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LETTER TO THE EDITOR

Incommensuration in quantum antiferromagnetic chain

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Abstract. A dimerized quantum Heisenberg or XY antiferromagnetic chain has a gap in the spectrum. We show that a weak incommensurate modulation around a dimerized chain produces a zero-temperature quantum critical point. As the incommensuration wavelength is varied, there is a transition to a modulated gapless state. The critical behaviour is in the universality class of the classical commensurate–incommensurate (Pokrovsky–Talapov) transition. An analogous metal–insulator transition can also take place for an incommensurate chain.

The one-dimensional $S = \frac{1}{2}$ quantum antiferromagnetic Heisenberg model is a prototypical example of quantum fluctuations destroying the classical ground state [1–6]. Such a uniform chain, with gapless excitations, can undergo a spin–Peierls (SP) transition to a lattice dimerized state via the interplay of spins and lattice distortion, going over to an incommensurate phase in large magnetic fields [7–10]. The SP state has a gap in the spectrum. However, specific heat measurements in the incommensurate phase of the inorganic insulator $CuGeO_3$ [10] hint [11, 12] towards a gapless phase. This, then, raises a few basic questions. Can a weak incommensuration around a dimerized Heisenberg (or XY) chain support *gapless* excitations, even though the dimerized case *does not*? If it is true, then is there a quantum critical point (QCP) separating a gapless state and a gappy state (a state with a gap)? What would be the nature of the quantum critical point?

In order to address these issues for the incommensurate phase, and to gain an understanding of the underlying phenomena, one may consider a simpler situation of a static case where the coupling constant follows the incommensurate modulation of the lattice. We therefore consider a model Hamiltonian

$$H = \sum_{j=1}^{N} \left[\frac{J_j}{2} (S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) \right] + h \sum_j S_j^z \tag{1}$$

where $S_j^{\pm} = S_j^x \pm \mathrm{i} S_j^y$ are the spin raising and lowering operators at site j, and h is the magnetic field in the z-direction. The case of interest in this paper is $J_j = J + \delta \cos(\pi + q)\, j$, with $\delta \ll J > 0$. This corresponds to a weak incommensuration around the dimer phase ($q = 0$). For $\delta = 0$, the system is gapless (uniform chain). For $q = 0$, a gap develops in zero field for $\delta \neq 0$ but a gapless phase is recovered above a critical magnetic field h_c [13]. Our aim is to get the phases in the (q, h) plane for $\delta \ll 1$, based on low-energy excitations.

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We are considering the XY model, because, so far as the gap is concerned the difference between XY and Heisenberg chain is not crucial (see equation (6)). Admittedly, for the SP problem, the spin–lattice interaction and the magnetic field play important roles [14] and correlate [15] q and h. A real system would follow a particular trajectory $q = q(h)$ in the (q, h) phase diagram. We therefore take q and h as independent parameters.

Equation (1) also describes, via a Jordon Wigner transformation [16], spinless fermions on a one-dimensional lattice—a description we use in this paper. By defining $C_j = K(j)S_j^-$ as the fermionic annihilation operator, where $K(j) = \exp(\mathrm{i}\pi \sum_{n=1}^{j-1} S_n^+ S_n^-)$ is the nonlocal kink operator, the spin Hamiltonian of equation (1) can be written as

$$H = \tfrac{1}{2} \sum J_j (C_j^\dagger C_{j+1} + C_{j+1}^\dagger C_j) - h \sum_j C_j^\dagger C_j. \tag{2}$$

Note that the fermions have *incommensurate hopping* rates, and h acts as a chemical potential.

A QCP is a phase transition point with a diverging length scale induced by a change of a parameter of the Hamiltonian at zero temperature (Chakrabarti *et al* [1]). Since quantum fluctuation is responsible for such criticality, the dynamic exponent z, determining the scaling of time and space, becomes more important than in thermal critical points ($\tau \sim \xi^z$ with τ and ξ as characteristic diverging time- and length scales). In the spin–chain context, a well known QCP is the dimerization point $\delta = 0$ for $q = h = 0$ for equation (1) or (2). This critical point (separating a gapless state and a gappy state) corresponds to free fermions with $z = 1$ and a correlation length diverging as $\xi = \delta^{-1}$. The spin–spin correlation function $C(r, \delta) = \langle S_i^z S_{i+r}^z \rangle$ has a scaling behaviour $C(r, \delta) = r^{-\eta} f(r\delta)$ with $\eta = 2$ [17]. For the QCP of concern in this paper, we start from the dimerized gappy state and change the incommesuration q keeping δ fixed.

A QCP for $q = 0$ at $\delta = 0$ ensures the existence of a continuum limit of the lattice problem. We use this continuum limit to study the effect of q on the phase diagram, and in a renormalzation group (RG) framework only the relevant terms need to be kept. To go to the continuum limit, we adopt the technique of bosonization for the low-energy excitations around the fermi points [18, 16, 19]. Also since wavenumber is no longer a good quantum number, we work in the real space. The low-energy excitations of equation (2) across the fermi surface on the two branches can be described by L (left) or R (right) moving particles with linear spectrum. This gives $z = 1$. In the continuum limit, the Hamiltonian is written in terms of the (bosonic) phase variables. The free bosonic theory corresponding to J_j = constant, $h = 0$ turns out to be just the harmonic lattice Hamiltonian, which forms the basis for the subsequent analysis of the remaining terms such as dimerization, incommensuration around the dimerized case and the magnetic field. The relevance or irrelevance of various terms come from their scaling behaviour on a long length and timescale. In the RG approach, the scaling behaviour is obtained by integrating out the short distance fluctuations in both directions and incorporating their effects in the parameters of the problem. This is implemented by studying the Euclidean version of the problem (i.e. imaginary time, $t \to \mathrm{i}t$).

For low-energy excitations, we define new operators $a_j = (i)^{-j} C_j$ to eliminate the fast variation at the Fermi vector. From these, right and left movers are defined by the chiral transformation $R(j) = (a_{2j} - a_{2j-1})/\sqrt{2}$ and $L(j) = (a_{2j} + a_{2j-1})/\sqrt{2}$ so that the continuum version of the Hamiltonian can be written as

$$H = \mathrm{i} \int \mathrm{d}x \, J[L^\dagger(x)\partial_x L(x) - R^\dagger(x)\partial_x R(x)] \tag{3a}$$

$$-\frac{\mathrm{i}}{2}\int \mathrm{d}x\, \partial J(x)(R^{\dagger}(x)R(x) - L^{\dagger}(x)L(x)) \tag{3b}$$

$$+\frac{\mathrm{i}}{2}a_0\int \mathrm{d}x\, \partial^2 J(x)(R^{\dagger}(x)L(x) - L^{\dagger}(x)R(x)) \tag{3c}$$

where for simplicity the modulated part of the coupling has been ignored in equation (3*a*). This is justified by the modified Harris criterion of [22] since incommensuration $\delta\cos(2k_f + q)x$ is bounded. The notation $\partial J(x)$ and $\partial^2 J(x)$ denote the appropriate continuum limit of the discrete difference of the modulation of the couplings.

The bosonic operators are obtained from the phases [8, 23] of $R(x)$ and $L(x)$,

$$R(x) = \frac{1}{\sqrt{2\pi a_0}}\exp(\mathrm{i}k_f x - \phi_1(x)) \tag{4}$$

$$L(x) = \frac{1}{\sqrt{2\pi a_0}}\exp(-\mathrm{i}k_f x - \phi_2(x)) \tag{5}$$

with $k_f = \pi/2$, so that $\theta(x) = \mathrm{i}(\phi_1(x) + \phi_2(x))$, and the conjugate momentum p are related to the density and current respectively as $\partial\theta/\partial x = R^{\dagger}R + L^{\dagger}L$ and $p = R^{\dagger}R - L^{\dagger}L$. With this choice, the free part of the bosonic Hamiltonian (analogous to the first term, equation (3*a*)) is the standard harmonic chain Hamiltonian

$$H_0 = \frac{1}{2\pi}\int \mathrm{d}x\, \left[\frac{1}{K}\left(\frac{\mathrm{d}\theta}{\mathrm{d}x}\right)^2 + K(\pi p)^2\right] \tag{6}$$

in units of $\hbar = 1$ and spin wave velocity = 1. Here, $K = 4$ for the XY model. For the full isotropic Heisenberg Hamiltonian or interacting fermions in the fermionic language, $K = 2$. The second term, equation (3*b*), is analogous to a current-type term which is absent if one goes over to the dimer limit (recovering translational symmetry) and is expected in the incommensurate case on symmetry grounds (or lack of it). In the bosonic variables, the current term in equation (3*b*) is like $\delta q \sin Qxp(x)$, where $Q = 2k_f + q$, and it vanishes in the limit $q \to 0$. However, because of the oscillatory coefficient with average zero over a period, we ignore this term in the present analysis. The third term (3*c*) shows that a spatially varying J gives rise to a umklapp scattering process which apparently violates momentum conservation by $2k_f$. This is a special term needed mainly because of the underlying lattice in the problem. Considering only slow variations in the bosonic field θ, the umklapp term can be written [23] as $\approx \frac{\delta}{4\pi}\int \mathrm{d}x\, Q^2\cos(\theta(x) - [2k_f - Q]x)$, by shifting $\theta \to \theta - \pi/2$. The bosonized version of the incommensurate Hamiltonian is therefore (prime denoting spatial derivative)

$$H = \frac{1}{2\pi}\int \mathrm{d}x\, \left[\frac{1}{K}(\theta')^2 + K(\pi p)^2\right] - \frac{\delta\pi}{4}\int \mathrm{d}x\, \cos(\theta(x) + qx). \tag{7}$$

The dimer limit is restored by taking $q = 0$ and in this limit with $k_f = \pi/2$ the umklapp term agrees with Nakano and Fukuyama [23] who obtained a similar term in the presence of a constant bond alteration. The above bosonic Hamiltonian has resemblance with the Hamiltonian that appears in theory of incommensurate crystals [24]. In those problems q plays the same role of incommensuration vector. Such a Hamiltonian also occurs in the Frenkel–Kontorowa model [25] of a harmonic chain in an external cosine potential. This similarity shows that the solitons expected in such cosine potentials are also important in the spin–chain problem.

To study the relevance or irrelevance of the sine-Gordon term, we implement a RG analysis, well documented in [26, 24]. The basic steps involve obtaining a functional integral $\int \mathrm{e}^{\mathrm{i}S(\theta)}\,\mathrm{d}\theta$ where $S(\theta)$ is a dimensionless action. By going over to imaginary time $\tau = \mathrm{i}t$

the integral is written as a partition function of a classical two-dimensional problem. A further shift of the field variable $\theta(x,\tau) = \theta(x,\tau) - qx$, gives the classical Hamiltonian† as

$$H = \frac{1}{\pi K}\int \mathrm{d}\tau\, \mathrm{d}x\, [\tfrac{1}{2}\dot{\theta}^2 + \tfrac{1}{2}(\theta' - q)^2 - \Delta\cos\theta] \tag{8}$$

where $\Delta = \delta\pi^2 K/4$.

The RG procedure [26] for $q = 0$ involves decomposing the cosine term into fast and slowly varying components of θ for $\Delta \ll 1$ and then averaging out the fast varying component with respect to its Gaussian distribution. Absorbing the contribution from the averaged fast component in Δ we can have the renormalization of the Δ as $\Delta_R = \Delta^{1/(1-\beta^2/8\pi)}$, where $\beta^2 = \pi K$. For $\beta < \sqrt{8\pi}$, the sine-Gordon term is relevant and yields a massive theory. The Heisenberg or the XY model belongs to this category and, as expected, any dimerization produces a gap in the spectrum, with the gap scaling as Δ_R, and therefore scaling as $\delta^{8/(8-K)}$. With the incommensurate term, the system can disregard the potential if $q\theta'$ is comparable to the cosine potential energy. This gives the phase transition point [24] as $q_c \sim \delta^{4/(8-K)}$. For the XY model, the transition to the gapless phase is in the same universality class as the commensurate–incommensurate transition in two dimensions [24, 27]. For this universality class, the relativistic invariance leading to $z = 1$ is lost. The spatial length scale exponent is $\nu = \frac{1}{2}$ with $z = 2$ [29, 28].

The results imply that the gap at the Fermi level persists for small q incommensurations around the dimerized phase. Isolated states might well appear in the gap but they do not destroy the gap. The spins basically follow a dimerized lattice. For larger incommensuration, i.e. for $q > q_c$, the spins follow the dimerized lattice over a finite length scale separated by defects or solitons. Such (spin $\frac{1}{2}$) solitons do exist for the dimerized chain [23]. Though the solitons cost energy, a many soliton state for large q would be favourable compared with, say, following the dimerized lattice over the whole length (a no soliton state) because of the energy gain through the 'q' term in equation (8). In this phase with a finite density of solitons, translational invariance is recovered because these solitons are not bound to the underlying lattice, and one gets back a massless mode. The density ρ of these solitons is given by $\langle\theta'\rangle$, and this density can act as the order parameter for the transition. In the gappy phase, ρ is zero (no soliton or domain wall), while ρ is nonzero in the gapless phase. The dependence of ρ on the deviation from the critical point is obtained by matching the chemical potential to the relativistic Fermi energy. This leads to a density $\sim(q - q_c)^\beta$ with $\beta = \frac{1}{2}$. In one dimension, a length scale l can also be defined from ρ as the average separation of the solitons. This length l diverges ($l \sim (q - q_c)^{-\nu}$) with an exponent $\nu = \beta = \frac{1}{2}$ as the critical point is reached on the gapless side. Because of the high energy involved in the soliton formation, there will be no critical divergences in the gappy state [28, 29, 27]. The gapless phase is not identical to the free fermion phase, mainly because of the existence of a length scale l for the average domain size within which the system follows the dimerized lattice. For example, the equal time spin–spin correlation function $C(r, q)$ would have an algebraic decay as for free fermions or the dimerization QCP with $\eta = 2$, but for the incommensurate QCP, there will be an additional oscillatory factor $\cos(r/l)$ [28, 29]. Such oscillatory factors would be detectable in scattering experiments.

For the spin system, the phase transition induced by the incommensuration q signals the formation of a band at the fermi surface (in zero field) through the wandering of the solitons which in one dimension also act like noninteracting fermions [28, 27]. The low-lying spectrum therefore becomes gapless. A simple dimensional analysis suggests that

† Note that the current term would have changed the $\dot{\theta}$ term as well, and the general form of the square gradient term would have been $(\nabla\theta - \boldsymbol{A}(x))^2$ with $\boldsymbol{A}$ depending only on the space coordinate.

the width of the band formed around the Fermi level is $w \sim 1/l^2$. We, therefore, expect the bandwidth to vanish as $w \sim |q - q_c|^{2\beta}$, i.e. linearly on the gapless side. According to the bosonization rules the local magnetization is proportional to $\langle\theta'\rangle$ so that the soliton density also determines the magnetization in the phase. Therefore the gappy phase will be nonmagnetic but the gapless phase is magnetic and the magnetization vanishes with the Pokrovsky–Talapov exponent $\beta = \frac{1}{2}$.

So far we have considered the zero-field case. The magnetic field acts as the chemical potential of the fermions, as seen in equation (2), and so long as the Fermi surface is in a band, the equivalent bosonized Hamiltonian will be of the form equation (6), with a renormalized K and the spin wave velocity (taken to be unity). Since h couples to $\partial\theta/\partial x$, such a magnetic field for a dimerized chain would have an equivalent bosonized Hamiltonian as equation (8) with h replacing q. The critical behaviour as the Fermi surface reaches the boundary of the gap will therefore be similar to what we have already studied. This has explicitly been shown in [13]. If the band formed by the solitons lies entirely in the original gap, then by shifting the Fermi level the system can go from a gapless to a gappy state and then again to a gapless phase.

Our analysis though aimed at the spin problem is equally valid for hopping spinless fermions on a one-dimensional incommensurate lattice, i.e. on a lattice with incommensurate hopping rates, as given by equation (2). We can therefore conclude that for a half-filled lattice, there will be an insulator–metal transition as the incommensuration wavelength is varied. One-dimensional incommensurate systems can therefore be classified as metals or insulators based on the incommensuration. It might be possible to observe such a metal–insulator transition in an incommensurate crystal (incommensuration around dimerized lattice) by changing say temperature or other external parameters that control the incommensuration of the lattice.

As emphasized at the beginning, our analysis is tied to the dimerized gappy phase, the existence of a continuum limit, and the perturbative RG (i.e. $\delta \ll 1$). From the similarity with the Frenkel–Kontorowa model in the continuum limit, equation (7), and the possibility of a gap in the original Hamiltonian of equation (1) whenever the wavevector $Q = \pi + q$ is a rational fraction of the Fermi wavevector, it is expected to have stable lock-in phases [24, 25] around certain rational fractions. Our procedure would then yield similar critical behaviour around each such lock-in gappy phase. To get the full phase diagram (and the possibility of a Devil's staircase [24, 25]) one needs to study the original lattice model as the strength of the incommensuration δ is increased. Also strong incommensuration may completely destroy the band structure yielding point spectrum as known for quasiperiodic systems [30]. These remain to be studied.

To summarize, we have studied the effect of incommensuration in a quantum antiferromagnetic Heisenberg or XY chain and found a quantum critical behaviour induced by incommensurability q around dimerization. Using RG results we find that, in zero magnetic field, with the increase of the lattice incommensurability the massive theory reduces to a massless theory through a *continuous* transition at zero temperature. This indicates a transition from a nonmagnetic gappy (as in the dimerized case) to a gapless magnetic phase. The critical behaviour of this transition is found to be in the same universality class as the two-dimensional commensurate–incommensurate transition, with all singular features appearing *only* on the incommensurate gapless state. Correlation functions will have characteristic oscillatory factors that distinguish the incommensurate phase from the gapless free fermion phase. This prediction could be tested in synthetic one-dimensional magnetic chains. We have also pointed out that our results are equally valid for spinless fermions on special types of incommensurate crystals. Therefore the prediction and critical

nature of the metal–insulator transition induced by incommensuration around a dimerized lattice can be tested in properly fabricated incommensurate heterojunctions [31].

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