value of ρ shown in Fig. 6, a crossover effect is noted, i.e., the behavior at earlier time appears to be consistent with $t^{0.5}$. This is because at small ρ, the walker continues as a free walker for a considerable period of time and exhibits the corresponding behaviour.

The behavior of $\sigma_1(t)$ with time t has been studied for values of ρ even smaller than 0.1 in smaller lattices and it appears that for any finite ρ, however small, $\theta \simeq 0.25$ is valid at longer times always. We conclude that there is a transition point at $\rho = 0$ for any $\rho \neq 0$, the random walker exponent is $\simeq 0.25$ while for $\rho = 0$, it is 0.5. The results for σ_2 are consistent with the above observations. Both σ_1, $\sigma_2 = At^\theta$ with $\theta = 0.25$ independent of ρ (for $\rho \neq 0$), while A depends on ρ. In Fig. 7, we plot $A(\rho)$ against ρ for both σ_1 and σ_2. $A(\rho)$ decereases monotonically with ρ and follows a rough exponential decrease as $A(\rho) \simeq \exp(-2\rho)$ except for values very close to 1, where one can expect anomalous behavior.

We investigate the behavior of another quantity $D(t)$, which we define as the fluctuation of the distance $d(t)$ between two neighbouring walkers at time t with respect to its initial value $d(0)$. Precisely,

$$D(t) = \sqrt{\langle (d(t) - d(0))^2\rangle}. \tag{10}$$

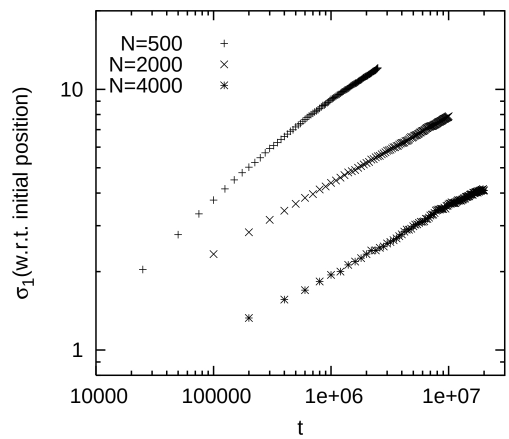

FIG. 6: Fluctuation σ_1 of the position of a walker w.r.t. its initial position as a function of time t for different no. of walkers on a lattice of size 5000. The best fit curves have a slope $\simeq 0.25$ for the higher densities.

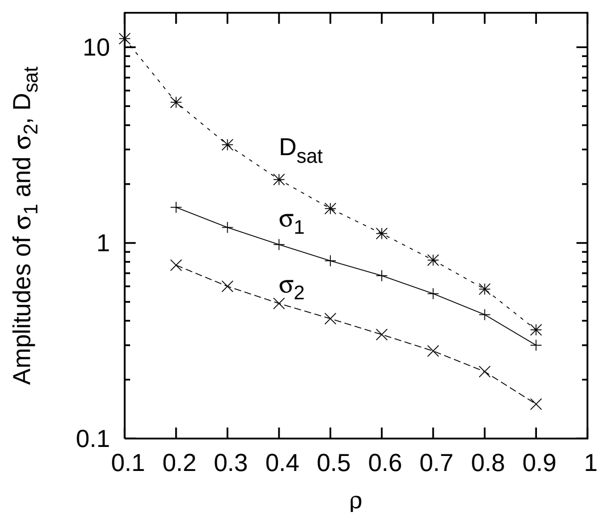

FIG. 7: Amplitudes (A) of σ_1,σ_2($= At^\theta$) and D_{sat} as function of ρ. The dashed lines are guides to the eye.

$D(t)$ shows an initial increase with t and reaches a time independent equilibrium value D_{sat} at larger times. This equilibrium value D_{sat} (calculated from the mean value of the last 100 Monte Carlo steps), when plotted against ρ, again shows a monotonic decay with ρ (Fig. 7). Hence, in contrast to the factor α appearing in the persistence dynamics, we do not find non-monotonic behavior in the factors appearing in the other dynamical features.

V. SUMMARY AND CONCLUSIONS

In summary, we have considered the dynamics of N mutually avoiding random walkers on a one dimensional chain of length L which simulates the quenching dynamics in the ANNNI model for a particular value of $\rho \simeq 0.54$. For this value of ρ, we verify that the survival probability $S(t)$ which corresponds to the persistence probability in the ANNNI model follows a stretched exponential behavior consistent with the ANNNI model dynamics. We also observe very good quantitative agreement for the exponent β and slope α. On generalising the value of ρ, we find that the behavior $S(t) \sim \exp(-\alpha t^{\beta})$ is valid for all ρ with β showing a universal value of $0.50 \pm .02$.

Observing that the time dependence in $S(t)$ is identical to that in $S'(t)$ (the corresponding quantity in presence of non-interacting walkers) for all ρ, we have shown that a mapping between the two indeed exist which remains exact for small ρ as far as the behaviour of α is concerned.

We have considered two different pictures while computing the persistence probability; in the spin (random walker) picture the sites initially occupied by the walkers are assumed to be not visited (visited) and the behaviour of α as a function of ρ is sensitive to this difference. In the SP, it has a non-monotonic behaviour. Such non-monotonic behaviour emerges in the case of interacting walkers only. However, when other dynamical phenomena in presence of interacting walkers are studied, no such non-monotonic behaviour is found. Thus we find that the persistence dynamics in a system with a finite density of mutually avoiding random walkers calculated in terms of the fraction of sites unvisited till time t, shows a unique behavior compared to other dynamical quantities. This again supports the fact that persistence is a phenomenon which cannot be directly connected to other dynamical features of a system.

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