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

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Abstract

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 behaviour of the nuclear spin relaxation rate $T_1^{-1}$. We discuss the results obtained here for the special cases of the dimerised chain, frustrated chain and the spin-$\frac{1}{2}$ ladder.

I. INTRODUCTION

Quantum spin chains have been a field of intense theoretical activity for the past decade. This seems pertinent in the face of the tremendous advance made in the fabrication of quasi-one dimensional systems. There are a lot of compounds like $(TMTTF)_2X$ which are essentially spin-$\frac{1}{2}$ chains, NENP - a spin-1 chain and a host of other organic compounds whose behaviours can be adequately described within the framework of interacting spin systems. The Heisenberg model with purely nearest neighbour interactions has been instrumental in understanding various properties of these spin systems. In addition to these, there are compounds with alternation in the nearest neighbour bonds (arises as a result of interactions with phonons) eg TMTTF, strong single ion anisotropies etc. The effects of spin-Peierls dimerization, interchain interactions and competing nearest neighbour interactions have been reasonably well understood in the spin-$\frac{1}{2}$ case. 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 Neel order to spiral order or spontaneously dimerise 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 Neel (C) zero uniform magnetisation phase to an incommensurate phase (IC) with non-zero magnetisation. As the magnetic field is increased, the magnetisation 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 $Cu_2(C_5H_{12}N_2)_2Cl_4.5\overline{2}$ and the quasi one-dimensional spin-$\frac{1}{2}$ systems $TTF-CuBDT$. The C-IC transition seen in $CuGeO_3$ 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 behaviours 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 magnetisation, 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 dimerised, frustrated and ladder systems. We find that though magnetisation 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 organised as follows: Sec. 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 behaviour of the same for the cases of the dimerised, frustrated and ladder models. Sec. 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 summarise certain results relevant to the work presented here. The main hamiltonian of interest is the Heisenberg model:

$$\mathcal{H} = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$  \hspace{1cm} (1)
where the $\vec{S}_i$ is a localised 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. Eventhough 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 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 $k_F = \frac{\pi}{2}$. We then perform a linearisation 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. We just present the final expressions obtained for the spin $\frac{1}{2}$ operators in terms of the bose field $\phi$ and its dual $\theta$

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

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

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

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

where $u$ is the spin wave velocity, $\Pi$ is the momentum conjugate to the field $\phi$ 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 $\phi$ 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 behaviour of spin-$\frac{1}{2}$ chains, it has often been found that there are many other interactions between spins, apart from the the isotropic interaction summarised 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 renormalisation 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 dimerisation and frustration arising from next nearest neighbour interactions.
We first consider a small dimerization \( \delta \), which arises from spin-lattice interactions. The corresponding perturbation to the Hamiltonian given in Eq.(1) is

\[
\mathcal{H}_D = (-1)^i \delta \vec{S}_i \cdot \vec{S}_{i+1}
\]

(4)

Using Eqs.(2) the bosonized continuum version of (4) is

\[
\mathcal{H}_D = \delta \int dx \cos(2\phi)
\]

(5)

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

\[
\mathcal{H}_F = J_2 \vec{S}_i \cdot \vec{S}_{i+2}
\]

(6)

For classical spins, the ground state retains its Neel 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 behaviour 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)

\[
\mathcal{H}_F = (J_2 - J_{2c}) \int dx \cos(4\phi)
\]

(7)

Apart from the cosine terms mentioned above, these spin interactions also renormalise the velocity \( u \) in (3). We now analyse the effects of the interactions given by Eqs.(6,7). In the free boson theory of Eq.(3), the anomalous dimensions of the operators \( \cos(n\phi) \) are given by \( \frac{n^2 K}{4} \). 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 \( \delta \). 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 \( J_2 < 0.2411 \). Therefore, we can see that both \( \delta \) 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 \( \delta \) and \( J_2 > J_{2c} \).

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

\[
\mathcal{H}_{\text{gap}} = \frac{1}{2\pi} \int dx [uK(\pi\Pi)^2 + \frac{u}{K}(\partial_x \phi)^2 + \nu \cos(n\phi)]
\]

(8)

The 2-parameter space spanned by \( K \) and \( n \) correspond to various spin-\( \frac{1}{2} \) systems with gaps in their spectra. For example, \( K = \frac{1}{2}, n = 2 \) corresponds to the dimerised 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 that apart from the magnons and solitons there exist certain excitations called breathers. These are non-linear 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. 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

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

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 magnetisation i.e., $\sum S_i^z = 0$. This corresponds to a completely filled lower band for fermions with a gap $\Delta$ 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 non zero magnetisation $m$. The zero magnetisation 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 magnetised, 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. IIIA).  

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 magnetisation 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).

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

This hamiltonian has the same form as 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 a discrete symmetry (C) to a phase with a continuous symmetry(IC). Note that the gradient term in Eq.(10) can be eliminated by a simple shift of the $\phi$ field i.e., $\phi \rightarrow \phi + \pi K g\mu_B H x$. Since the only effect of $H$ below $H_{c1}$ is to renormalise the gap, we can replace this shift by $\phi \rightarrow \phi + \pi mx$ where $m$ is the magnetisation. 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 \( \pm k_F' \), linearise 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 behaviour in the gapless IC region is governed by the Hamiltonian

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

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.

Before we proceed with the calculation of \( \tilde{K} \), we first study how the magnetisation rises above \( H_{c1} \). Using the results on the C-IC transition, the magnetisation increases from its zero value as a square root near \( H_{c1} \). A similar square root behaviour is seen near \( H_{c2} \) if one approaches this critical point from the ferromagnetic side. Here it is the decrease in magnetisation from the full ferromagnetic value that shows the square root behaviour. In Fig.2, we have shown the behaviour of the magnetisation 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 magnetisation increases in a nearly linear fashion with \( H \). The interval of \( H \) in which the square root behaviour of the magnetisation 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 \( \Delta \) 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 behaviour is not observed in Ref. [7]. Since the behaviour of the magnetisation given by Eq.(12) is generic to all the gapped systems studied here, it follows that a measurement of the magnetisation will not be able to qualitatively differentiate between the various models.

The magnetisation 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-\( \frac{1}{2} \) chain. Since the spin-\( \frac{1}{2} \) ladder and the spin-1 chain belong to the same universality class [25], Eq.(12) describes the magnetisation in the spin-1 chain also. This agrees
well with the result for $m$ in spin-1 chains obtained in Ref. [20, 21]. In Ref. [21] a mapping of a phenomenological Hamiltonian of interacting magnons onto a system of bosons with repulsive $\delta$-fn interactions was used to obtain the magnetisation and the correlations in the IC regime.

Naively one might expect that these gapped systems in a magnetic field have the same qualitative behaviour 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 behaviours in the IC regime depending on the value of $n$. For a generic interaction of the form $\cos(n\phi)$ (where $n^2 K \leq 8$) and $H$ close to $H_{c_1}$ on the IC side,

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

Here $\Delta$ is the gap and $\gamma$ is a positive constant which depends on the parameters of the theory but is independent of $H$. $\theta$ is defined by $\exp(-2\theta) = n^2 K^4$. At the transition $H_{c_1}$, $\tilde{K}$ goes to a universal value $\frac{4}{n^2}$ independent of the value of $K$. As $H$ increases, there is a non-zero magnetisation $m$ and the change in $\tilde{K}$ is completely governed by $n$ and $K$ in that $\tilde{K}$ could increase or decrease depending on the value of $K$. For example, for the frustrated $(J_2)$ model $\tilde{K} = \frac{1}{4}$ at $H = H_{c_1}$ and increases as $H$ increases and for the case of the dimerised ($\delta$) model, $\tilde{K} = 1$ at $H = H_{c_1}$ and decreases with increasing $H$. Here we have shown that though the magnetisation has the same qualitative behaviour for all the models, the value of $\tilde{K}$ 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 magnetisation 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 $\phi \to \phi + \pi mx$, it is clear that since for $H < H_{c_1}$ there is no net magnetisation, the form of the correlators is unaffected and only the gap is renormalised. However, in the IC phase, the presence of a non-zero magnetisation $m$ results in $\phi \to \phi + \pi mx$. The dual field $\theta$ 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

$$\langle S^z(x, t)S^z(0, 0) \rangle = m^2 + f_1(x, t) + \cos(1 - 2m)f_2(x, t)$$
$$\langle S^+(x, t)S^-(0, 0) \rangle = \cos(2\pi mx)g_1(x, t) + \cos(\pi x)g_2(x, t)$$  \hfill (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 magnetisation or equivalently a $Q = 0$ mode while the staggered part is shifted from $Q = \pi$ to $Q = \pi - 2\pi m$. 

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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 magnetisation (\( Q = 0 \)) 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),(14) and the result of Eq.(13). The correlation functions are found to be as follows:

\[
\langle \tilde{S}^z(x, t) \tilde{S}^z(0) \rangle = \langle (S^z(x, t) - m)(S^z(0) - m) \rangle
\]

\[
= \cos(\pi x(1 - 2m))(x^2 - t^2) - \tilde{K} + \text{cste.} \frac{\tilde{K}}{4\pi^2}(\frac{1}{(x - t)^2} + \frac{1}{(x + t)^2})
\]

\[
\langle S^+(x, t) S^-(0) \rangle = (-1)^x(x^2 - t^2) - \frac{\tilde{K}}{x^2} + \text{cste.} \cos(2\pi m x)(x^2 - t^2) - (\frac{1}{4\pi} + \tilde{K} - 1).
\]

\[
\left[ \exp(2i\pi mx)\frac{1}{(x - t)^2} + \exp(-2i\pi mx)\frac{1}{(x + t)^2} \right]
\]  \( \text{(15)} \)

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 dimerised 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 dimerised 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 \((q, \omega)\) 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

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

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., \( \langle S^i S^j \rangle = 0 \) 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 \( \hat{z} \)

\[
\chi^{Q=0}_{\parallel}(q, \omega, T) = \frac{q^2}{(vq)^2 - \omega^2}
\]

\[
\chi^{Q=\pi(1-2m)}_{\parallel}(q, \omega, T) = NT^2\tilde{K}^{-2}B(\frac{\tilde{K}}{2} - i\frac{(\omega + v(q - Q))}{4\pi T}, (1 - \tilde{K})) B(\frac{\tilde{K}}{2} - i\frac{(\omega - v(q - Q))}{4\pi T}, (1 - \tilde{K}))
\]  \( \text{(17)} \)

For the perpendicular susceptibility \( \chi_{\perp} \equiv \chi_{+-} \) i.e., in the \( x - y \) plane
the excitations has the form

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

$$+ B(\frac{\omega + v(q - Q)}{4\pi T} - (1 - \beta))B(\frac{\omega - v(q - Q)}{4\pi T} - (1 - \beta))]$$

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

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

where $\alpha = \frac{1}{2\tilde{K}}$, $B(x, y)$ is the Beta function and $v$ is the effective magnetisation dependent spin velocity. $N$ and $N'$ are velocity and hence field dependent pre-factors. These expressions for the susceptibilities are valid as long $T < (H - H_{c1})$. This is because above this temperature the hamiltonian in Eq.(11) obtained by linearising 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 behaviour 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 fermionised version of spin chains with a gap the complete dispersion for the excitations has the form $\omega_k = \pm \sqrt{\tilde{T}^2 k^2 + \Delta^2}$. These two branches constitute the lower and upper bands with a gap $2\Delta$ separating the two bands. With the full dispersion, the magnetisation is given by a function which depends on two parameters $\frac{\tilde{T}}{\tilde{T}}$ and $\frac{H}{\tilde{T}}$. The different regimes to be discussed below will be characterised by the varied behaviour 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 characterised 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 the incommensurate or Luttinger liquid I regime as was already discussed in Sec. IIIB (cf. Fig.3). The dynamical exponent is $z=1$ here. The susceptibilities in Eqs.(17-19) are valid in this Luttinger liquid regime.

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 region defined by $|H - H_{c1}| < T$. In the quantum critical region the physics is governed by the fixed point at $H = H_{c1}$ where $\tilde{K}$ has a universal value $\frac{1}{\pi T}$. A simple way of understanding the behaviour in this region is presented below. Firstly, 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 $\omega_k$ in $\Delta$ to obtain $\omega_k^{QC} = \Delta + \frac{k^2}{2\Delta}$ in the quantum critical region. The dynamical exponent $z = 2$ in this region. A direct consequence of the quadratic dispersion is that $\frac{\Delta}{T}$ and $\frac{H}{T}$ are
no longer independent scaling variables and only occur in the combination $H - H_{c1}$ and the magnetisation $m$ which is just the number of fermions in the upper band has the scaling form $m(T) = T^{\frac{1}{2}} f(\frac{H - H_{c1}}{T})$. Analogous scaling functions exist for the spin-spin correlations also. The scaling functions for the correlators are functions of $k^2 T$, $\omega T$ and $H - H_{c1}$. Note that $\Delta T$ 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. 23. The quantum critical behaviour 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. 23 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. 23 because the form $\omega_k^{QC}$ 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 magnetisation 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 dispersion becomes linear in $k$. This crossover should occur for temperatures $T$ of the order of twice the gap $\Delta$ but much lesser than the exchange couplings such that the interaction becomes irrelevant and the resulting behaviour is that of a Luttinger liquid. We denote this regime as the Luttinger liquid II. Classical behaviour 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. 23. 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 $\Delta$. This width can be increased or decreased by tuning the ratio $\frac{\Delta}{J}$. Applying these arguments to the case of spin-1 chains where the gap 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 susceptibilities 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 $(q, \omega)$ fourier transform of the full spin-spin correlator $\langle S(x, t) \cdot S(0, 0) \rangle$. 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 $\omega$ for some fixed $q$, should in addition to the peak generated by the massless
excitations near $Q = 0$ contains 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. Another probe is electron spin resonance (ESR) which can be used to directly probe the nature of the continuum of excitations at $Q = 2\pi m$.

One interesting question is whether the propagating modes corresponding to the uniform and staggered magnetisation 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 susceptibilities. First consider the case of the isotropic spin-$\frac{1}{2}$ chain in zero magnetic field. Here it is known that the uniform magnetisation component of the $S^z$ correlator diverges as $\frac{1}{x^2}$. The corresponding uniform and staggered susceptibilities at finite temperatures are given by Eqs.(17) with $m = 0$ and $\tilde{K} = \frac{1}{2}$. Isotropy results in the same expressions for the perpendicular susceptibility. In this context $v$ is the spinon velocity. The dependence of $\chi^{Q=\pi}_{\|}$ on temperature tells us that the $Q = \pi$ mode is damped at finite $T$. The temperature independence of the $\chi^{Q=0}_{\|}$ implies that there is no damping of the $Q = 0$ mode at finite $T$. This can also be understood from the fact that the exponent $\beta$ in Eq.(18) is zero at $K = \frac{1}{2}$. 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 magnetisation 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 magnetisation 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 non-integral exponent $\beta$ in $\chi^{Q=2\pi m}_{\perp}$ results in the $Q = 2\pi m$ mode being damped at finite temperatures by a factor proportional to $T^{2\beta}$. Similarly the behaviour of the $Q = \pi(1 - 2m)$ mode is dictated by $\chi^{Q=\pi(1-2m)}_{\|}$ 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 $\chi^{Q=0}_{\|}$. From Eqs.(17), we find that the parallel susceptibility does not damp the $Q = 0$ modes because $\chi^{Q=0}_{\|}$ is still independent of temperature. Because the system is not isotropic we need to check whether there is a sub-dominant 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 \( \omega \) is fixed at \( v\delta q \). The low temperature behaviour of the imaginary part of the susceptibility is given by

\[
\frac{\beta}{2} \omega^{\beta-1} T^{\beta+1} + \frac{2}{\beta} \omega^{\beta+1} T^{\beta-1}
\]

This expression implies that there is a thermal broadening of the \( Q = 0 \) or uniform magnetisation mode i.e., \( \delta q = -2 \pi m \). Nevertheless, using the fact that the total magnetisation in the \( \hat{z} \)- direction still commutes with the hamiltonian even in the presence of the magnetic field and that the time evolution of \( \sum_i S_i^z \) involves only \( \sum_i S_i^+ \) we conclude that there is no thermal broadening of the uniform mode (\( Q = 0 \)) mode. If \( \omega \) is not at the resonance frequency then for low \( T \), there is no obvious thermal broadening and \( \text{Im} \chi_{Q=2\pi m} \) 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 bosonisation 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 linearising at \( k'_F \) we take into account a lot of spurious states at the bottom of the band. To summarise, we find that the \( Q = 0 \) mode is undamped whereas the gapless modes at \( Q = 2\pi m, \pi(1 - 2m) \) and \( \pi \) are all damped.

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

Another system which exhibits a behaviour 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 that in chain 2, \( \vec{S}_2 \). We bosonize this system in the same manner as above. We refer the reader to Ref.\[20,27,28\] for details. We adopt the notations of these references and introduce the symmetric (triplet) and antisymmetric (singlet) combinations of the fields: \( \phi_{s,a} = \frac{\phi_1 \pm \phi_2}{\sqrt{2}} \) and their respective duals \( \theta_s \) and \( \theta_a \). The hamiltonian for the ladder is

\[ H = H_a + H_s \]  

where

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

\[
H_s = \frac{1}{2\pi} \int dx [Ku(\pi \Pi_s)^2 + \left( \frac{u}{K} \right)(\partial_x \phi_s)^2 + g_3 \cos(\sqrt{8} \phi_s)]
\]  

where \( K = \frac{1}{2}, g_1 = g_2 = g_3 = \frac{J_1 J_2}{2\pi} \) and \( J_1 \) is the interchain coupling and \( \lambda \) some constant. All the cosine operators are relevant operators of dimension one. Eqs.(22) have the same form as the hamiltonian for an isotropic spin-1 system written in terms of two spin-$\frac{1}{2}$ operators\[20\]. 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 \( J_1 \). 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
non-zero values of $J_{\perp}$ in the spectra of both the fields $\phi_a$ and $\phi_s$. The ground state of the ladder is a spin singlet and there exists a gap to the triplet excited state characterised by $\phi_s$. Therefore, analogous to the dimerised 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 $\phi_s$ field

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

(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 $\phi_s$ field becomes massless while in the antisymmetric sector the $\theta_a$ field acquires a non-zero expectation value and the $\phi_a$ still has a gap. As a result the correlations of the $\phi_a$ field decay exponentially. The value of $\tilde{K}$ for the $\phi_s$ 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 summarise the results for the various correlators below. Since we are concerned only with the asymptotic behaviours we present only the power law contributions to these correlators.

$$\langle S^+_r(x, t)S^+_t(0, 0) \rangle = m^2 + \frac{1}{8\pi^2} \left[ \frac{1}{(x-t)^2} + \frac{1}{(x+t)^2} \right]$$

(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

$$\langle S^+_1(x, t)S^-_1(0, 0) \rangle = \langle S^+_2(x, t)S^-_2(0, 0) \rangle$$

$$= (-1)^x(x^2 - v^2t^2)^{-\frac{1}{4\tilde{K}}}$$

$$\langle S^+_1(x, t)S^-_2(0, 0) \rangle = i(-1)^x(x^2 - v^2t^2)^{-\frac{1}{4\tilde{K}}}$$

(25)

Here again the uniform component is shifted to $Q = 2\pi m$ and decays exponentially. The fact that $\phi_a$ 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 behaviours. 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]. The dominant contribution to the perpendicular susceptibility for the ladder has the same form as that given in Eq.(19) with $\alpha = \frac{1}{8\tilde{K}}$ and that to the parallel susceptibility by $\chi^Q=0$ of Eq.(17). At the critical point $H = H_{c1}$, the exponent $\alpha = \frac{1}{4}$ for the ladder as well as the dimerised model. However, there is one big difference between the two models. In the dimerised model, the incommensurate parts of the $\langle S^zS^z \rangle$ and $\langle S^+S^- \rangle$
also show power law behaviours whereas, in the ladder they decay exponentially. This has a serious consequence for neutron scattering intensities. This is because for the dimerised 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 \( \phi_a \) 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 susceptibilities 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 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:

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

Here the \( F_{ij} \) are hyperfine form factors and \( \chi_{ij} \) 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 non-interacting spins, \( (T_1 T)^{-1} \) 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 non-zero 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 magnetisation \( m \) 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 susceptibilities 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 neighbouring 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 susceptibilities 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 behaviour for the single chain models:

\[
\left[ \frac{1}{T_1} \right]^{\text{single chain}} = A_{\perp} T_{2K}^{-1} + A_{\parallel} T^{2K-1} + B_{\parallel} T \tag{27}
\]
where $\tilde{K}$ 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

$$\left[\frac{1}{T_1}\right]^{\text{ladder}} = A_\perp T_1 \tilde{K}^{-1} + B_\parallel T$$

(28)

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

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

Dimerised ($\delta$):

$$\frac{1}{T_1} = (A_\parallel + B_\parallel) T + A_\perp T_1^{-\frac{1}{2}}$$

(29)

Frustrated models ($J_2$):

$$\frac{1}{T_1} = A_\parallel T_1^{-\frac{1}{2}} + (A_\perp + B_\parallel) T$$

(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 $T^{-\frac{1}{2}}$ for the three models. However, the divergent behaviour at low temperature in the frustrated model arises from the parallel susceptibility whereas in the ladder and dimerised systems it is the perpendicular susceptibility which leads to the divergent behaviour. 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 $\tilde{K}$ increases for the frustrated model and the divergence becomes weaker. Coincidentally $\tilde{K}$ decreases for the dimerised system and the divergence of $T_1^{-1}$ becomes weaker too. For the ladder, $\tilde{K}$ does not change with $H$ and the divergence persists and one has to go to higher fields to see a deviation from the $T^{-\frac{1}{2}}$ behaviour. If for some value of $H$, $\tilde{K}$ decreases to $\frac{1}{2}$ in the dimerised 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 behaviour 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 $T^{-\frac{1}{2}}$ for the dimerised 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 non-zero constant as $T \to 0$ as it does in the case of the Heisenberg model. 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 $T^{-\frac{1}{2}}$ divergence survives in the ladder but for dimerised 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 $T^{-\frac{1}{2}}$ at $H = H_{c2}$ for all the models irrespective of their values of $n$.

Even though both the ladder and the dimerised systems have the same divergence at the critical point, one can differentiate between these two systems by studying the non-divergent contributions to $T_1^{-1}$. For example, for the frustrated model, there exists a correction to $T_1^{-1}$ proportional to $T^{2\tilde{K} + \frac{1}{2\pi} - 1}$. 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 $T_1^{-1} = cste$ for all the models studied in this paper. A similar behaviour should be seen in the gapped phase i.e., $H < H_{c1}$ also. To summarise, 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 Neel order at a certain temperature $T_N$, results in $T_1^{-1}$ diverging as $(T - T_N)^{-\frac{1}{2}}$ for $T > T_N$. This behaviour is valid for a temperature range of size $T_N$. Since this divergence is the same as seen in the ladder, dimerised 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 behaviours 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 magnetisation is zero below $H_{c1}$ and rises as a square root above it. We found that the gapless behaviour 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. We then discussed the implications of the finite magnetisation for the correlation functions. We found that the effect of the finite magnetisation 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 $T, \omega, q$ and the magnetisation $m$. 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 dimerised, 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. where the system stays in the quantum critical regime for a wide range 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. This intermediate temperature behaviours follow from the form of the dispersion spectrum of fermions with a gap due to interactions. Lastly, even though we have given the exact values of the exponents at the critical point $H_{c1}$ alone, a knowledge of the magnetisation $m$ 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 magnetisation 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) and Raman scattering. These methods might also be able to directly differentiate between the dimerised and ladder systems. We conclude by observing that it should be possible to verify the results obtained here in NMR measurements being done on $\text{CuGeO}_3$ and $\text{Cu}_2(\text{C}_{5}\text{H}_{12}\text{N}_2)_2\text{Cl}_4$. 

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REFERENCES

1 I. Affleck in Fields, Strings and Critical Phenomena, ed E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1990), 563 and references therein.
2 J.P. Renard et al, Europhys. Lett. 3, 945 (1987).
3 L.J. de Jongh and A.R. Miedma, Adv. Phys. 23, 1 (1974).
4 J.C. Bonner and M.E. Fisher, Phys. Rev B 22, 5274 (1980).
5 F.D.M. Haldane, Phys. Lett. 93A, 464 (1983); I. Affleck, Nucl. Phys. B265, 409 (1986).
6 C.K. Majumdar and D.K. Ghosh, J. Math. Phys. 10, 1388 (1969).
7 G. Chaboussant et al, preprint LCMI /Meso-95-3.
8 V. Kiryukhin, B. Keimer and Moncton, Phys. Rev. Lett. 74, 1669 (1995).
9 M. Hase et al., Phys. Rev. Lett. 70, 3651 (1993).
10 J.P. Pouget et al, Phys. Rev. Lett. 72, 4037 (1994) and references therein.
11 T.M. Brill et al Phys. Rev. Lett. 73, 1545 (1994).
12 K. Okamoto and K. Nomura, Phys. Lett. 169A, 433 (1992).
13 R.F. Dashen, B. Hasslacher and A. Neveu, Phys. Rev D 10, 4130 (1974).
14 K. Maki and H. Takayama, Phys. Rev B 22, 5302 (1980).
15 D. Reich, L.P. Levy and T. Giamarchi Phys. Rev. Lett. 67, 2207 (1991).
16 R. Chitra et al Phys. Rev B 52, 6581 (1995).
17 T. Tonegawa and I. Harada, J. Phys. Soc. Jpn. 56, 2153 (1987).
18 V.L. Pokrovsky and A.L. Talapov, Phys. Rev. Lett. 42, 65 (1979).
19 H.J. Schulz Phys. Rev. B 22, 5274 (1980).
20 H.J. Schulz Phys. Rev B. 34, 6372 (1986).
21 I. Affleck, Phys. Rev. B 43, 3215 (1991).
22 M.C. Cross and D.S. Fisher, Phys. Rev. B 19, 402 (1979).
23 S. Sachdev, T. Senthil and R. Shankar, Phys. Rev. B 50, 258 (1994).
24 C. Broholm (private communication) and D.C. Dender, D.H. Reich, C. Broholm and G. Aeppli, unpublished (1996).
25 W. Palme et al, Phys. Rev. Lett. 76, 4817 (1996).
26 S. Sachdev, Phys. Rev. B 50, 13006 (1994).
27 D.G. Shelton, A.A. Nersesyan and A.M. Tsvelik, Phys. Rev. B 53, 8521 (1996).
28 S.P. Strong and A.J. Millis, Phys. Rev. Lett. 69, 2419 (1992).
29 T. Moriya, J. Phys. Soc. of Jpn. 18, 516 (1963).
30 T. Moriya and K. Ueda, Sol. State Comm. 15, 169 (1964).
31 P.M. Richards and M.B. Salamon, Phys. Rev. B 9, 32 (1974).
32 I.S. Jacobs et al, Phys. Rev. B 14, 3036 (1976).
33 G. Chaboussant, L. Levy et al (unpublished).
Table I

Temperature dependence of $T^{-1}_1$ at $H = H_{c1}$

| Model                  | $K$ at $H_{c1}$ | $T^{-1}_{1\parallel}$ | $T^{-1}_{1\perp}$ |
|------------------------|-----------------|------------------------|-------------------|
| Spin-Peierls ($\delta$)| 1               | $T$                    | $T^{-\frac{1}{2}}$ |
| Frustration ($J_2$)    | $\frac{1}{4}$   | $T^{-\frac{1}{2}}$    | $T$               |
| Ladder                 | $\frac{1}{2}$   | $T$                    | $T^{-\frac{1}{2}}$ |
Figure Captions

1. Schematic picture of the field dependent dispersion in the IC phase as seen by \( S^z S^z \) 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.

2. Plot of the magnetisation \( m \) (apart from an overall normalisation) versus magnetic field \( H \) for \( \Delta = 0.4J \) at various temperatures \( T \). \( H \) and \( T \) have been normalised by the exchange coupling \( J \). The solid line corresponds to \( T = 0 \), the dashed line at \( T = 0.05 \) and the dashed dot 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.

3. Phase diagram of gapped spin-\( \frac{1}{2} \) chains in a magnetic field \( H \) as a function of temperature \( T \). There are essentially 5 regions and all the lines indicate crossovers between these regions.
$E(q)$
Quantum Critical Luttinger Liquid

Classical Luttinger Liquid

Gapped

Quantum Critical

H_{c1}

J

T

Δ

H