

Time evolution of a single spin inhomogeneously coupled to an interacting spin environment

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(Received 22 December 2005; accepted 13 March 2006; published online 14 April 2006)

We study the time evolution of a single spin coupled by exchange interaction to an environment of interacting spin bath modeled by the XY Hamiltonian. By evaluating the spin correlator of the single spin, we observed that the decay rate of the spin oscillations strongly depends on the relative magnitude of the exchange coupling between the single spin and its nearest neighbor J' and coupling among the spins in the environment J . The decoherence time varies significantly based on the relative coupling magnitudes of J and J' . The decay rate law has a Gaussian profile when the two exchange couplings are of the same order $J' \sim J$ but converts to exponential and then a power law as we move to the regimes of $J' > J$ and $J' < J$. We also show that the spin oscillations propagate from the single spin to the environmental spins with a certain speed. The effect of varying the anisotropic parameter, external magnetic field, and temperature on the decaying rate of the spin state is also discussed. © 2006 American Institute of Physics. [DOI: 10.1063/1.2192778]

I. INTRODUCTION

As classical computers are approaching their limits in terms of size and capabilities soon, there has been increasing demand on developing new powerful computing systems that would fulfill the expected gap. This demand leads to the birth of the new paradigm of quantum computing and quantum information processing.^{1–4} Different experimental systems have been proposed over the last few years as reliable candidates for implementing quantum computing algorithms.^{5–12}

In particular, there has been a special interest in solid state systems as they facilitate the fabrication of large integrated networks that would be able to implement realistic quantum computing algorithms on a large scale. On the other hand, the strong coupling between a solid state system and its complex environment makes it a significantly challenging mission to achieve the high coherence control required to manipulate the system. Decoherence is considered as one of the main obstacles toward realizing an effective quantum computing system.^{13–16} The main effect of decoherence is to randomize the relative phases of the possible states of the isolated system as a result of coupling to the environment. By randomizing the relative phases, the system loses all quantum interference effects and may end up behaving classically.

In recent years, there has been an increasing focus on the spin dynamics of electrons in semiconductor structures as a

result of the shift in interest from the charge degree of freedom of the electron to the spin one, which led to the new emerging field of spintronics (spin-based electronics).¹⁷ Adding the spin degree of freedom to conventional charge-based systems or even replacing it entirely results in significant advantages. In quantum information and quantum computing fields there have been proposals for using the electron spin S itself as the qubit (the basic unit of quantum information in the quantum computer) or as an intrinsic components of qubit gates specially in semiconductor quantum dots.^{18,19} This is in contrast to previous proposals based on the charge (orbital) degrees of freedom for constructing the qubit,²⁰ which has much shorter decoherence time (nanoseconds) compared to the spin one (microseconds). As a system of special interest, there has been great efforts to study the mechanism of electron phase decoherence and determine the time scale for such process (the decoherence time) in solid state quantum dots both theoretically^{21–24} and experimentally.^{25–29} The main source of electron spin decoherence in a quantum dot is the inhomogeneous hyperfine coupling between the electron spin and the nuclear spins. The interaction has a Gaussian decay profile over the quantum dot. The mutual interaction among the nuclear spins, due to direct dipole interaction, is ignored in most of theoretical works because it is orders of magnitude weaker than the hyperfine one and because of the complexity that it may add to the problem.³⁰ In fact, the exponential size of the Hilbert space in such solid state systems and the different types of possible decoherence channels make it eventually impossible to have an exact analysis of the decoherence mechanism or to obtain an estimate for the relaxation time taking these

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effects into account. Therefore it becomes a necessity to impose different approximations in order to tackle the problem.

The longitudinal T_1 and transverse T_2 relaxation times are very important quantities in NMR experiments.^{31,32} T_1 is considered as the characteristic time for recovery of the magnetization along the static field to its thermal equilibrium value. Modeling the revolution of spin in the magnetic field direction will help us understand this process and provide us insight to increase the relaxation time. Motivated by these developments and facts, in this paper we investigate the dynamics of a single spin S that is coupled inhomogeneously to an interacting environment of spin bath. The single spin, which is considered as the quantum system of interest, is centered in a one-dimensional spin chain. It is coupled to its nearest neighbor spins through exchange interaction while its nearest neighbors are in turn coupled to their nearest neighbors through exchange interaction as well and so on. We made the relative magnitudes of the coupling of the single spin to its nearest neighbors and the coupling among the other spins (constituting the environment) a varying parameter. In addition, we consider anisotropic coupling and study the time evolution of the centered spin at different strengths of that anisotropy. The composite system (single spin and the environment) is coupled to a transverse external magnetic field. The centered single spin can be considered as directly coupled to its nearest neighbors but indirectly to all other spins in the environment, through its nearest neighbors, in a way that the coupling is weakened as it propagates along the chain. Though this investigation is of fundamental interest in its own right, it also bears strong resemblance to and can give good insight about real systems of interest such as the single electron spin coupled to nuclei in a quantum dot³³ and other localized impurities in host materials, for instance, an electron bounded to a phosphorous atom inserted as an impurity into a silicon matrix³⁴ or Si in a GaAs or Ge matrix.

In our results, we observe a decay in the centered single spin state, represented by a spin correlator, as a function of time. The spin exhibits an oscillatory motion with an overall decaying behavior. An interesting observation is that the decay rate of the spin oscillations strongly depends on the relative magnitude of the exchange coupling between the single spin and its nearest neighbors and the coupling among the spins in the environment. It is largest when the two exchange couplings are of the same order while it decreases when either of them is larger than the other. We also observe that the decay rate law shows different profiles in different regimes of relative coupling magnitudes. This means that the decoherence time varies significantly based on the relative coupling magnitudes. By comparing to the spin oscillation of environmental spin without introducing single spin, we found the spin coherence propagates from the single spin to the environmental spin with certain speed. Also the anisotropic parameter plays an important role in the decaying rate of the spin state, where steeper decaying rate is obtained as the strength of anisotropy is reduced reaching maximum value for complete isotropic coupling.

This paper is organized as follows. In Sec. II we briefly describe the details of our model and the calculations of the spin correlator. In Sec. III we present our numerical results

stressing on the role that the different parameters of the problem play in determining the spin decay rate. We close with our conclusions in Sec. IV.

II. MODEL AND CALCULATIONS

In this section, we briefly present our model and the numerical calculations. We consider a single spin centered in a one-dimensional XY type spin chain in an external transverse magnetic field. The Hamiltonian for such system is given by^{35,36}

$$H = -\frac{1+\gamma}{2} \sum_{i=1}^N J_{i,i+1} \sigma_i^x \sigma_{i+1}^x - \frac{1-\gamma}{2} \sum_{i=1}^N J_{i,i+1} \sigma_i^y \sigma_{i+1}^y - \sum_{i=1}^N h_i \sigma_i^z, \quad (1)$$

where $J_{i,i+1}$ is the exchange interaction between sites i and $i+1$, h_i is the strength of the external magnetic field on site i , σ^a are the Pauli matrices ($a=x,y,z$), γ is the degree of anisotropy, and N is the number of sites.

We consider the centered spin on the l_{th} site as the single spin quantum system and the rest of the chain as its environment, where in this case $l=(N+1)/2$. The single spin directly interacts with its nearest neighbor spins through exchange interaction $J_{l-1,l}=J_{l,l+1}=J'$.

We assume that exchange interactions between spins in the environment are uniform, and simply set it as $J=1$. The centered spin is considered as inhomogeneously coupled to all the spins in the environment by being directly coupled to its nearest neighbors and indirectly to all other spins in the chain through its nearest neighbors. The coupling is weakened as it propagates through the chain. We assume periodic boundary conditions, so that

$$\sigma_{N+1}^x = \sigma_1^x, \quad \sigma_{N+1}^y = \sigma_1^y, \quad \sigma_{N+1}^z = \sigma_1^z. \quad (2)$$

We apply the standard procedures to solve the Hamiltonian [Eq. (1)] by transforming the spin operators into fermionic operators.^{36,37} We first perform the transformation

$$a_i^+ = \frac{1}{2}(\sigma_i^x + i\sigma_i^y), \quad a_i^- = \frac{1}{2}(\sigma_i^x - i\sigma_i^y). \quad (3)$$

Then, we introduce Fermi operators c_i , and c_i^+ , defined by

$$a_i^- = \exp\left(-\pi i \sum_{j=1}^{i-1} c_j^+ c_j\right) c_i, \quad a_i^+ = c_i^+ \exp\left(\pi i \sum_{j=1}^{i-1} c_j^+ c_j\right), \quad (4)$$

so that the Hamiltonian assumes the following form:

$$H = -\sum_{i=1}^N J_{i,i+1} [(c_i^+ c_{i+1} + \gamma c_i^+ c_{i+1}^+) + \text{H.c.}] - 2 \sum_{i=1}^N h_i \left(c_i^+ c_i - \frac{1}{2} \right). \quad (5)$$

This Hamiltonian has the form

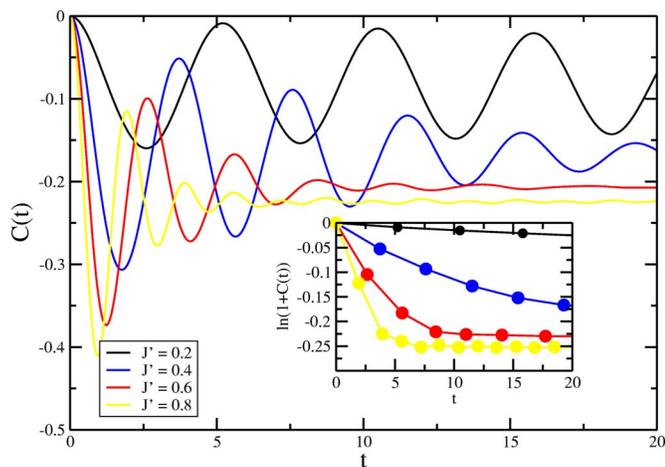


FIG. 1. The spin correlation function $C(t)$ of centered spin for $N=501$, $h=0.5$, and $\gamma=1.0$ versus time t for different values of the coupling $J' \leq J$ at zero temperature. The decay profile for each case is shown in the inner panel.

of time since it is proportional to $\langle \hat{S}_z(t) - \hat{S}_z(0) \rangle$. To investigate the decay law of the single spin and have an estimate for the relaxation time scale we study $\ln(1+C(t))$ as a function of time as well.

III. RESULTS AND DISCUSSIONS

The Ising system, corresponding to $\gamma=1$ in our Hamiltonian, is known to undergo a quantum phase transition at $\lambda_c = J/2h = 1$.^{38,39} The magnetization $\langle \sigma^x \rangle$ is different from zero for $\lambda > 1$ and it vanishes at the transition. However, the magnetization $\langle \sigma^z \rangle$ is different from zero for any value of λ . At the quantum phase transition the correlation length diverges as $\xi \sim |\lambda - \lambda_c|^{-1}$. When $\lambda \rightarrow 0$, the ground state becomes a product of spins pointing in the positive z direction. However, in the limit $\lambda \rightarrow \infty$, the ground state becomes again a product of spins pointing in the positive x direction. In both limits the ground state approaches a product state, thus the entanglement vanishes. When $\lambda = 1$, a fundamental transition in the form of the ground state occurs and the system develops a nonzero magnetization $\langle \sigma^x \rangle \neq 0$ which grows as λ is increased. The calculations of entanglement show that it rises from zero in the two limits $\lambda \rightarrow 0$ and $\lambda \rightarrow \infty$ to a maximum value near the critical point $\lambda_c = 1$. On the other hand, the centered spin in the quantum dot or NMR experiment directly interacted with the nuclear spins through hyperfine interactions. Though compared to external magnetic field, this interaction is weak, it has a large impact on the dephasing of the consider spin due to the large amounts of nuclei exist around the spin. In our model we include this effect by setting the value of coupling constant of centered spin and environmental spins close to the external magnetic field. In order to investigate the decay of the centered spin under the effect of the environment while at the critical point, we set the external magnetic field $h=0.5$ with $J=1.0$ in most of our calculations except when otherwise is stated.

We first study the dynamics of the centered spin while weakly coupled ($J' < 1$) with the environment within a short time period. In Fig. 1 we show $C(t)$ as a function of time

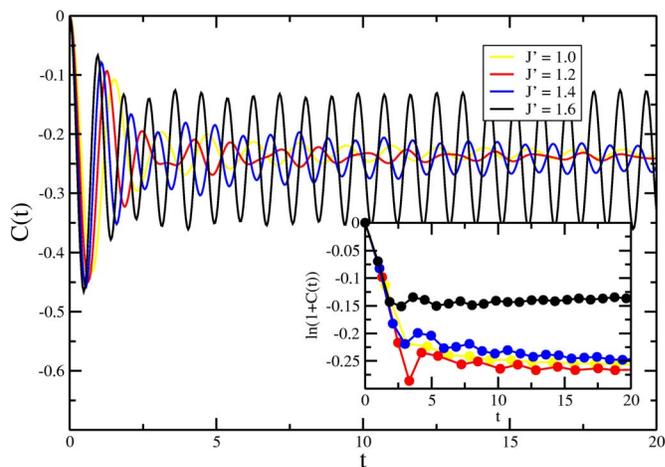


FIG. 2. The spin correlation function $C(t)$ of centered spin for $N=501$, $h=0.5$, and $\gamma=1.0$ vs time t for different values of the coupling $J' \geq J$ at zero temperature. The decay profile for each case is shown in the inner panel.

with different coupling constant values $J' < 1$ at zero temperature ($\beta \rightarrow \infty$). As expected, $C(t)$ maintains the value zero when $J' = 0$ since the centered spin stays in its initial state with no coupling to environment. When the interaction between the centered spin and its environment is turned on, for $t > 0$, it starts to exhibit an oscillatory motion. For instance, at $J' = 0.2$, the spin maintains its oscillation behavior for a long time until it reaches the saturation value $C_s = -0.08$.

Increasing the coupling between the centered spin and the environment, but keeping J' less than J , we find that the spin oscillates with smaller amplitude and higher frequency. But the decay rate becomes much steeper reaching a saturation state very rapidly. It is remarkable that the larger the coupling between the spin and its environment, the greater the magnitude of the saturation value C_s is, the more decoherence taking place in the spin state. Which means that more entanglement between the system and its environment leads to more decoherence introduced into the system as expected.

In order to figure out the decay law that the system obeys at different values of J' , we selectively pick up the points that make up the envelope of $C(t)$ and use them to plot $\ln(1.0+C(t))$ as a function of time in the inner panel. Interestingly, we find the decay rate obeys different laws depending on the value of the coupling constant J' (relative to J). So, when J' is small (0.2) the decay law is a power law and as J' gets larger (0.6 for instance) it becomes an exponential decay law. Finally, when J' is close to one, i.e., the coupling between the centered spin and the environment is of same order as the coupling between the spins in the environment, the decay law has a Gaussian decay profile. In fact, this variation in the decay behavior is expected, because the strength of interaction between the centered spin and its environment decides how fast the spin gets entangled to the environment and loses its identity. Therefore it should be expected that the centered single spin suffers more rapid decay with an increasing coupling constant value.

In Fig. 2 we show the decay behavior of the centered spin in the strong interaction regime ($J' > J$) at zero temperature. We observe that for $J' \sim J$ the decay behavior is still

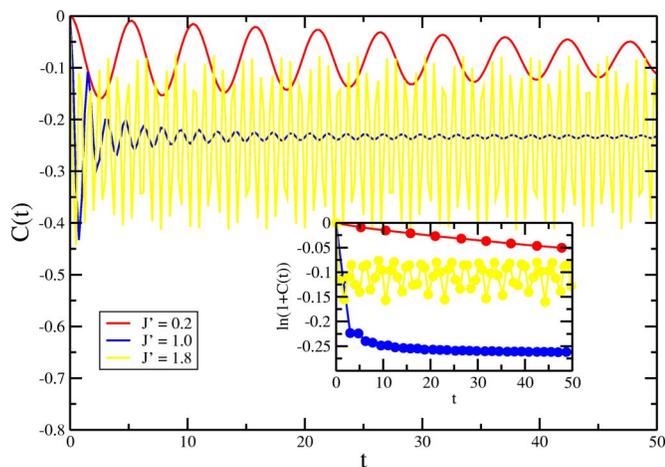


FIG. 3. The spin correlation function $C(t)$ vs time t for different values of the coupling $J' < J$ (red), $J' \approx J$ (blue), and $J' > J$ (yellow) with $N=501$, $h=0.5$, and $\gamma=1.0$.

Gaussian but as we increase J' it converts to an exponential and then to a power law. For larger values of J' the oscillations persist for a very long time and its amplitude and frequency get larger and they decay much slower. Remarkably the spin oscillates about the same average value for this large J' values. The decaying profile collapses into one line when $J' > 1.6$, which suggests for this region that the decoherence time is not significantly affected by the magnitude of interaction between the centered spin and the environment. This is because the coupling between spins in the environment is weaker compared to the coupling between the centered spin and its nearest neighbor, which leads to stronger entanglement between the spins in the environment compared to the entanglement between centered spin and its nearest neighbors. So that the centered spin will lose its identity quickly through its nearest neighbors to the environment, the coupling between spins in the environment decides the decay rate of centered spin. However, when we decrease the entanglement between the centered spin and its nearest neighbors by further increasing the J' value, the decay rate of the centered spin becomes smaller.

To compare the decay rates in the two different regimes of weak and strong couplings, we plot $C(t)$ versus time for $J' < J$, $J' \approx J$, and $J' > J$ at zero temperature in Fig. 3. As it has been observed in the previous figures the decay rate behaves differently in each region. For $J' < J$ the spin decays with a slow power law for $J'=0.2$. When J' is close to J , the decay is Gaussian (or exponential depending on the value of J'). For the region $J' > J$ it oscillates with higher frequency and the envelope of $C(t)$ decays slowly according to a power law and maintains the oscillations for a long time.

In Fig. 4, we study the propagation of spin coherence at zero temperature in the spin chain. The red lines represent $C(t)$ versus time for $J'=1.5$, and black lines for $J'=J$. The different dynamic behaviors of the centered spin can be seen in the top left panel. The centered spin starts oscillating shortly after $J'=1.5$ is applied. In the top right panel we plot the $C(t)$ as the function of time for site which is link with center spin with extra four environmental spins in the middle. When $t < 10$, the red line and black line collapsing

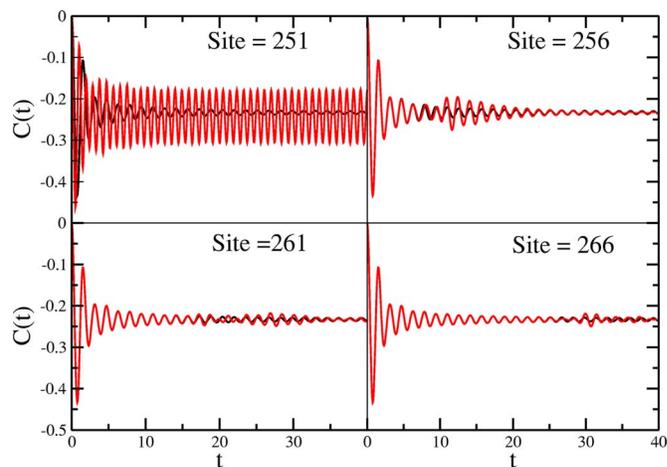


FIG. 4. The spin correlation function $C(t)$ vs time t with $J'=1.0$ (black) and $J'=1.5$ (red) for the centered spin (upper left) and the spin at site 256 (upper right), 261 (lower left), and 266 (lower right) in the environment. $N=501$, $h=0.5$, and $\gamma=1.0$.

into same line show that the environmental spin does not feel the existence of center spin at this moment. When t closes to 10, we start to see the spin correlation function of $J'=1.5$ vibrates away from $J'=1.0$, which indicates the environmental spin at site 256 start to be disturbed by the centered spin at this moment. In the bottom left panel, the correlators' curve becomes different when t is around 20 for the spin 9 sites away from the centered spin, and they show different when t is near 30 for environment spin 14 away from the centered spin. This evidence shows that the spin coherence propagates from the centered spin to the environment with certain speed.

We show the spin correlation function as a function of time with different temperatures for the weaker coupling between the centered spin and environment in Fig. 5. We find that the temperature does not lead to a significant change in the decay rate, but the saturated decoherence increases as temperature increases, when external magnetic field h is small. For the larger value of h , the spin correlation functions

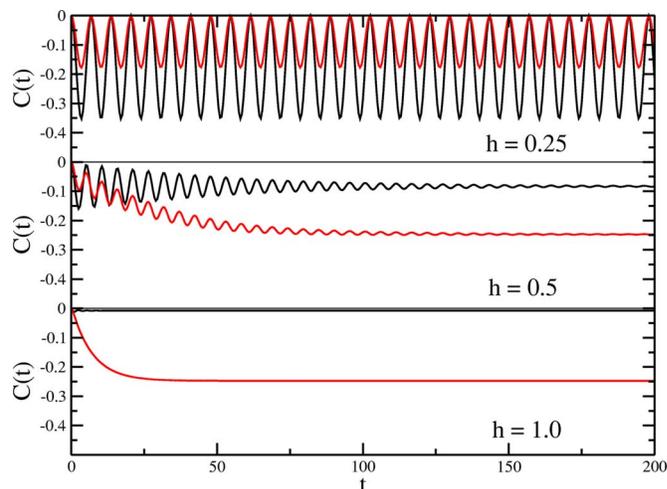


FIG. 5. The spin correlation function $C(t)$ of the centered spin vs time t for $N=501$, $J=1.0$, $J'=0.2$, and $\gamma=1.0$ at different temperatures $\beta \rightarrow \infty$ (black lines) and $\beta=0.1$ (red lines) with external magnetic field $h=0.25$, $h=0.5$, and $h=1.0$.

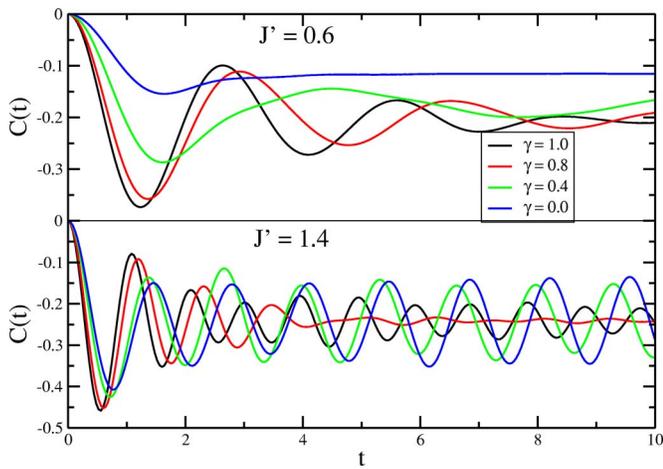


FIG. 6. The spin correlation function $C(t)$ of the centered spin vs time t with $N=501$, $h=0.5$, and $\gamma=1.0$ for different anisotropic parameter γ values at zero temperature. $J'=0.6$ for the upper panel and $J'=1.4$ for the lower panel.

drop significantly when we increase the temperature, and the decay rate of the centered spin changes from the power law to the exponential law. We also observe that the temperature has slightly impact on the decay rate and saturated decoherence of the centered spin when the coupling between the centered spin and its nearest neighbor becomes larger because the entanglement between the centered spin and neighbor becomes smaller.

In Fig. 6, we show the spin decay at different degrees of anisotropy in both the weak and strong coupling regimes, where for $\gamma=1.0$ the coupling becomes an Ising one while for $\gamma=0$ becomes of XY type. Interestingly, weak and strong interactions show different behaviors. We find the oscillations decrease when we decrease γ from 1 to 0 in the weak interaction case, and less amount of saturated decoherence is induced to the spin state for full isotropic case. Particularly, $C(t)$ decays from 0 and reaches saturated decoherence value shortly around $t=3$ in the XY model (full isotropy). Nevertheless, in the strong coupling case, while the degree of anisotropy has no effect on the saturated decoherence level, it leads to a peculiar effect on the amplitude of oscillations. The amplitude reduces as anisotropy increases reaching minimum value at $\gamma=0.8$ then it starts to raise up again for higher γ .

The size effect on the spin entanglement has been reported in our previous work.⁴⁰ In Fig. 7, we show how the size also has an influence on the spin dynamics. As we can see, at $N=201$, the oscillations starts at $t>0$, and reaches a saturated value when $t>30$. We observe them starting again at the critical time $t_c=200$. Afterwards, the oscillations never reaches the saturation value again. But by increasing the size N of the environment, we find the critical time increases linearly. As $N \rightarrow \infty$, $t_c \rightarrow \infty$. This indicates that the system will stay in a saturated decoherence state as t goes to infinity for a large enough environment. However, the oscillation of the consider spin after a specific time t_c is not caused by the propagation of the observed spin coherence. As we can see the propagation of decoherences decreases quickly when the distance from considered spin becomes large. Moreover, the

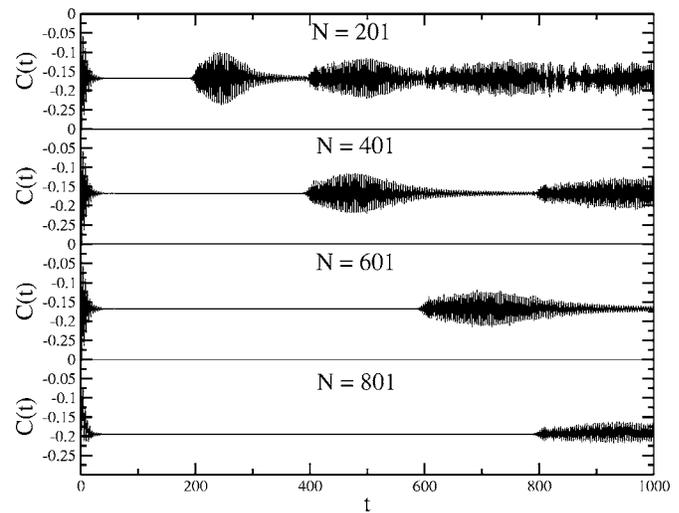


FIG. 7. The spin correlation function $C(t)$ of the centered spin vs time t with $J'=0.4$, $h=0.5$ and $\gamma=1.0$ for different number of spins N in the environment at zero temperature.

propagation speed of spin coherence from the impurity is too slow to interfere with the considered spin at the time when spin oscillations start.

In order to see the external magnetic field h effect we plot the spin correlation function with different h in the Fig. 8. As we can see when $\lambda=J/2h$ is much smaller than the critical point of phase transition $\lambda_c=1$, the spin correlation function starts oscillations with large magnitude and decays very slowly to reach the saturated decoherence due to the lower entanglement between spins. However, the spin correlation function decays to larger saturated decoherence rapidly when λ is close to critical point since the entanglement reaches maximum in this region. Further increasing the λ where the entanglement between spins vanishes, the spin correlation functions decay very slowly as we expected.

IV. CONCLUSIONS

In summary we have studied the time evolution of a single spin inhomogeneously coupled to an interacting spin

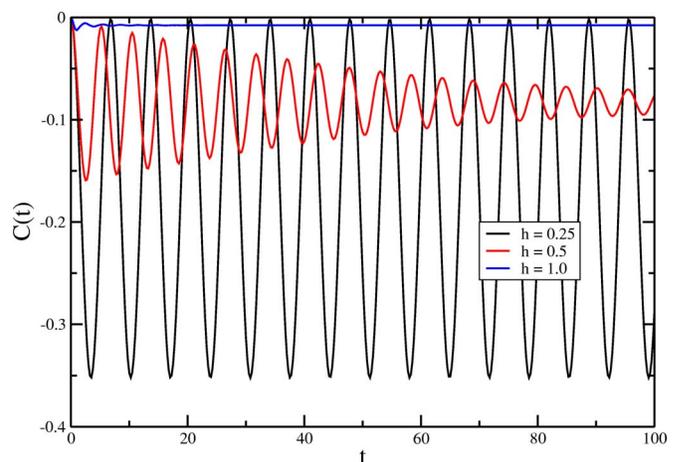


FIG. 8. The spin correlation function $C(t)$ of the centered spin vs time t with $N=501$, $\gamma=1.0$ $J=1.0$, and $J'=0.2$ for different external magnetic field h at zero temperature.

environment. Our main observation is that the relative magnitude of the coupling between the single spin and its environment to the coupling between the spins within the environment plays a significant role in determining the dynamics of the single spin and its decay rate. While for a small value of this relative magnitude the decay rate follows a power law it converts to an exponential and then Gaussian as it approaches unity. For greater relative magnitude corresponding to stronger coupling between the single spin and the environment compared to that among the spins within the environment the decay rate reduces again approaching slow power law as the relative magnitude becomes significantly higher than unity. Also the amount of saturated decoherence induced into the spin state depends on this relative magnitude and approaches maximum value for a relative magnitude of unity. Our results suggest that setting the interaction within the environment in such a way that its magnitude is much higher or lower than the interaction with the single spin may reduce the decay rate of the spin state. The reason behind this phenomenon could be that the variation in the coupling strength along the chain at one point (where the single spin exits) blocks the propagation of decoherence along the chain by reducing the entanglement among the spins within the environment which reduces its decoherence effect on the single spin in return. This result might be applicable in general to similar cases of a centered quantum system coupled inhomogeneously to an interacting environment with large degrees of freedom.

ACKNOWLEDGMENTS

This work has been supported in part by the Purdue Research Foundation. One of the authors (S.K.) thanks the John Simon Guggenheim Memorial Foundation for financial support.

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