Critical Behaviour of Structure Factors at a Quantum Phase Transition

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We discuss the critical behaviour of structure factors at a quantum phase transition, for quantum spin models at temperature T = 0. The theory is reviewed, and compared with exact or numerical results for various specific models. The differing behaviour of the 1-particle residue and structure functions are highlighted.

1. Introduction

Modern probes of material properties, such as the new inelastic neutron scattering facilities, are reaching such unprecedented sensitivity that they can measure the spectrum not only of a single quasiparticle excitation, but even two-particle excitations (see e.g. [1]). These quasiparticles can collide, scatter, or form bound states just like elementary particles in free space. The spectrum of the multiparticle excitations is a crucial indicator of the underlying dynamics of the system.

The experiments measure scattering cross-sections, which are proportional to the appropriate 'structure factor' for the system or material at hand. It is therefore of particular interest to explore the critical behaviour of these structure factors in the vicinity of a quantum phase transition. We compare the theoretical predictions with some exact analytic results and numerical calculations for various models. We will only consider temperature T=0.

2. Review of Theory

The neutron scattering cross section is proportional to the dynamical structure factor [2]

$$S^{\alpha\gamma}(\mathbf{k},\omega) = 1/2\pi N \sum_{i,j} \int_{-\infty}^{\infty} dt \exp[i(\omega t - \mathbf{k}.(\mathbf{r_j}-\mathbf{r_i}))] < S^{\alpha}_j(t) S^{\gamma}_i(0) >_0 \qquad (1)$$

where α,γ label Cartesian components of the spin operator S_i at site i, N is the number of lattice sites, and the angular bracket denotes the ground-state expectation value. Introduce a complete set of energy eigenstates $|n\rangle$ in equation (1) and integrate over time to obtain a sum over 'exclusive' structure factors or 'spectral weights' $S^{\alpha\gamma}{}_n$,

$$S^{\alpha\gamma}(\mathbf{k},\omega) = \sum_n S^{\alpha\gamma}{}_n(\mathbf{k},\omega), \qquad S^{\alpha\gamma}{}_n(\mathbf{k},\omega) = 1/N \sum_n \delta(\omega - E_n + E_0) \left|\sum_i \langle\psi_n|S^{\gamma}_i|\psi_0\rangle \exp[i\mathbf{k}.\mathbf{r}_i]\right|^2 \quad (2)$$

where E_n is the energy of the nth eigenstate, and $|\psi_0\rangle$ is the ground state (here we assume S^{α} and S^{γ} are Hermitian conjugates). The intermediate states n can be classified into 1-particle, 2-particle or many-particle states. Integrating over energy gives the `integrated' or 'static' structure factor, the spatial Fourier transform of the 2-spin correlator at equal times:

$$S^{\alpha\gamma}(\mathbf{k}) = \int_{-\infty}^{\infty} d\omega\, S^{\alpha\gamma}(\mathbf{k},\omega) = 1/N \sum_{i,j} \exp[i\mathbf{k}.(\mathbf{r_i}-\mathbf{r_j})] < S^{\alpha}_j S^{\gamma}_j >. \qquad (3)$$

Critical Behaviour near a Quantum Phase Transition

Now let us suppose that a quantum spin model undergoes a quantum phase transition as a function of some coupling λ at temperature T=0. In the continuum approximation near the critical point, equation (3) reduces to

$$S^{\alpha\gamma}(\mathbf{k}) = \int d^d r \exp[[i\mathbf{k}.\mathbf{r}] < S^{\alpha}(\mathbf{r}) S^{\gamma}(0) >_0 \qquad (4)$$

where d is the number of spatial dimensions. The oscillating factor exp[i**k**.**r**] will kill off the

contributions from large distances unless it is compensated by a corresponding oscillation exp[-i$\mathbf{k_0}$.$\mathbf{r}$] in the correlation function. Then we can write

$$S^{\alpha\gamma}(\mathbf{k}) = \int d^d r \exp[i\mathbf{q}.\mathbf{r}]\, g(r) \qquad (5)$$

where $\mathbf{q} = \mathbf{k}-\mathbf{k_0}$, and g(r) is a smooth function. Scaling theory then tells us that in the vicinity of the critical point $g(r) \sim r^{-(d+z-2+\eta)}\, f(r/\xi)$, where ξ is the correlation length, and z is the dynamic critical exponent. Hence one can show that as the coupling $\lambda \to \lambda_c$, corresponding to a quantum phase transition, we expect

$$S^{\alpha\gamma}(\mathbf{k}_0) \sim |\lambda_c - \lambda|^{-(2-z-\eta)\nu}. \qquad (6)$$

For the 1-particle exclusive structure factor, Sachdev [3] shows the following, assuming relativistic invariance of the effective field theory (i.e. z =1), which applies to many though not all models. Let the 1-particle energy be $E(\mathbf{k}) = \sqrt{(c^2k^2 + \Delta^2)}$ near the critical point, then we can write the dynamic structure factor for the 1-particle state

$$S^{\alpha\gamma}{}_{1p}(\mathbf{k},\omega) = A^{\alpha\gamma}(\mathbf{k})/(2E(\mathbf{k}))\, \delta(\omega-E(\mathbf{k})) \qquad (7)$$

and hence the static structure factor

$$S^{\alpha\gamma}{}_{1p}(\mathbf{k}) = \int_{-\infty}^{\infty} d\omega\, S^{\alpha\gamma}{}_{1p}(\mathbf{k},\omega) = A^{\alpha\gamma}(\mathbf{k})/(2E(\mathbf{k})) \qquad (8)$$

where $A^{\alpha\gamma}(\mathbf{k})$ is the 1-particle residue function, which in general may be a function of $\mathbf{k}$. From renormalization group theory, the scaling dimension of the residue function is expected to be $\dim[A^{\alpha\gamma}] = \eta$, or in other words we expect near the critical point $A^{\alpha\gamma}(\mathbf{k}_0) \sim |\lambda_c - \lambda|^{\eta\nu}$, $E(\mathbf{k}_0) \sim |\lambda_c - \lambda|^{\nu}$, and hence $S^{\alpha\gamma}{}_{1p}(\mathbf{k}) \sim |\lambda_c - \lambda|^{-(1-\eta)\nu}$, just as for the total structure factor (recall here z=1). In many cases, the 1-particle contribution will dominate the structure factor, but this is not always true, as we shall see.

3. Comparison with Exact Results

The transverse Ising chain model is exactly solvable, and expressions for the energy spectrum, magnetization, etc. have been given by Pfeuty [4]. Our aim is to confirm the scaling behaviour of the structure factors for this model. In the disordered phase, the Hamiltonian for the model can be written as

$$H = \sum_i (1-\sigma^z_i) - \lambda \sum_{<ij>} \sigma^x_i\, \sigma^x_j \qquad (9)$$

where the $\sigma^\alpha_i = 2S^\alpha_i$ are Pauli operators and the second sum is over nearest neighbour pairs. The critical point lies at $\lambda = 1$, and the 1-particle energy is

$$E(k) = 2\Lambda(k) = 2[1+\lambda^2-2\lambda \cos(k)]^{1/2}, \qquad (10)$$

so that the 'critical wavevector' is $k_0 = 0$ and the energy gap is $\Delta = 2(1-\lambda)$. The 1-particle exclusive structure factors have been discussed by Hamer et al. [5]. From the results of Vaidya and Tracy [6], one can obtain the 1-particle contributions to the structure factors:

$$S^{xx}{}_{1p}(k) = (1-\lambda^2)^{1/4}/(4\Lambda(k)), \qquad S^{yy}{}_{1p}(k) = (1-\lambda^2)^{1/4}\Lambda(k)/4\,. \qquad (11)$$

In the vicinity of $\lambda \to 1$, $k \to 0$, the 1-particle structure factor $S^{xx}{}_{1p}(k) \sim (1-\lambda)^{-3/4}$, which agrees with the expected scaling form (c.f. equation (6)), with d=1, z=1, $\eta = 1/4$, the transverse Ising model values. The other transverse structure factor $S^{yy}{}_{1p}(k) \sim (1-\lambda)^{5/4}$, and has a sub-leading critical index, two powers of Δ smaller than $S^{xx}{}_{1p}$. The quasiparticle residue for the dominant spectral weight S^{xx} at k=0 is independent of k in this case:

$$A(k) = (1-\lambda^2)^{1/4} \sim [2(1-\lambda)]^{1/4}\,, \qquad \lambda \to 1, \qquad (12)$$

4. Comparison with Numerical Results

The Alternating Heisenberg Chain

Schmidt and Uhrig [7] and Hamer et al. [8] have investigated the spectral weights of the alternating Heisenberg chain, which can be described by the following Hamiltonian

$$H = \sum_i (\mathbf{S}_{2i} \,.\, \mathbf{S}_{2i+1} + \lambda\, \mathbf{S}_{2i-1} \,.\, \mathbf{S}_{2i}) \qquad (13)$$

where the $\mathbf{S}_i$ are spin-1/2 operators at site i, and λ is the alternating coupling. Here we assume that the distance between two successive dimers is d. At λ = 0, the system consists of a chain of decoupled dimers, and in the ground state each dimer is in a singlet state. Excited states are made up from the three triplet excited states on each dimer, with a finite energy gap between the singlet ground state and the triplet excited states. This scenario is believed to hold right up to the uniform limit λ = 1, which corresponds to a critical point. At λ = 1, we regain the uniform Heisenberg chain, which is gapless.

Analytic studies of the critical behaviour near λ = 1 indicate that the ground-state energy per site $\varepsilon_0(\lambda)$, and the energy gap Δ(λ) should behave as

$$\varepsilon_0(\lambda) - \varepsilon_0(1) \sim \delta^{4/3}/|\ln(\delta/\delta_0)|, \qquad \Delta(\lambda) \sim \delta^{2/3}/\sqrt{|\ln(\delta/\delta_0)|}, \qquad (14)$$

as $\lambda \to 1$, where $\delta = (1-\lambda)/(1+\lambda)$. This corresponds to critical exponents $\alpha = 2/3$, $\nu = 2/3$. The logarithmic terms in (14) are due to the existence of a marginal variable in the model. For the uniform chain λ = 1, and near $kd \to 2\pi$, Affleck [9] has obtained expressions for the correlation functions in the model, which correspond to an exponent η = 1: note that in this case $(1-\eta)\nu = 0$, so there is no power-law divergence in the structure factor, but rather a logarithmic one. This implies that for $kd = 2\pi$ and as $\lambda \to 1$, the asymptotic form for $S(2\pi)$ diverges as $S(2\pi) \sim [-\ln(1-\lambda)]^{3/2}$, $\lambda \to 1$. For $0 < kd < 2\pi$, one expects S to be finite for any λ.

For fixed values of k, Fig. 1 shows the integrated structure factor S versus λ. The logarithmic divergence as $\lambda \to 1$ for the case $kd = 2\pi$ is clearly evident. For wavevectors other than 2π, an analysis of the series for the 1-particle structure factor S^{-+}_{1p} using Dlog Padé approximants by Schmidt and Uhrig [7] appeared to show that it vanishes with a behavior close to $(1-\lambda)^{1/3}$. Since S remains finite, one would thus expect that S_{1p}/S vanishes like $(1-\lambda)^{1/3}$. If the residue function A(k) behaved in the same way as at $kd = 2\pi$, however, we would expect it to vanish with exponent $\eta\nu = 2/3$.

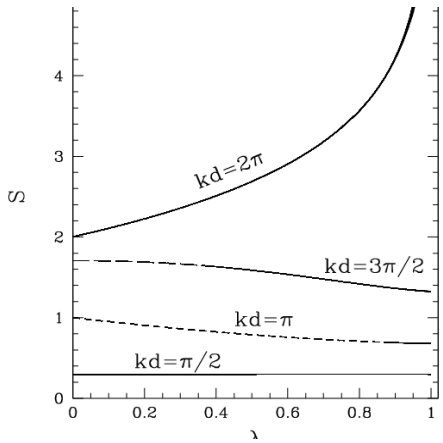

Figure 1. The integrated structure factor S for the alternating chain versus λ for kd = π/2, π, 3π/2 and 2π. From Ref. [8].

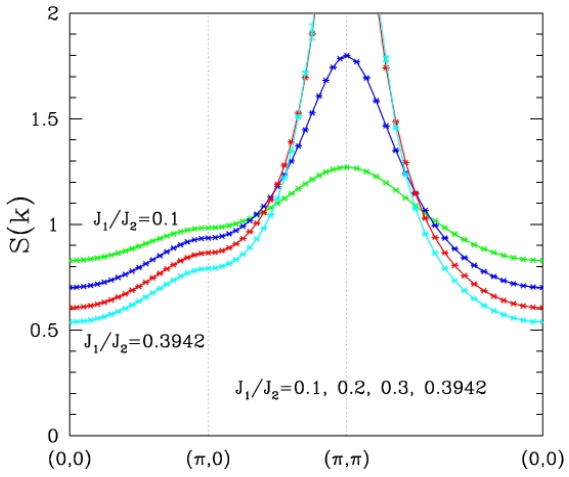

Figure 2. The total static structure factor S(**k**) for the bilayer model as a function of **k** at various couplings $\lambda = J_1/J_2$. From Ref. [10].

Heisenberg Bilayer Model

As our final example, we consider the Heisenberg bilayer antiferromagnet on the square lattice, with Hamiltonian

$$H = J_1 \sum_{m=1,2} \sum_{<ij>} \mathbf{S_{mi}} \cdot \mathbf{S_{mj}} + J_2 \sum \mathbf{S_{1i}} \cdot \mathbf{S_{2i}} \qquad (15)$$

where m = 1,2 labels the two planes of the bilayer. The physics then depends on the coupling ratio $\lambda = J_1/J_2$. At $\lambda = 0$, the ground state consists of S = 0 dimers on each bond between the two layers, and the excitations are S = 1 'triplon' states on bonds. At large λ the ground state will be a standard Néel state, with S = 1 'magnon' excitations. At some intermediate critical value λ_c, a phase transition will occur between these two phases.

Figure 2 shows some series results for the total static transverse structure factor $S(\mathbf{k}) \equiv S^{+-}(\mathbf{k})$ as a function of $\mathbf{k}$ at various couplings $\lambda = J_1/J_2$. All results are for $k_z = \pi$, probing intermediate states antisymmetric between the planes, and we only refer to $\mathbf{k} = (k_x,k_y)$ hereafter. The critical point is estimated as $\lambda_c = 0.3942$. The dominant feature is a large peak at the Néel point $\mathbf{k} = (\pi,\pi)$, which appears to become divergent as $\lambda \rightarrow \lambda_c$, as we would expect. From scaling theory, both the 1-particle structure factor and the total structure factor in the vicinity of the critical point should scale like $(\lambda_c - \lambda)^{(\eta-1)\nu}$, at the critical (Néel) momentum. We expect this transition to belong to the universality class of the O(3) model in 3 dimensions, which has critical exponents $\nu = 0.707(4)$, $\eta = 0.036(3)$, hence we expect $(\eta-1)\nu = -0.682(5)$, which is quite compatible with the numerical estimates.

How does S_{1p} behave at the critical coupling away from the Néel momentum? Here the behaviour is quite different from the previous models. The ratio S_{1p}/S decreases smoothly towards the critical coupling, but shows no sign of vanishing there. In fact the 1-particle structure factor is dominant everywhere, remaining at 80% of the total or more.

4. Conclusions

We have focused here on quantum spin models, but the conclusions should apply more generally. The structure factors at the 'critical wavevector' generally conform with theoretical expectations. At general wavevectors, however, the 1-particle residue functions and structure factors show quite distinct differences for the various models. For the exactly solvable transverse Ising chain, the residue function is independent of wavevector, and the 1-particle structure factor vanishes at the critical point with exponent $\eta\nu$ for all noncritical wavevectors. For the alternating Heisenberg chain, the 1-particle structure factor vanishes similarly, but with an exponent apparently different from $\eta\nu$. Finally, for the bilayer Heisenberg model, the renormalized residue function and the 1-particle structure function remain finite at the critical point, everywhere except at the critical wavevector, and the 1-particle state dominates the total structure factor. The 'triplon' state smoothly continues into the 'magnon' state across the transition in this case.

Acknowledgements

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