Critical properties of gapped spin-$\frac{1}{2}$ chains and ladders in a magnetic field

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(Received 25 October 1996)

An interesting feature of spin-$\frac{1}{2}$ chains with a gap is that they undergo a commensurate-incommensurate transition in the presence of an external magnetic field H. The system is in a gapless incommensurate regime for all values of the magnetic field between the lower critical field H_{c1} and an upper critical field H_{c2}, where it is gapless and has power-law correlations. We calculate the critical exponents for such a generic gapped system in the incommensurate regime at the critical field H_{c1} and in its vicinity. Our analysis also applies to the spin-$\frac{1}{2}$ ladder. We compute the full dynamical susceptibilities at finite temperature. We use the same to discuss the thermal broadening of various modes and obtain the low-temperature behavior of the nuclear spin relaxation rate T_1^{-1}. We discuss the results obtained here for the special cases of the dimerized chain, frustrated chain, and the spin-$\frac{1}{2}$ ladder. [S0163-1829(97)05509-4]

I. INTRODUCTION

Quantum spin chains have been a field of intense theoretical activity for the past decade.[1] This seems pertinent in the face of the tremendous advance made in the fabrication of quasi-one-dimensional (1D) systems. There are a lot of compounds like $(TMTTF)_2X$ which are essentially spin-$\frac{1}{2}$ chains, NENP—a spin-1 chain,[2] and a host of other organic compounds whose behaviors can be adequately described within the framework of interacting spin systems.[3] The Heisenberg model with purely nearest-neighbor interactions has been instrumental in understanding various properties of these spin systems.[4] In addition to these, there are compounds with alternation in the nearest-neighbor bonds (arises as a result of interactions with phonons), e.g., TMTTF, strong single-ion anisotropies, etc. The effects of spin-Peierls dimerization, interchain interactions, and competing nearest-neighbor interactions have been reasonably well understood in the spin-$\frac{1}{2}$ case.[5] These are known to drive phase transitions in the pure spin-$\frac{1}{2}$ model. The basic issue addressed is whether there exists a gap above the singlet ground state to the first excited state which is a triplet. Apart from these, the ground state could also exhibit crossovers from short-range Néel order to spiral order or spontaneously dimerize[6] but these are not signals of any kind of quantum phase transitions.

More interesting phases can be obtained by placing these gapped systems in a magnetic field. For some critical value of the field H_{c1}, the system undergoes a continuous phase transition from a commensurate Néel (C) zero uniform magnetization phase to an incommensurate phase (IC) with nonzero magnetization. As the magnetic field is increased, the magnetization increases and saturates at some critical H_{c2} where the ground state is fully ferromagnetic but differs from the XXX ferromagnet in that it has a finite gap to the first excited state. The intermediate region (between H_{c1} and H_{c2}) is completely gapless and the pitch vector Q (the value of the momenta at which the static structure factor shows a peak) decreases continuously from $Q=\pi$ at H_{c1} to $Q=0$ at H_{c2}. Evidence for such transitions were seen in the spin-$\frac{1}{2}$ ladder compound $Cu_2(C_5H_{12}N_2)_2Cl_4$ (Ref. 7) and the quasi-one-dimensional spin-$\frac{1}{2}$ systems TTF-CuBDT.[8] The C-IC transition seen in $CuGeO_3$ (Refs. 9–11) can be understood in a similar manner if it is treated as a spin chain with spin-Peierls interactions alone. However, because of the presence of strong phonon interactions in $CuGeO_3$, various complications can arise, in particular, the transition becomes first order.

In this paper, we are concerned with the properties of a generic gapped spin-$\frac{1}{2}$ system in the presence of an external magnetic field. Though the naive expectation is that all gapped systems might exhibit similar behaviors in the presence of the field, we find that they have very different properties depending on the nature of the interaction which creates the gap. In particular we focus on experimentally measurable quantities like the total magnetization, NMR relaxation rates, and neutron scattering intensities. To do this we calculate various spin-spin dynamic correlation functions in the gapless region between H_{c1} and H_{c2}. We calculate various exponents in the IC regime close to H_{c1} and use these to calculate the temperature dependence of the NMR rates (T_1). We also discuss in detail the consequences of our results for the dimerized, frustrated, and ladder systems. We find that though magnetization measurements will not help differentiate between these systems, neutron scattering and NMR can. Since the models studied in this paper directly describe the compounds mentioned above, the results obtained here are of immediate relevance to experiments.

The paper is organized as follows. Section II contains a very brief review of spin-$\frac{1}{2}$ chains and the technique of bosonization used in this paper. In Sec. III, we introduce our Hamiltonian for a generic gapped spin-$\frac{1}{2}$ chain and discuss the effects of the applied magnetic field and the consequences of incommensurability induced by the magnetic field. We present in Sec. IV our results for the dynamic correlations and the values of the exponents near the transition at H_{c1} for a generic gapped spin-$\frac{1}{2}$ chain. We also discuss the generic phase diagram as a function of magnetic field and temperature. The spin ladder is treated separately in Sec. V. In Sec. VI, we calculate the temperature dependence of the NMR rate T_1^{-1} and discuss the behavior of the same for the cases of the dimerized, frustrated, and ladder models. Section VII contains the concluding remarks.

II. INTRODUCTION TO SPIN-$\frac{1}{2}$ SYSTEMS

Here we present a brief introduction to the physics of spin-$\frac{1}{2}$ chains and summarize certain results relevant to the work presented here. The main Hamiltonian of interest is the Heisenberg model:

$$\mathcal{H}=J\sum_i \vec{S}_i\cdot\vec{S}_{i+1} \tag{1}$$

where the $\vec{S}_i$ is a localized spin $\frac{1}{2}$ operator. We set $J=1$ in the rest of the calculation. This model is Bethe ansatz soluble and is known to be gapless. A lot is known about the static and dynamic properties of this system. Even though there are various methods used to study spin-$\frac{1}{2}$ chains, in this paper we use the machinery of bosonization since this enables us to deduce various properties in a relatively easy manner. Since this is an oft used method we sketch the details briefly. We first use the Jordan-Wigner transformation[1,5] which essentially maps the spin problem onto a problem of interacting fermions on a lattice. For the spin-$\frac{1}{2}$ system considered here, the corresponding fermionic problem has Fermi momentum $k_F=\pi/2$. We then perform a linearization around the free Fermi points given by $\pm k_F$, to obtain an effective low-energy continuum fermionic theory and then bosonize using the standard dictionary of Abelian bosonization.[1,5] We just present the final expressions obtained for the spin-$\frac{1}{2}$ operators in terms of the bose field ϕ and its dual θ

$$S^z(x)=(-1)^x\cos(2\phi)+\frac{1}{2\pi}\partial_x\phi,$$

$$S^-(x)=\exp(i\theta)[(-1)^x+\cos(2\phi)]. \tag{2}$$

Finally, Eqs. (2) can be used to obtain the bosonized version of the Hamiltonian given in Eq. (1), i.e.,

$$\mathcal{H}=\frac{1}{2\pi}\int dx\left[uK(\pi\Pi)^2+\left(\frac{u}{K}\right)(\partial_x\phi)^2\right], \tag{3}$$

where u is the spin-wave velocity, Π is the momentum conjugate to the field ϕ, and $K=\frac{1}{2}$ for the isotropic Hamiltonian of Eq. (1). $\mathcal{H}$ is just the Hamiltonian for free bosons. Note that $K=1$ for the case of the XX antiferromagnet which in turn is equivalent to a theory of free fermions via the Jordan-Wigner transformation. Other values of K correspond to having a J_z coupling and hence to interacting fermions. Since there is no mass term for the ϕ field, it is clear that there is no gap to the first excited state from the singlet ground state. Since a free boson theory given by Eq. (3) is trivially solvable, it is fairly straightforward to calculate the dynamic correlation functions using Eqs. (2).

III. SPIN-$\frac{1}{2}$ SYSTEMS WITH A GAP IN A MAGNETIC FIELD

A. Zero magnetic field case

In many compounds which mimic the behavior of spin-$\frac{1}{2}$ chains, it has often been found that there are many other interactions between spins, apart from the isotropic interaction summarized in the Hamiltonian of Eq. (1). These could be anisotropies, frustration, impurities, and interchain couplings. More often than not, it is found that these interactions are small and can be treated as perturbations of the above gapless system. Within the framework presented here, the effects of these perturbations can be gauged from whether they are relevant, marginal, or irrelevant in the renormalization group sense. Depending on whether the perturbations are relevant or irrelevant, a gap opens in the spectrum. In this paper we are interested in a weak spin-Peierls dimerization and frustration arising from next-nearest-neighbor interactions.

We first consider a small dimerization δ, which arises from spin-lattice interactions. The corresponding perturbation to the Hamiltonian given in Eq. (1) is

$$\mathcal{H}_D=(-1)^i\delta\vec{S}_i\cdot\vec{S}_{i+1}. \tag{4}$$

Using Eqs. (2) the bosonized continuum version of Eq. (4) is[1]

$$\mathcal{H}_D=\delta\int dx\ \cos(2\phi). \tag{5}$$

It is equally interesting to study the effect of a competing next-nearest-neighbor interaction J_2. Such an interaction tends to frustrate the system. The addition to Eq. (1) is

$$\mathcal{H}_F=J_2\vec{S}_i\cdot\vec{S}_{i+2}. \tag{6}$$

For classical spins, the ground state retains its Néel-like order for all $J_2<0.25$ and exhibits spiral order for $J_2>0.25$. This is just a crossover as it is not possible for J_2 to drive a zero-temperature phase transition in the classical system. What is the behavior of the quantum spin-$\frac{1}{2}$ system? To study this we again take recourse to Eqs. (2) and write down the bosonized version of Eq. (6) (Ref. 1)

$$\mathcal{H}_F=(J_2-J_{2c})\int dx\ \cos(4\phi). \tag{7}$$

Apart from the cosine terms mentioned above, these spin interactions also renormalize the velocity u in Eq. (3). We now analyze the effects of the interactions given by Eqs. (6) and (7). In the free boson theory of Eq. (3), the anomalous dimensions of the operators $\cos(n\phi)$ are given by $n^2K/4$. Using this at the isotropic point $K=\frac{1}{2}$, we see that $\mathcal{H}_D$ given by Eq. (5) has dimension $\frac{1}{2}$ and hence is relevant for all values of δ. Similarly $\mathcal{H}_F$ described in Eq. (7) is found to have dimension 2 and is marginal. Numerically it has been shown that $\mathcal{H}_F$ is marginally relevant for $J_2>J_{2c}=0.2411$ and irrelevant for $J_2<0.2411$.[12] Therefore, we can see that both δ and J_2 drive a quantum phase transition from a gapless phase to a phase where a gap opens in the dispersion for all values of δ and $J_2>J_{2c}$.

Instead of restricting ourselves to the dimerized and frustrated models in this paper, we study the following Hamiltonian generic to gapped spin-$\frac{1}{2}$ chains in a magnetic field:

$$\mathcal{H}_{\rm gap}=\frac{1}{2\pi}\int dx\left[uK(\pi\Pi)^2+\left(\frac{u}{K}\right)(\partial_x\phi)^2+\nu\ \cos(n\phi)\right]. \tag{8}$$

The two-parameter space spanned by K and n correspond to various spin-$\frac{1}{2}$ systems with gaps in their spectra. For ex-

ample, $K=\frac{1}{2}, n=2$ corresponds to the dimerized model and $K=\frac{1}{2}, n=4$ is the frustrated antiferromagnet.

We see that though all these models have a gap, we can differentiate between them by studying their excitation spectra, the nature of which depends on the values of K and n. For instance, it is known from the study of excitations in the sine-Gordon theories[13] that apart from the magnons and solitons there exist certain excitations called breathers. These are nonlinear like the solitons and manifest themselves as discrete levels in excitation spectrum. These breathers have energies higher than the singlet-triplet gap but lie below the continuum part of the spectrum generated by the solitons. The number N of such breather modes is given by $N<(8-n^2K)/n^2K$. For example, we see that the frustrated model has no breather modes in its excitation spectrum. On the other hand, the spin-Peierls system has two breather modes in its spectrum: the $N=1$ breather is just a renormalized magnon and the $N=2$ breather is a bound state of two magnons. This extra bound state is found to affect the spin-correlation function at finite temperatures.[14] Optical experiments on the lines of Ref. 15, where breathers in quasi-1D ferromagnets were detected, can be used to directly detect these breathers.

B. Effects of a magnetic field

We now study the effect of a magnetic field on these gapped systems. To do so, we turn on a magnetic field H in the $\hat{z}$ direction. Note that the magnetic field breaks the SU(2) symmetry. The interaction with the spins on the lattice is

$$\mathcal{H}_m=\sum_i g\mu_B H S_i^z. \tag{9}$$

A simple understanding of the effect of the field can be obtained in the fermionic picture. First of all, the application of the magnetic field is equivalent to a chemical potential for the fermions. When $H=0$ we have zero uniform magnetization, i.e., $\Sigma_i S_i^z=0$. This corresponds to a completely filled lower band for fermions with a gap Δ separating the lower and the upper bands and the Fermi energy lying in the middle. As we increase H, we are in effect shifting the Fermi energy. A point is reached where the Fermi energy crosses the gap and lies at the bottom of the upper band. This value of H corresponds to H_{c1}, i.e., $\Delta=g\mu_B H_{c1}$. When H is increased beyond H_{c1}, the upper band is partially filled resulting in a nonzero magnetization m. The zero magnetization region with a gap below H_{c1} is the commensurate (C) regime in that short-range antiferromagnetic order still persists. Above H_{c1}, the ground state is magnetized, has no gap and canted. This is what we call the incommensurate (IC) phase. This is a quantum phase transition and S^z is the relevant order parameter. This is what makes it different from the incommensurate (spiral) phases seen in frustrated systems (Sec. III A).[16,17]

Now that we have a heuristic understanding of the effect of the magnetic field we now proceed to calculate various quantities of interest like the magnetization and exponents in the vicinity of H_{c1}, within the continuum approximation. Using Eqs. (2) we can see that Eq. (9) corresponds to adding a gradient term $g\mu_B H\partial_x\phi$ to the Hamiltonian of Eq. (8)

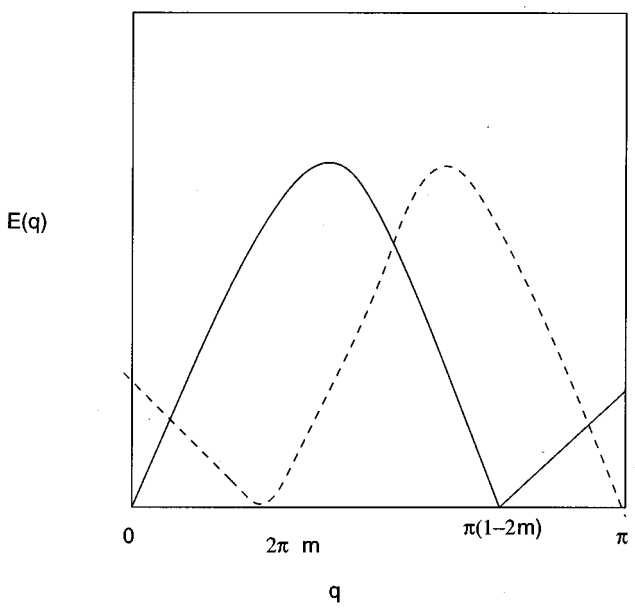

FIG. 1. Schematic picture of the field-dependent dispersion in the IC phase as seen by S^zS^z correlations (bold line) and S^+S^- correlations (dashed line). $Q=0$ and $Q=\pi$ are the usual commensurate modes and $Q=2\pi m$ and $Q=\pi(1-2m)$ are the incommensurate modes.

$$\mathcal{H}_{\rm tot}=\mathcal{H}_{\rm gap}+\frac{1}{2\pi}\int dx g\mu_B H\partial_x\phi. \tag{10}$$

This Hamiltonian has the same form as that for ffermions with attractive interactions in a magnetic field[18] and also the one used in the context of the C-IC transition in two-dimensional systems where it is a transition from a phase with a discrete symmetry (C) to a phase with a continuous symmetry (IC).[19,20] Note that the gradient term in Eq. (10) can be eliminated by a simple shift of the ϕ field, i.e., $\phi\rightarrow\phi+\pi K g\mu_B H x$. Since the only effect of H below H_{c1} is to renormalize the gap, we can replace this shift by $\phi\rightarrow\phi+\pi m x$ where m is the magnetization. The cosine term, however, is not invariant under this shift. From the analogy with the chemical potential in fermionic systems, we infer that the magnetic field changes the Fermi momentum. We can redefine new Fermi points $\pm k_F'$, linearize around these points, and obtain a new effective massless free boson theory, albeit with a different value of K. It has gapless modes at $q=0$ and $q=2k_F'=\pi(1-2m)$. A schematic plot of the field dependent dispersion for the spins in the IC phase is given in Fig. 1. The behavior in the gapless IC region is governed by the Hamiltonian

$$\tilde{\mathcal{H}}=\frac{1}{2\pi}\int dx\left[v\tilde{K}(\pi\Pi)^2+\left(\frac{v}{\tilde{K}}\right)(\partial_x\phi)^2\right]. \tag{11}$$

The quantities v and $\tilde{K}$ are dependent on H. Although it is difficult to obtain the dependences for the entire range of H between H_{c1} and H_{c2}, one can compute the exact values for the exponents (equivalently the $\tilde{K}$) at the critical point H_{c1} and see how they change as we move away from these points.

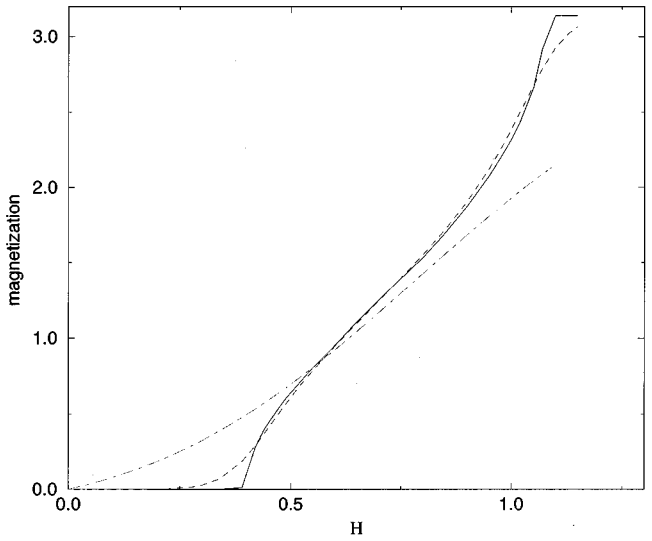

FIG. 2. Plot of the magnetization m (apart from an overall normalization) vs magnetic field H for $\Delta=0.4J$ at various temperatures T. H and T have been normalized by the exchange coupling J. The solid line corresponds to $T=0$, the dashed line at $T=0.05$, and the dashed-dotted line to $T=0.25$. We see that even at sufficiently low temperatures the square root regime gets wiped out and m increases in a nearly linear fashion.

Before we proceed with the calculation of $\widetilde{K}$, we first study how the magnetization rises above H_{c1}. Using the results on the C-IC transition[20]

$$m=\eta\sqrt{\frac{K}{n}}\sqrt{(H^2-H_{c1}^2)}=\eta\sqrt{\frac{K}{n}}\sqrt{(H-H_{c1})(H+H_{c1})}$$
$$\simeq\eta\sqrt{\frac{K}{n}}\sqrt{(H-H_{c1})2\Delta}, \tag{12}$$

where n is the coefficient of ϕ in the argument of the cosine interaction and η is a constant of proportionality which depends on the renormalized velocities. The magnetization increases from its zero value as a square root near H_{c1}. A similar square root behavior is seen near H_{c2} if one approaches this critical point from the ferromagnetic side. Here it is the decrease in magnetization from the full ferromagnetic value that shows the square root behavior. In Fig. 2, we have shown the behavior of the magnetization with temperature and the field in units of $g\mu_B$. This was done using the analogy with the case of fermions with a gap and a chemical potential. We assumed a dispersion for the fermions of the form $\omega_k=\pm\sqrt{(Jk)^2+(\Delta)^2}$. Here the two square root regimes near H_{c1} and H_{c2} (0.4 and 1.1 in the figure) are joined by a region in which the magnetization increases in a nearly linear fashion with H. The interval of H in which the square root behavior of the magnetization is seen and also the range where the nearly linear regime is seen, depend on the parameters like the couplings and the gap. For certain ranges of these parameters where the gap Δ is of the order of the exchange couplings one obtains a scenario where the width of the square root regime is quite small so that even experiments done at reasonably low temperatures could entirely miss the detection of this region. This might be the reason as to why the square root behavior is not observed in Ref. 7. Since the behavior of the magnetization given by Eq. (12) is generic to all the gapped systems studied here, it follows that a measurement of the magnetization will not be able to qualitatively differentiate between the various models.

The magnetization derived in Eq. (12) applies to the ladder also. This is because, as we will later show in Sec. V, the effective Hamiltonian for the ladder has the same form as given in Eq. (10). Another system which exhibits a similar transition in the magnetic field is the spin-1 chain. Since the spin-$\frac{1}{2}$ ladder and the spin-1 chain belong to the same universality class,[21] Eq. (12) describes the magnetization in the spin-1 chain also. This agrees well with the result for m in spin-1 chains obtained in Refs. 21 and 22. In Ref. 22 a mapping of a phenomenological Hamiltonian of interacting magnons onto a system of bosons with repulsive δ-fn interactions was used to obtain the magnetization and the correlations in the IC regime.

Naively one might expect that these gapped systems in a magnetic field have the same qualitative behavior for correlation functions and that quantitative features like H_{c_1} and thermodynamic quantities like m are model dependent. We shall see below that this is not true and that these models have dynamically different physical behaviors in the IC regime depending on the value of n. For a generic interaction of the form $\cos(n\phi)$ (where $n^2K\leqslant 8$) and H close to H_{c1} on the IC side,[20]

$$\widetilde{K}=\frac{4}{n^2}\left(1-\frac{um\gamma\sinh(2\theta)}{\Delta}\right). \tag{13}$$

Here Δ is the gap and γ is a positive constant which depends on the parameters of the theory but is independent of H. θ is defined by $\exp(-2\theta)=n^2K/4$. At the transition H_{c1}, $\widetilde{K}$ goes to a universal value $4/n^2$ independent of the value of K. As H increases, there is a nonzero magnetization m and the change in $\widetilde{K}$ is completely governed by n and K in that $\widetilde{K}$ could increase or decrease depending on the value of K. For example, for the frustrated (J_2) model $\widetilde{K}=\frac{1}{4}$ at $H=H_{c1}$ and increases as H increases and for the case of the dimerized (δ) model, $\widetilde{K}=1$ at $H=H_{c1}$ and decreases with increasing H. Here we have seen that though the magnetization has the same qualitative behavior for all the models, the value of $\widetilde{K}$ is model dependent because it is determined by the anomalous dimensions of the perturbing operators. As a consequence the exponents in these models will be radically different as will be shown in the following section.

IV. CORRELATION FUNCTIONS IN THE CRITICAL REGION

In this section, we first study how the structures of the correlation functions are altered by the magnetization in the IC phase. Later we will calculate the various commensurate and incommensurate contributions to the finite temperature dynamic susceptibility. From the magnetic interaction given by Eq. (9) and the field shift $\phi\rightarrow\phi+\pi mx$, it is clear that since for $H<H_{c1}$ there is no net magnetization, the form of the correlators is unaffected, and only the gap is renormalized. However, in the IC phase, the presence of a nonzero magnetization m results in $\phi\rightarrow\phi+\pi mx$. The dual field θ is

insensitive to this shift. Incorporating this field shift in the expressions for the spin operators given in Eq. (2), we find that the generic form of the spin-spin correlation function in the IC region is

$$\langle S^z(x,t)S^z(0,0)\rangle = m^2 + f_1(x,t) + \cos\pi(1-2m) f_2(x,t),$$
$$\langle S^+(x,t)S^-(0,0)\rangle = \cos(2\pi m x) g_1(x,t) + \cos(\pi x) g_2(x,t), \tag{14}$$

where f_1, f_2, g_1, and g_2 are monotonic, decreasing, power-law functions of space and time and they go to zero asymptotically. From the above expressions we deduce the following: the correlation function parallel to the field, i.e., $\langle S^z S^z\rangle$, has a uniform magnetization or equivalently a $Q=0$ mode while the staggered part is shifted from $Q=\pi$ to $Q=\pi-2\pi m$. This is in contrast to the correlation in the plane perpendicular to the field, $\langle S^+S^-\rangle$, where the staggered mode is unshifted and remains at $Q=\pi$ and the uniform magnetization ($Q=0$) mode is shifted to $Q=2\pi m$. We call $Q=2\pi m$ and $Q=\pi(1-2m)$ the incommensurate modes.

With the results obtained above, we now proceed with our calculation of experimentally relevant quantities like the dynamic susceptibilities at finite temperatures. As a first step we compute the associated unequal time correlation functions using Eqs. (2) and (14) and the result of Eq. (13). The correlation functions are found to be as follows:

$$\langle \tilde{S}^z(x,t)\tilde{S}^z(0)\rangle = \langle (S^z(x,t)-m)(S^z(0)-m)\rangle = \cos(\pi x(1-2m))(x^2-t^2)^{-\tilde{K}} + \text{const}\frac{\tilde{K}}{4\pi^2}\left(\frac{1}{(x-t)^2}+\frac{1}{(x+t)^2}\right)$$
$$\langle S^+(x,t)S^-(0)\rangle = (-1)^x(x^2-t^2)^{-1/4\tilde{K}} + \text{const}\cos(2\pi m x)(x^2-t^2)^{-(1/4\tilde{K}+\tilde{K}-1)}$$
$$\times\left[\exp(2i\pi m x)\frac{1}{(x-t)^2}+\exp(-2i\pi m x)\frac{1}{(x+t)^2}\right], \tag{15}$$

with $\tilde{K}$ being specified by Eq. (13). It is not surprising that the exponents are different in the directions parallel and perpendicular to the external field. This is because the magnetic field breaks the SU(2) spin-rotational invariance. For the case of the dimerized model at the critical magnetic field $H=H_{c1}$, we found in Sec. III that $\tilde{K}=1$. An interesting coincidence is that the exponents and hence the correlation functions calculated here for the dimerized model at $H=H_{c1}$ are the same as that for the XX antiferromagnet in a zero magnetic field. The correlation functions of the XX model (which is in turn equivalent to a theory of free fermions) can be obtained by substituting $m=0$ and $\tilde{K}=1$ in Eqs. (15). Note that this correspondence holds only at the critical point.

Using the above results we can also evaluate the (q,ω) dependent susceptibility at finite temperatures, both in the direction of the applied magnetic field and in the direction perpendicular to it. A knowledge of this quantity helps us extract various measurable quantities like neutron scattering intensities, absorption, and nuclear magnetic resonance (NMR) rates. The susceptibilities are given by the following expression:

$$\chi_{ij}(q,\omega,T) = -i\int dt dx\ \exp i(\omega t - qx)\,\theta(t)\langle[S^i(x,t),S^j(0,0)]\rangle_T. \tag{16}$$

Here i,j refer to the components of the spin and the subscript T implies that the correlator is evaluated at finite temperature. Since rotations in the x-y plane still leave the Hamiltonian invariant, there are no cross correlations, i.e., $\langle S^iS^j\rangle=0$ for $i\neq j$. For the susceptibility $\chi_{zz}\equiv\chi_\parallel$ in the $\hat{z}$ direction parallel to the direction of the applied field[21,23]

$$\chi_\parallel^{Q=0}(q,\omega,T) = \frac{q^2}{(vq)^2-\omega^2}, \tag{17}$$

$$\chi_\parallel^{Q=\pi(1-2m)}(q,\omega,T) = NT^{2\tilde{K}-2}B\left(\frac{\tilde{K}}{2}-i\frac{(\omega+v(q-Q))}{4\pi T},(1-\tilde{K})\right)B\left(\frac{\tilde{K}}{2}-i\frac{(\omega-v(q-Q))}{4\pi T},(1-\tilde{K})\right).$$

For the perpendicular susceptibility $\chi_\perp\equiv\chi_{+-}$, i.e., in the x-y plane,

$$\chi_\perp^{Q=2\pi m}(q,\omega,T) = -N'T^{2\beta}\left[B\left(\frac{\beta+2}{2}-i\frac{(\omega+v(q-Q))}{4\pi T},(-1-\beta)\right)B\left(\frac{\beta}{2}-i\frac{(\omega-v(q-Q))}{4\pi T},(1-\beta)\right)\right.$$
$$\left.+B\left(\frac{\beta}{2}-i\frac{(\omega+v(q-Q))}{4\pi T},(1-\beta)\right)B\left(\frac{\beta+2}{2}-i\frac{(\omega-v(q-Q))}{4\pi T},(-1-\beta)\right)\right], \tag{18}$$

where $2\beta=2\tilde{K}+1/2\tilde{K}-2$,

$$\chi_{\perp}^{Q=\pi}(q,\omega,T)=NT^{2\alpha-2}B\left(\frac{\alpha}{2}-i\frac{(\omega+v(q-Q))}{4\pi T},(1-\alpha)\right)B\left(\frac{\alpha}{2}-i\frac{(\omega-v(q-Q))}{4\pi T},(1-\alpha)\right), \quad (19)$$

where $\alpha=1/4\tilde{K}$, $B(x,y)$ is the β function, and v is the effective magnetization-dependent spin velocity. N and N' are velocity- and hence field-dependent prefactors. These expressions for the susceptibilites are valid as long as $T<(H-H_{c1})$. This is because above this temperature the Hamiltonian in Eq. (11) obtained by linearizing the Fermi surface around k_F' is no longer valid.

Though we have explicitly calculated the susceptibilities only in the IC regime for low temperatures, it is nonetheless interesting to study the behavior outside this IC phase. For example, one can study how the system crosses over to the high-temperature classical limit as a function of the parameters of the theory. We present a phase diagram as a function of T and H in Fig. 3. This phase diagram is true only for $H<H_{c2}$ because at H_{c2} the system makes a transition to another gapped phase. For temperatures smaller than the exchange J one obtains four regimes as indicated in Fig. 3. All the lines indicate crossovers and are not phase transitions. This phase diagram can be easily understood within the fermionic picture. Note that for the fermionized version of spin chains with a gap the complete dispersion for the excitations has the form $\omega_k=\pm\sqrt{J^2k^2+\Delta^2}$. These two branches constitute the lower and upper bands with a gap 2Δ separating the two bands. With the full dispersion, the magnetization is given by a function which depends on two parameters Δ/T and H/T. The different regimes to be discussed below will be characterized by the varied behavior of this function. For all $T<H_{c1}-H$ one gets the gapped phase where the chemical potential, i.e., H lies in the gap and the temperature is still small enough and does not excite particles to the upper band. This phase is characterized by an exponential decay of all correlation functions. When $H>H_{c1}$ and $T<(H-H_{c1})$, the chemical potential lies in the upper band and we get the incommensurate or Luttinger liquid I regime as was already discussed in Sec. III B (cf. Fig. 3). The dynamical exponent is $z=1$ here. The susceptibilites in Eqs. (17)–(19) are valid in this Luttinger liquid regime.

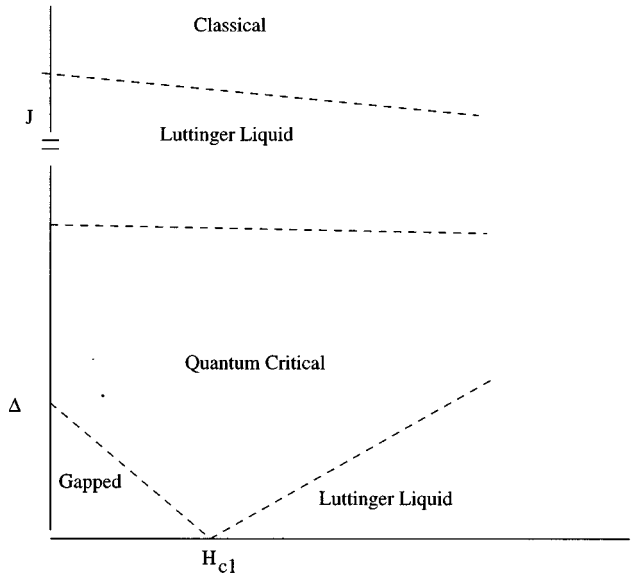

FIG. 3. Phase diagram of gapped spin-$\frac{1}{2}$ chains in a magnetic field H as a function of temperature T. There are essentially five regions and all the lines indicate crossovers between these regions.

If the chemical potential lies at the bottom of the upper band and $T\sim 0$ or equivalently when temperature is such that it can excite particles at the Fermi level to the bottom of the upper band, one obtains the quantum critical regime[24] defined by $|H-H_{c1}|<T$. In the quantum critical region the physics is governed by the fixed point[24] at $H=H_{c1}$ where $\tilde{K}$ has a universal value $4/n^2$. A simple way of understanding the behavior in this region is presented below. First, the curvature of the bottom of the band becomes very important in that the effective dispersion seen by the excitations is quadratic. Here one can expand ω_k in Δ to obtain $\omega_k^{\mathrm{QC}}=\Delta+k^2/2\Delta$ in the quantum critical region. The dynamical exponent $z=2$ in this region. A direct consequence of the quadratic dispersion is that Δ/T and H/T are no longer independent scaling variables and only occur in the combination $(H-H_{c1})/T$ and the magnetization m which is just the number of fermions in the upper band has the scaling form $m(T)=T^{1/2}f((H-H_{c1})/T)$. Analogous scaling functions exist for the spin-spin correlations also. The scaling functions for the correlators are functions of k^2/T, ω/T, and $(H-H_{c1})/T$. Note that Δ/T and H/T are no longer independent scaling variables and only occur in the combination $(H-H_{c1})/T$. The spins are complicated functions of the fermions and this results in the scaling functions being difficult to obtain for reasons described in Ref. 24. The quantum critical behavior holds only as long as the quadratic form of the dispersion assumed is valid, or in other words, only as long as temperature is such that the bulk of the excitations is confined to the bottom of the upper band. Similar phases were obtained in Ref. 24 in the context of spin-1 chains in a magnetic field, using a phenomenological theory of magnons with repulsive interactions. Here starting from a microscopic description, we find that these phases are generic to all gapped chains in a field and we have also obtained the exponents in the Luttinger liquid regime I.

Now if temperature is increased further, there is a crossover to a fourth region. This regime was not obtained in Ref. 24 because the form ω_k^{QC} was assumed for all values of k. Above a certain temperature excitations to higher k states occur and one starts probing the deviation from a quadratic dispersion and the k^2 approximation is no longer valid. As a result the quantum critical scaling for the magnetization, etc., will no longer be valid above these temperatures. The system then crosses over to a new region where temperature is large enough such that in addition to the excitations which now involve states way above the bottom of the upper band, there are transitions between the lower and the upper bands. This implies that the gap becomes irrelevant and the effective dis-

persion becomes linear in k. This crossover should occur for temperatures T of the order of twice the gap Δ but much lesser than the exchange couplings such that the interaction becomes irrelevant and the resulting behavior is that of a Luttinger liquid. We denote this regime as the Luttinger liquid II. Classical behavior sets in for temperatures greater than the exchange couplings. The widths of all these regions are dictated by the values of the gaps and the exchange coupling. For instance, the width of the quantum critical regime is fixed by the gap alone, and for magnetic fields away from H_{c1} this width is quite small and not as large as purported to be in Ref. 24. As a consequence, the scaling arguments apply only in the vicinity of the fixed point at H_{c1} where the width of the quantum critical regime is appreciable and not for fields far away from it. In contrast, the width of the Luttinger liquid II regime is given by the relative sizes of J and Δ. This width can be increased or decreased by tuning the ratio Δ/J. Applying these arguments to the case of spin-1 chains where the gap is of the order of the exchange coupling J, one finds that for small fields the classical limit sets in soon and there are no sharp crossovers between the quantum critical, Luttinger liquid II, and classical regimes.

In the following paragraphs we discuss the physical significance of the susceptibilites calculated above. The susceptibilities are directly relevant to inelastic neutron scattering measurements where apart from certain magnetic form factors, the intensity is proportional to the (q,ω) Fourier transform of the full spin-spin correlator $\langle \mathbf{S}(x,t)\cdot\mathbf{S}(0,0)\rangle$. From Eqs. (17), we can see that the scattering intensity in the IC phase due to the S^z correlator, obtained as a function of ω for some fixed q, should in addition to the peak generated by the massless excitations near $Q=0$ contain an extra peak corresponding to the massless modes at the incommensurate $Q=\pi(1-2m)$. Similarly, for the correlations perpendicular to the field, peaks are seen at the staggered mode $Q=\pi$ and at $Q=2\pi m$. These peaks are divergent at $T=0$ because of the power-law correlations present at these values of Q. At finite temperatures the peak heights are finite and are determined by the T dependence of Eqs. (17)–(19). Such incommensurate features have been observed in inelastic neutron scattering data from copper benzoate which is a $s=\frac{1}{2}$ system in a magnetic field.[25] Another probe is electron spin resonance (ESR) which can be used to directly probe the nature of the continuum of excitations at $Q=2\pi m$.[26]

One interesting question is whether the propagating modes corresponding to the uniform and staggered magnetization are damped at finite temperature, or in other words, is there any thermal broadening? This can be answered by studying the temperature dependence of the imaginary parts of the corresponding susceptibilites. First consider the case of the isotropic spin-$\frac{1}{2}$ chain in zero magnetic field. Here it is known that the uniform magnetization component of the S^z correlator diverges as $1/x^2$. The corresponding uniform and staggered susceptibilities at finite temperatures are given by[21,23] Eqs. (17) with $m=0$ and $\tilde{K}=1/2$. Isotropy results in the same expressions for the perpendicular susceptibility. In this context v is the spinon velocity. The dependence of $\chi_{\parallel}^{Q=\pi}$ on temperature tells us that the $Q=\pi$ mode is damped at finite T. The temperature independence of the $\chi_{\parallel}^{Q=0}$ implies that there is no damping of the $Q=0$ mode at finite T.[27] This can also be understood from the fact that the exponent β in Eq. (18) is zero at $K=1/2$. There is no damping of this mode within the continuum approximation where the fermionic dispersion was assumed to be linear. Taking into account a small curvature of the fermion dispersion spectrum does not alter this result because the height of the peak which is given by the lifetime of the quasiparticles in the fermionic picture becomes infinite as $q\to 0$ even at finite temperatures. Another way of understanding this absence of damping of the uniform mode is by noting the fact that the total magnetization in all the directions commutes with the Hamiltonian which in turn implies that there is no damping of this mode in the lattice spin system.

We now discuss the damping of the various modes in the IC phase. The modes are the uniform magnetization mode $Q=0$, the staggered mode $Q=\pi$, and the incommensurate modes at $Q=2\pi m$ and $Q=\pi(1-2m)$. From Eqs. (17)–(19) we see that the dominant contribution to the $Q=\pi$ and $Q=2\pi m$ modes is from the perpendicular susceptibility. As in the Heisenberg case discussed above, the staggered mode at $Q=\pi$ has a damping factor proportional to $T^{2\alpha-2}$. Similarly the presence of a nonintegral exponent β in $\chi_{\perp}^{Q=2\pi m}$ results in the $Q=2\pi m$ mode being damped at finite temperatures by a factor proportional to $T^{2\beta}$. Similarly the behavior of the $Q=\pi(1-2m)$ mode is dictated by $\chi_{\parallel}^{Q=\pi(1-2m)}$ in Eq. (17) and has a damping factor $T^{2\tilde{K}-2}$. We now consider the $Q=0$ mode. The dominant contribution to the damping of this mode arises from $\chi_{\parallel}^{Q=0}$. From Eqs. (17), we find that the parallel susceptibility does not damp the $Q=0$ modes because $\chi_{\parallel}^{Q=0}$ is still independent of temperature. Because the system is not isotropic we need to check whether there is a subdominant contribution from the perpendicular susceptibility which damps this mode. To do this we first study the damping for other values of Q between 0 and $2\pi m$. Note that this damping can be studied at the resonance frequencies $\omega=v(Q-q)$ or away from resonance. To obtain the leading temperature dependence of the damping of these modes at resonance, we substitute $q-2\pi m=\delta q$ in Eq. (18). The resonance frequency ω is fixed at $v\,\delta q$. The low-temperature behavior of the imaginary part of the susceptibility is given by

$$\frac{\beta}{2}\omega^{\beta-1}T^{\beta+1}+\frac{2}{\beta}\omega^{\beta+1}T^{\beta-1}. \tag{20}$$

This expression implies that there is a thermal broadening of the $Q=0$ or uniform magnetization mode, i.e., $\delta q=-2\pi m$. Nevertheless, using the fact that the total magnetization in the $\hat{z}$ direction still commutes with the Hamiltonian even in the presence of the magnetic field and that the time evolution of $\Sigma_i S_i^+$ involves only $\Sigma_i S_i^+$ we conclude that there is no thermal broadening of the uniform mode $(Q=0)$ mode. If ω is not at the resonance frequency then for low T, there is no obvious thermal broadening and $\mathrm{Im}\chi_{\perp}^{Q=2\pi m}$ is proportional to $[v\,\delta q(v\,\delta q-2\pi m)]^{\beta-1}$. This expression is not valid for $\omega-v\,\delta q<T$ and fails in the vicinity of $\delta q=2\pi m$. From these calculations we see that though bosonization describes the physics correctly near $Q=\pi$ and $Q=2\pi m$ for the perpendicular correlations it does not describe modes far away from these two points well. This is

not surprising in view of the fact that by linearizing at k_F' we take into account a lot of spurious states at the bottom of the band. To summarize, we find that the $Q=0$ mode is undamped whereas the gapless modes at $Q=2\pi m, \pi(1-2m)$ and π are all damped.

V. SPIN-$\frac{1}{2}$ LADDER

Another system which exhibits a behavior akin to the systems studied above is the spin ladder. Here we consider a ladder with two identical and isotropic chains. Let the spins in chain 1 be labelled $\vec{S}_1$ and those in chain 2, $\vec{S}_2$. We bosonize this system in the same manner as above. We refer the reader to Refs. 21, 28, and 29 for details. We adopt the notations of these references and introduce the symmetric (triplet) and antisymmetric (singlet) combinations of the fields: $\phi_{s,a}=(\phi_1 \pm \phi_2)/\sqrt{2}$ and their respective duals θ_s and θ_a. The Hamiltonian for the ladder is

$$\mathcal{H}=\mathcal{H}_a+\mathcal{H}_s, \tag{21}$$

where

$$\mathcal{H}_a=\frac{1}{2\pi}\int dx\left[Ku(\pi\Pi_a)^2+\left(\frac{u}{K}\right)(\partial_x\phi_a)^2+g_1\cos(\sqrt{8}\phi_a)+2g_2\cos(\sqrt{2}\theta_a)\right],$$

$$\mathcal{H}_s=\frac{1}{2\pi}\int dx\left[Ku(\pi\Pi_s)^2+\left(\frac{u}{K}\right)(\partial_x\phi_s)^2+g_3\cos(\sqrt{8}\phi_s)\right], \tag{22}$$

where $K=\frac{1}{2}$, $g_1=g_2=g_3=J_\perp\lambda/2\pi$ and $J_\perp$ is the interchain coupling and λ some constant. All the cosine operators are relevant operators of dimension one. Equations (22) have the same form as the Hamiltonian for an isotropic spin-1 system written in terms of two spin-1/2 operators.[21] We note that the spin-1 system has fixed values for g_1, g_2, and g_3 and has no analog of a tunable parameter like $J_\perp$. Nevertheless the results to be derived below apply to the spin-1 system in a magnetic field. From Eqs. (21) and (22) we can infer the existence of gaps for all nonzero values of $J_\perp$ in the spectra of both the fields ϕ_a and ϕ_s. The ground state of the ladder is a spin singlet and there exists a gap to the triplet excited state characterized by ϕ_s. Therefore, analogous to the dimerized chains, we expect the vanishing of the gap and the onset of a gapless incommensurate phase for some critical value of the magnetic field. Since the magnetic field acts on both chains equally, we can easily see from the bosonization formulas that H affects only the ϕ_s field

$$\mathcal{H}_s\rightarrow\mathcal{H}_s+\sqrt{2}H\partial_x\phi_s. \tag{23}$$

Note that this Hamiltonian has the same form as Eq. (10). Therefore, using the results obtained in Sec. III, we can immediately see that the ϕ_s field becomes massless while in the antisymmetric sector the θ_a field acquires a nonzero expectation value and the ϕ_a still has a gap. As a result the correlations of the ϕ_a field decay exponentially. The value of $\tilde{K}$ for the ϕ_s field at $H=H_{c1}$ is $\tilde{K}=\frac{1}{2}$. From Eq. (13), we find that $\tilde{K}=\frac{1}{2}$ above H_{c1} also. This is because $\sinh(2\theta)=0$ for the ladder. However, one should note that this is valid only in the region close to H_{c1} and provided that the gaps and the magnetic field are small compared to the intrachain exchange coupling. Using the above results we can compute the spin-correlation functions. There are two kinds of correlations: correlations within a chain and between chains. Here again the magnetic field changes the structure of the correlation functions in a manner analogous to that described in Eqs. (14). We summarize the results for the various correlators below. Since we are concerned only with the asymptotic behaviors we present only the power-law contributions to these correlators:

$$\langle S_z^r(x,t)S_z^t(0,0)\rangle=m^2+\frac{1}{8\pi^2}\left[\frac{1}{(x-t)^2}+\frac{1}{(x+t)^2}\right]. \tag{24}$$

Here r,t denote the chain labels. Unlike in the single chain case, in the ladder *the alternating part at $Q=\pi$ which is now shifted to $Q=\pi(1-2m)$ by the magnetic field decays exponentially*. Similarly

$$\langle S_1^+(x,t)S_1^-(0,0)\rangle=\langle S_2^+(x,t)S_2^-(0,0)\rangle=(-1)^x(x^2-v^2t^2)^{-1/8\tilde{K}},$$

$$\langle S_1^+(x,t)S_2^-(0,0)\rangle=i(-1)^x(x^2-v^2t^2)^{-1/8\tilde{K}}. \tag{25}$$

Here again *the uniform component is shifted to $Q=2\pi m$ and decays exponentially*. The fact that ϕ_a is massive results in an exponential decay of all the incommensurate contributions to the correlations. This exponential decay of all the incommensurate correlations in the ladder is in contrast to the single chain systems studied in the previous sections. Also note that except for certain exponentially decaying corrections, the interchain and intrachain correlators have essentially the same asymptotic behaviors. As already mentioned, the spin ladder in the magnetic field has the same exponents as that of the spin-1 chain in a magnetic field.[21,22] The dominant contribution to the perpendicular susceptibility for the ladder has the same form as that given in Eq. (19) with $\alpha=1/8\tilde{K}$ and that to the parallel susceptibility by $\chi_\parallel^{Q=0}$ of Eq. (17). At the critical point $H=H_{c1}$, the exponent $\alpha=\frac{1}{4}$ for the ladder as well as the dimerized model. However, there is one big difference between the two models. In the dimerized model, the incommensurate parts of the $\langle S^zS^z\rangle$ and $\langle S^+S^-\rangle$ also show power-law behaviors, whereas in the ladder they decay exponentially. This has a serious consequence for neutron scattering intensities. This is because for the dimerized system, at $T=0$ the power-law divergences of the incommensurate parts of the dynamic correlations will result in a divergent peak at the incommensurate wave vector Q. On the other hand, the exponential decay of the incommensurate correlations results in much smaller peaks at incommensurate Q whose finite height and width are determined by the gaps in the ϕ_a field. Though away from the critical point the exponents for the two models are no longer identical, the discussion presented above for the neutron scattering still holds.

VI. NMR RELAXATION RATES

With the help of the susceptibilites derived above, we can easily compute various quantities that can be studied by neutron scattering and nuclear magnetic resonance (NMR). Here, we focus on NMR and in particular the spin-lattice relaxation time T_1. The dominant contribution to T_1 comes from the coupling of the nuclei to the lattice spins. Therefore, it is a good probe to study the nature of the lattice-spin system. To obtain the temperature dependence of T_1 we use the following formula in terms of the local susceptibility to calculate the same:[30]

$$\frac{1}{T_1}=\lim_{\omega\to 0}\frac{2k_BT}{\hbar^2\omega}\int\frac{dq}{2\pi}F_{ij}(q)\chi_{ij}(q,\omega,T). \tag{26}$$

Here the F_{ij} are hyperfine form factors and χ_{ij} has been defined in Eq. (16). In general these form factors are diagonal in i,j and do not vary much with q. For a system of noninteracting spins, $(T_1T)^{-1}$ is a constant. For interacting spin systems, the dependence on temperature could be more complicated because the underlying magnetic order plays a very important role in that it changes the effective magnetic field seen by the nuclei. Examples are the isotropic Heisenberg model where ${T_1}^{-1}$ goes to a nonzero value as $T\to 0$ and the spin-Peierls system where T_1^{-1} goes to zero at $T=0$ because of the gap to spin excitations.

We now use the results obtained in the previous section to calculate the NMR rates. We first note that the magnetization m only shifts the resonance frequency and does not change the form of the expressions for T_1^{-1}. Depending on the kind of NMR done, one can probe specific correlations. This is especially useful for anisotropic spin systems and also isotropic systems in a magnetic field where the perpendicular and parallel susceptibilites are different. For instance, if the NMR was done on the nucleus of the lattice spin, then the relaxation occurs through a contact interaction and T_1^{-1} depends on $\chi_\perp$ alone. On the other hand, if it is done on other neighboring nuclei in the compound, the relaxation is through dipolar interactions and T_1^{-1} depends on $\chi_\perp$ and $\chi_\parallel$. An amalgam of the two methods will be useful in isolating the two susceptibilites experimentally.

Substituting the expressions for $\chi_\perp$ and $\chi_\parallel$ derived in Eqs. (17), (18), and (19) in Eq. (26), we find that a straightforward power counting yields the following leading low-temperature behavior for the single chain models:

$$\left[\frac{1}{T_1}\right]^{\text{single chain}}=A_\perp T^{(1/2\widetilde{K})-1}+A_\parallel T^{2\widetilde{K}-1}+B_\parallel T, \tag{27}$$

where $\widetilde{K}$ is given by Eq. (13). $A_\perp$, $A_\parallel$, and $B_\parallel$ are constants independent of temperature. The suffixes $\perp$ and $\parallel$ refer to the contributions from the perpendicular and parallel susceptibilities. It is easy to see that the staggered susceptibilities dominate in T_1^{-1}. For the ladder model, T_1^{-1} is given by

$$\left[\frac{1}{T_1}\right]^{\text{ladder}}=A_\perp T^{(1/4\widetilde{K})-1}+B_\parallel T. \tag{28}$$

The contribution coming from the $A_\parallel$ term has not been explicitly written because it goes to zero exponentially as $T\to 0$.

TABLE I. Temperature dependence of T_1^{-1} at $H=H_{c1}$.

Model	$\widetilde{K}$ at H_{c1}	$T_{1\parallel}^{-1}$	$T_{1\perp}^{-1}$
Spin-Peierls (δ)	1	T	$T^{-1/2}$
Frustration (J_2)	$\frac{1}{4}$	$T^{-1/2}$	T
Ladder	$\frac{1}{2}$	T	$T^{-1/2}$

The temperature dependences of these rates for the dimerized and frustrated models at the critical point H_{c1} are given below.

Dimerized (δ):

$$\frac{1}{T_1}=(A_{\delta\parallel}+B_{\delta\parallel})T+A_{\delta\perp}T^{-1/2}. \tag{29}$$

Frustrated models (J_2):

$$\frac{1}{T_1}=A_{f\parallel}T^{-1/2}+(A_{f\perp}+B_{f\parallel})T. \tag{30}$$

In Table I, we present the leading low-T contributions to T_1^{-1} at the transition, for the three models considered in this paper. There are other temperature-dependent contributions to the NMR rate, but these go to zero at $T=0$. As mentioned earlier there are two possible scenarios. One is that the nucleus probed does not correspond to the spins and the interactions are dipolar. Here at $H=H_{c1}$, the T_1^{-1} diverges as $T^{-1/2}$ for the three models. However, the divergent behavior at low temperature in the frustrated model arises from the parallel susceptibility whereas in the ladder and dimerized systems it is the perpendicular susceptibility which leads to the divergent behavior. This feature can be used to differentiate between the models as will be discussed in the following paragraph. As H is increased, we can see from Eq. (13) that $\widetilde{K}$ increases for the frustrated model and the divergence becomes weaker. Coincidentally $\widetilde{K}$ decreases for the dimerized system and the divergence of T_1^{-1} becomes weaker too. For the ladder, $\widetilde{K}$ does not change with H and the divergence persists and one has to go to higher fields to see a deviation from the $T^{-1/2}$ behavior. If for some value of H, $\widetilde{K}$ decreases to $\frac{1}{2}$ in the dimerized model and increases to $\frac{1}{2}$ in the frustrated system, we see that T_1^{-1} does not diverge and T_1^{-1} goes to a constant $A_\parallel+A_\perp$ as $T\to 0$. This behavior occurs because at some point the magnetic field becomes large enough such that the interaction which generates the gap becomes unimportant and should recover the exponents for the chain without the interaction, i.e., the Heisenberg chain where T_1^{-1} is a constant. For fields greater than this value of H, the exponents vary like those of a Heisenberg chain in a magnetic field. The exponent approaches that of the XX chain or free fermions for sufficiently large fields.

Another way of differentiating between the three models is if the NMR involves the nuclei of the relevant spins. Here, only the perpendicular local susceptibilities matter and a very interesting picture unfolds. At $H=H_{c1}$, T_1^{-1} diverges as $T^{-1/2}$ for the dimerized and ladder models whereas it approaches zero linearly in T for the frustrated model. Naively, for gapless systems, we would have expected T_1^{-1} to diverge or go to a nonzero constant as $T\to 0$ as it does in the case of

the Heisenberg model.[27] This T dependence in the frustrated model is indeed strange because it is reminiscent of the T_1^{-1} rates for spin chains with gaps where T_1^{-1} also goes to zero as $T\to 0$ but exponentially. A divergence will be seen in the frustrated system if H is such that $\tilde{K}>\frac{1}{2}$. For increasing H the $T^{-1/2}$ divergence survives in the ladder but for dimerized systems T_1^{-1} becomes less and less divergent as $T\to 0$ and later saturates to a constant $A_\perp$ at $T=0$ for some value of H. This is very similar to what was seen in the case of dipolar interactions discussed above. However, note that the saturation values are different in both cases. We also note that the above discussion rests on the fact that these fields are smaller than H_{c2} which need not necessarily be the case. As mentioned above, for magnetic fields close to H_{c2} where the ground state is nearly ferromagnetic, we expect the system to approach the free fermion limit, i.e., $\tilde{K}\to 1$. As a result T_1^{-1} is expected to diverge as $T^{-1/2}$ at $H=H_{c2}$ for all the models irrespective of their values of n.

Even though both the ladder and the dimerized systems have the same divergence at the critical point, one can differentiate between these two systems by studying the nondivergent contributions to T_1^{-1}. For example, for the frustrated model, there exists a correction to T_1^{-1} proportional to $T^{2\tilde{K}+(1/2\tilde{K})-1}$. This exponent changes with increasing magnetic field and corrections of a similar nature do not exist in the ladder. These corrections should manifest themselves at not too low temperatures. However, inelastic neutron scattering should be able to differentiate between them as previously discussed in Sec. V. At temperatures large compared to the exchange couplings and the gap, from the analogy with fermions we expect that $T_1^{-1}=\text{const}$ for all the models studied in this paper. A similar behavior should be seen in the gapped phase, i.e., $H<H_{c1}$ also. To summarize, we find that the kind of NMR experiments done can result in drastically different T_1^{-1} for the three models.

The results derived here can be checked in $CuGeO_3$ and various other quasi-1D systems. However, with most compounds being 3D the results obtained in this paper are applicable only in the temperature interval where the compound is effectively 1D and that there is no 3D magnetic ordering. Such a magnetic ordering in 3D could also result in divergent NMR rates. For instance, the onset of 3D Néel order at a certain temperature T_N results in T_1^{-1} diverging as $(T-T_N)^{-1/2}$ for $T>T_N$.[31] This behavior is valid for a temperature range of size T_N. Since this divergence is the same as seen in the ladder, dimerized, and frustrated systems at $H=H_{c1}$, it is important to establish whether such a divergence arises from the quasi-one-dimensional or the 3D nature of the compound. This can be checked by working in the appropriate temperature interval where there is no 3D ordering or by increasing the magnetic field. If the compound is in the 1D regime, its exponents vary with the field as predicted above and if it has 3D order the exponents do not vary with the field.

VII. CONCLUSIONS

We have studied the behaviors of various spin-$\frac{1}{2}$ models in the gapless IC phase induced by an external magnetic field. For a generic gapped spin-$\frac{1}{2}$ in a magnetic field, it was shown that the magnetization is zero below H_{c1} and rises as a square root above it. We found that the gapless behavior in the IC regime is determined by the dimension of the cosine operator and hence different systems have drastically different properties. The results presented here were obtained from a microscopic theory and not from a phenomenological theory as was done in the case of the spin-1 chain.[24] We then discussed the implications of the finite magnetization for the correlation functions. We found that the effect of the finite magnetization was to shift the $Q=\pi$ mode in the S^zS^z correlators to $Q=2\pi m$ and the $Q=0$ mode in the S^+S^- correlators to $Q=\pi(1-2m)$. We also calculated the unequal time correlation functions and have provided explicit formulas for the various susceptibilities as a function of T, ω, q, and the magnetization m. These were used to study the thermal broadening of the various modes in a single chain. We find that the modes at $Q=\pi$, $Q=2\pi m$, and $Q=\pi(1-2m)$ are broadened at finite temperatures whereas the $Q=0$ mode is not. Using the susceptibilities we also showed that neutron scattering intensities had extra peaks arising from the incommensurability in single chains but not in the ladder systems. We have also calculated the NMR relaxation rates as functions of temperature and have discussed the results for the dimerized, frustrated, and ladder systems in detail. Using the fermion analogy, we find that the phase diagram for a generic gapped chain as a function of field and temperature has five regions as shown in Fig. 3. In contrast to Ref. 24 where the system stays in the quantum critical regime for a wide range of temperatures before it crosses over to the classical high-temperature limit, we find that the system crosses over from the quantum critical regime to a second Luttinger liquid regime before it becomes classical. These intermediate temperature behaviors follow from the form of the dispersion spectrum of fermions with a gap due to interactions. Finally, even though we have given the exact values of the exponents at the critical point H_{c1} alone, a knowledge of the magnetization m from experiments can be used in conjunction with Eq. (13) to obtain the exponents and hence T_1^{-1} close to the transition at H_{c1}. We find that though magnetization measurements cannot distinguish between the various models, techniques like NMR or neutron scattering which probe the dynamical spin-spin correlations will be able to do so. Other frequently used methods to study spin systems are EPR (electron paramagnetic resonance) (Refs. 33 and 32) and Raman scattering. These methods might also be able to directly differentiate between the dimerized and ladder systems. We conclude by observing that it should be possible to verify the results obtained here in NMR measurements being done on $CuGeO_3$ and $Cu_2(C_5H_{12}N_2)_2Cl_4$.[34]

ACKNOWLEDGMENTS

We would like to thank J.P. Boucher, G. Chaboussant, and L. Levy for interesting discussions and for critical readings of the manuscript.

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