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Dynamic scaling for longitudinal critical dynamics of dilute Heisenberg and quantum XY chains

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Abstract. By averaging over chain segments, the response function and density of states is obtained for the longitudinal dynamics of two dilute one-dimensional models: the Heisenberg ferromagnet in the spin wave approximation and the quantum XY model in a transverse field. Dynamic scaling descriptions are derived, and the associated exponents and universal scaling functions obtained, for scaling limits where the percolation correlation length diverges and the wavevector tends to 0 or π.

1. Introduction: dynamic scaling

In lattice-based systems, such as localised magnets, dilution drives the system to a 'geometrical' critical point, the percolation threshold [1, 2]. At this point the divergence of the percolation correlation length ξ causes a crossover from normal to anomalous (critical) dynamics, and the description of this and associated effects has been the subject of much recent work [3-6].

In this paper we study the longitudinal dynamics of one-dimensional spin models of classical and quantum type near this dilution-induced critical point. We provide exact descriptions of the scaling regimes which confirm dynamic scaling hypotheses and yield explicit closed forms for scaling functions for dynamic response and density of states.

The discussion relies on the fact that in one dimension dilution breaks a chain into finite segments. By finding the Green functions on a segment of arbitrary length and averaging over configurations it is possible to obtain average correlation functions for diluted chains. This method was first used for the diffusion problem [7], and has since been used to calculate (in the linearised spin-wave approximation) the configurationally averaged transverse correlation function $\langle S_k^+ S_{-k}^- \rangle$ of the dilute classical Heisenberg ferromagnet in closed form in the scaling limit [8, 9]. It was verified that the result exhibits dynamic scaling, and the scaling function was given. A related approach treats the system away from the scaling limit by solving analytically for the transverse response of individual chain segments and then summing numerically over chain lengths [10]. Methods similar to those of Stinchcombe and Harris [8] and Harris [9] have also been

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used to treat the transverse correlations of the dilute Heisenberg chain antiferromagnet [11], and the results of this work agree, within the accuracy of the experiments, with neutron scattering measurements of the dynamic structure factor of diluted samples of the chain antiferromagnet TMCC [12-14]. Such experiments usually measure a mixture of transverse and longitudinal dynamic correlation functions, and so far no adequate theoretical treatment has been given of the longitudinal critical dynamics of dilute magnetic chains.

The present paper attempts to fill this gap by providing exact results, in the scaling limit, for the configurationally averaged longitudinal dynamic response function and longitudinal density of states for the following important types of dilute one-dimensional magnet:

(a) the Heisenberg ferromagnet in a linearised spin-wave approximation;

(b) the quantum XY chain in a transverse field h.

These are among the most fundamental types of classical and quantum spin system, respectively.

In dilute chains the criticality associated with the diverging percolation correlation length ($\xi \to \infty$) occurs near the pure limit [1, 2] and normally shows up in the dynamics at low frequency ($\omega \sim 0$) and small wavevector ($k \sim 0$). The simplest form of dynamic scaling hypothesis [15] supposes that in this scaling regime (ξ^{-1}, ω, k all small) the response occurs at a 'characteristic frequency' ω_c given by

$$w_c = k^z f(k\xi) \tag{1}$$

where z is the dynamic exponent and f is a universal scaling function. The more complete statement of the dynamic scaling hypothesis [15], containing a generalisation of (1), is that the response $R(\omega, k, \xi)$ (the imaginary part of an appropriate Green function) has the scaling form

$$R(\omega, k, \xi) = k^{-(z+2-\eta)} F(k\xi, \omega k^{-z}) \qquad \omega, k, \xi^{-1} \to 0 \tag{2}$$

where η is a (static) critical exponent and the two-variable scaling function F is again universal.

The dynamic scaling statement (2) will be explicitly verified for the longitudinal response of models (a) and (b). The scaling functions F are given as infinite sums, which are evaluated numerically for various values of their arguments (the scaling parameters) to provide plots of these universal functions. As in the above introductory discussion both models studied have a scaling regime where ξ^{-1}, k, are small; however, for this to occur in model (b) the field must satisfy $h = J$ (where J is the exchange constant). A dynamic scaling result also holds in both models in a second scaling limit where ξ^{-1}, $\pi - k$, $\omega - 4J$ are all small with, in model (b), h equal to zero.

Such results for the response also imply dynamic scaling statements and universal scaling functions for the (longitudinal) densities of states, and these are also obtained in this paper.

The outline of the paper is as follows. In § 2 we describe the basis of the method (averaging over chain segments) and give required properties of individual chain segments. The configurational averaging is carried out in § 3 to yield analytic expressions for the longitudinal dynamic response for each system in each of the two scaling regimes. In § 4 we give corresponding results for the densities of states. Plots of numerical evaluations of the analytic expressions are given in § 5, which concludes with an interpretation and discussion of these results.

2. Basis of method: longitudinal dynamic response of chain segment

In one dimension the percolation threshold is at $p_c = 1$ since any dilution breaks the system into independent segments. An expansion about the critical point is thus equivalent to expansion about the pure system. The full dynamic scaling behaviour is however non-trivial and is not accurately described by any effective medium theory or simple perturbative expansion. Instead one can exploit the separation of the chain, by dilution, into independent finite segments upon which it is possible to solve the dynamics of many systems exactly. The response of the ensemble of segments found in any realisation of the dilute system is then found as the configurational average of the response of the individual segments. In the limit of large percolation correlation length it is permissible to replace the sums which arise in these configurational averages by integrals from which the dynamic scaling can be exhibited and relevant exponents extracted. If the sums or integrals arising in the configurational average are not too difficult one then has the dynamic scaling function in closed form. Otherwise the scaling function can still be calculated numerically.

This is the method used here to calculate the critical dynamic response of the longitudinal degrees of freedom of dilute one-dimensional magnets in the scaling limit. The method clearly requires a knowledge of the dynamic response of finite chain segments for the models considered, and the rest of this section is devoted to providing this ingredient.

The two models considered here are the dilute Heisenberg ferromagnet in the linear spin-wave approximation and the dilute spin-$\frac{1}{2}$ XY chain. The longitudinal response, which will be calculated for both models in the limits $k \to 0$ and $k \to \pi$, is found from the imaginary part of the longitudinal Green function

$$G_{rr'}(t) = \langle\langle S_r^z(t);\, S_{r'}^z(0)\rangle\rangle \tag{3}$$

where r, r' are space coordinates. As remarked above, the procedure is to calculate the Green functions of a chain segment of arbitrary length and then to perform an average over all positions and lengths. The calculation for a particular chain segment is easy for the linearised Heisenberg ferromagnet, and is also possible for the XY chain, the longitudinal response of which can be found exactly in a long segment where end effects are small [16].

For the Heisenberg ferromagnet in the spin-wave approximation the operator S^z is found by expanding in terms of the transverse components using the fixed length of the spin vector. The Green function (1) can thus be approximated by a Green function involving four transverse operators [17]:

$$\begin{aligned} G_{rr'}(t) &\simeq (1/4S)\langle\langle S_r^+(t)S_r^-(t);\, S_{r'}^+(0)S_{r'}^-(0)\rangle\rangle \\ &\simeq \langle\langle a_r^+(t)a_r(t);\, a_{r'}^+(0)a_{r'}(0)\rangle\rangle. \end{aligned} \tag{4}$$

The usual boson operator a^+ has been defined as $S^+/\sqrt{2S}$ and a is its Hermitian conjugate. In terms of these operators the Hamiltonian takes the following diagonal form in the wavevector representation:

$$H = \sum_k \varepsilon_k a_k^+ a_k \qquad \varepsilon_k = 2J(1 - \cos k). \tag{5}$$

For convenience the spin magnitude S has been absorbed into J.

To perform the calculation of the response of an individual chain segment it is convenient to express the Green function (4) in terms of the basis which diagonalises the Hamiltonian, by taking matrix elements of the operators in (4) with the set of operators labelled by the eigenmodes of each segment:

$$G_{rr'} = \sum_{kk'} \langle q|r\rangle\langle r|q'\rangle\langle k|r'\rangle\langle r'|k'\rangle G_{qq'kk'} \tag{6}$$

where

$$G_{qq'kk'} \equiv \langle\langle a_q^+ a_{q'};\, a_k^+ a_{k'}\rangle\rangle. \tag{7}$$

The Green function $G_{qq'kk'}$ can be calculated using for example the equation of motion method. Differentiating with respect to t and then Fourier transforming gives the following standard expression [18] for such a free boson pair propagator

$$G_{qq'kk'}(\omega) = \frac{\delta_{qk'}\delta_{q'k}(n_q^{\mathrm{b}} - n_{q'}^{\mathrm{b}})}{\omega + \varepsilon_{q'} - \varepsilon_q} \tag{8}$$

where n_q^{b} is the Bose occupation function at energy ε_q. The inner products of (6) are the eigenvectors of the chain segments. For a segment of N bonds these are

$$\langle q|r\rangle = [2/(N+1)]^{1/2} \cos(r+\tfrac{1}{2})q \tag{9}$$

where the possible wavevectors, determined by the end conditions evident from the equations of motion of the $\{S^+\}$, are

$$q = m\pi/(N+1) \qquad m = 1, 2, \ldots, N. \tag{10}$$

On substituting these results into (6), the Green function for a single chain segment of the linearised Heisenberg ferromagnet is found in the form of the following double summation:

$$G_{rr'}(\omega) = 4\sum_{qq'} \frac{\cos(r+\frac{1}{2})q\, \cos(r+\frac{1}{2})q'\, \cos(r'+\frac{1}{2})q\, \cos(r'+\frac{1}{2})q'}{(N+1)^2}\, \frac{n_q^{\mathrm{b}} - n_{q'}^{\mathrm{b}}}{\omega - \varepsilon_q + \varepsilon_{q'}}. \tag{11}$$

A similar calculation can be performed for the quantum XY system described by the following spin-$\frac{1}{2}$ Hamiltonian

$$H = \sum_{\langle ij\rangle} J(S_i^X S_j^X + S_i^Y S_j^Y) - h\sum_i S_i^Z. \tag{12}$$

In this case an exact expression can be found [16] for the longitudinal response of a chain segment by introducing the Jordan–Wigner transformation [17]

$$S_j^+ = \exp\left(\mathrm{i}\pi \sum_{l=1}^{j-1} c_l^+ c_l\right) c_j^+ \qquad S_j^Z = c_j^+ c_j - \tfrac{1}{2} \tag{13}$$

where c are fermion operators. Provided we neglect the boundary term which will appear in the Hamiltonian after the introduction of the transformation, it can be diagonalised and the eigenfrequencies are in this case given by

$$\varepsilon_k = -h + J\cos k \tag{14}$$

with wavevectors given by

$$k = p\pi/(N+2) \qquad p = 1, \ldots, N+1. \tag{15}$$

It should be remarked that in the thermodynamic limit (N large, appropriate when the correlation length ξ is large) the neglected boundary term does not introduce any contribution to the longitudinal response, although it does for the transverse response.

The operators that describe the standing modes are related to the c_j^+ through the transformation

$$c_k^+ = \left(\frac{2}{N+2}\right)^{1/2} \sum_l \sin kl\, c_l^+. \tag{16}$$

Following the same procedure adopted for the linear spin-wave approximation we may write immediately for the XY system

$$G_{rr'}(\omega) = 4 \sum_{q,q'} \frac{\sin(r-\frac{1}{2})q \sin(r-\frac{1}{2})q' \sin(r'-\frac{1}{2})q \sin(r'-\frac{1}{2})q'}{(N+2)^2} \frac{n_q^{\mathrm{f}} - n_{q'}^{\mathrm{f}}}{\omega - \varepsilon_q + \varepsilon_{q'}} \tag{17}$$

where n_k^{f} is the Fermi function at the energy ε_k given by (14) and the wavevectors occurring in the summation are specified in (15).

Equations (11), (5), (10) and (17), (14), (15) are the input for the configurational averages to be performed in § 3.

3. Configurational average for the longitudinal dynamic response

In § 2 we have derived expressions for the longitudinal Green functions of single chain segments which apply respectively to a quantum XY chain (in a transverse field, h) and to the longitudinal correlations of a Heisenberg ferromagnet in a linearised spin-wave approximation. We now use these results to calculate the response of an ensemble of such segments as might be found in an experimental realisation where a pure chain-like system has been diluted with non-magnetic ions. We shall carry the calculation to its conclusion, and give plots, for four contrasting cases.

(i) Linearised approximation as $\omega \to 0$, $k \to 0$ and $\xi^{-1} \to 0$.
(ii) XY system as $\omega \to 0$, $k \to 0$, $\xi^{-1} \to 0$ and $h = J$.
(iii) Linearised system as $\omega \to 4J$, $k \to \pi$ and $\xi^{-1} \to 0$.
(iv) XY system as $\omega \to 4J$, $k \to \pi$, $\xi^{-1} \to 0$ and $h = 0$.

In each of these cases the final result exhibits dynamic scaling in the appropriate variables. The dynamic scaling function is given as an infinite sum which is evaluated numerically for various values of the scaling parameters.

Given the Green function G for a single chain segment of N bonds and $(N+1)$ sites the average response of the ensemble of such segments produced by random dilution is given by [7, 8, 9, 11]

$$R_k = \sum_N (1-p)^2 p^N \sum_{m=-N}^{N} \cos km \left(\sum_{r=0}^{N-|m|} \operatorname{Im} G_{r,r+|m|} \right). \tag{18}$$

The trigonometric manipulations required to perform the sums over r and m can be performed simultaneously for both the ferromagnet and the XY system by expanding the products of four sines or cosines in (11) and (17) as

$$\begin{aligned}\sum_{q,q'}^{\pi} &\tfrac{1}{8}[\cos(q+q')(2r+m+\alpha) + \cos(q-q')(2r+m+\alpha)]\\ &+ \tfrac{1}{4}[\cos qm \cos q'm - (-1)^\alpha \cos qm \cos q'(2r+m+\alpha)\\ &- (-1)^\alpha \cos q'm \cos q(2R+m+\alpha)].\end{aligned} \tag{19}$$

The parameter α is an indicator variable and is given by $\alpha = 0$ for the XY chain and $\alpha = 1$ for the linearised system. The sums over q and q' are given by either (10) or (15).

The summations over m and r of (18) are now easy. In general the expressions obtained after these summations have been performed are intractable to further simplifications but further progress can be made in the limits given above. In all four cases the dominant term is derived from the factor $\cos qm \cos q'm$ in (19). All other terms turn out to be of higher order in ξ^{-1}. We find that to leading order the summations over m and r in (18) give

$$\sum_{q,q'} \frac{1}{16}\left(\frac{\sin^2 \frac{1}{2}(k+q+q')(N+1)}{\sin^2 \frac{1}{2}(k+q+q')} + \frac{\sin^2 \frac{1}{2}(k+q-q')(N+1)}{\sin^2 \frac{1}{2}(k+q-q')} + \frac{\sin^2 \frac{1}{2}(k-q+q')(N+1)}{\sin^2 \frac{1}{2}(k-q+q')} + \frac{\sin^2 \frac{1}{2}(k-q-q')(N+1)}{\sin^2 \frac{1}{2}(k-q-q')}\right)(1+\mathrm{O}(\xi^{-1})). \tag{20}$$

This expression can be written in a much shortened form by noting that all four terms in the bracket of (20) can be accommodated by extending the range of summation over wavevectors to include both positive and negative q and q' so that for the rest of this section sums over q and q' will be given by $q = n\pi/(N+1)$, $n = \pm 1, \pm 2, \ldots, \pm N$ for the ferromagnet and $q = n\pi/(N+2)$, $n = \pm 1, \pm 2, \ldots, (N+1)$ for the XY chain (rather than by (10) and (15), which have been used up to this point). After further trigonometric manipulations we are led to a much shortened expression for the response function

$$R_k = \pi \sum_N (1-p)^2 p^N \sum_{q,q'} \frac{1}{(N+2-\alpha)^2} \frac{1-\cos(k+q+q')(N+1)}{8 \sin^2 \frac{1}{2}(k+q+q')} \times \delta(\omega - \varepsilon_q + \varepsilon_{q'})[n(q) - n(q')]. \tag{21}$$

We now simplify this in the appropriate limits of frequency and wavevector. We can assume, without loss of generality, that $\omega > 0$. R_k is reconstructed for negative ω by noting that $R_k(\omega) = -R_k(-\omega)$.

In cases (i) and (ii) listed at the beginning of this section both ω and k are small; the sum over q and q' is then dominated by those q and q' which are small compared to 1 so that we can expand the denominator and the energies of (21) to lowest order. Since the correlation length $\xi = -\ln p$ is large it is possible to replace the summation over chain lengths by an integral, freely substituting L for N, $N+1$ and $N+2$:

$$R_K = \pi \int_0^\infty \frac{1}{2\xi^2} \mathrm{e}^{-L/\xi}\, \mathrm{d}L \sum_{q,q'} \frac{1}{L^2} \frac{1-\cos(k+q+q')L}{(k+q+q')^2} \delta(\omega + Jq^2 - Jq'^2)[n(q) - n(q')]. \tag{22}$$

We would like to use the integral arising from the average over chain lengths to eliminate the δ function; to do this we interchange the order of summation and integration taking care to change the limits where necessary

$$R_k = \pi \sum_{\substack{|m|>|n|\neq 0 \\ -\infty}}^{+\infty} \int_{|m|}^\infty \frac{\mathrm{e}^{-L/\xi}}{2\xi^2}\left(\frac{1-(-1)^{m+n}\cos kL}{(kL + m\pi + n\pi)^2}\right)\delta\left(\omega - J\frac{(m^2-n^2)\pi^2}{L^2}\right)[n(n) - n(m)]. \tag{23}$$

It is now seen that the error made in replacing the lower limit of the integral by 0 rather than $|m|$ is of higher order in ξ^{-1}, and this allows the integral to be performed without difficulty.

Let us now distinguish between the linearised system where Bose statistics must be used and the XY chain where the elementary excitations are fermionic. For energies obeying the condition $\beta\omega \leqslant 1$ the difference $n(n)-n(m)$ of occupation factors can be expanded to give

$$n^{\mathrm{b}}(n)-n^{\mathrm{b}}(m)=\frac{1}{\beta J}\frac{(m^2-n^2)}{n^2m^2}\frac{L^2}{\pi^2} \qquad \text{for the Bose case} \tag{24}$$

$$n^{\mathrm{f}}(n)-n^{\mathrm{f}}(m)=\frac{(m^2-n^2)\pi^2\beta J}{4L^2} \qquad \text{for the Fermi case.} \tag{25}$$

We are now able to give the final answers for the dynamic response, in cases (i) and (ii), as infinite double summations:

$$R_k=\sum_{\substack{|m|>|n|\neq 0\\ -\infty}}^{+\infty}\frac{\sqrt{J}}{4\beta\xi^2}\frac{1}{n^2m^2}\left(\frac{m^2-n^2}{\omega}\right)^{5/2}\exp\{-\pi[J(n^2-m^2)/\omega\xi^2]^{1/2}\}$$
$$\times\frac{1-(-1)^{m+n}\cos k\pi[J(n^2-m^2)/\omega]^{1/2}}{\{k[J(n^2-m^2)/\omega]^{1/2}+n+m\}^2} \tag{26}$$

for the ferromagnet as $\omega\to 0$ (case (i));

$$R_k=\sum_{\substack{|m|>|n|\neq 0\\ -\infty}}^{+\infty}\frac{\beta\sqrt{J}}{16\xi^2}\left(\frac{m^2-n^2}{\omega}\right)^{1/2}\exp\{-\pi[J(n^2-m^2)/\omega\xi^2]^{1/2}\}$$
$$\times\frac{1-(-1)^{m+n}\cos k\pi[J(n^2-m^2)/\omega]^{1/2}}{\{k[J(n^2-m^2)/\omega]^{1/2}+n+m\}^2} \tag{27}$$

for the XY chain as $\omega\to 0$ (case (ii)).

We now turn to the other two cases (iii) and (iv) and obtain expressions for the linearised spin-wave system and (zero-field) XY chain in the limit $\omega\to 4J$, $k\to\pi$, $\xi^{-1}\to 0$. For the XY system this limit gives rise to a Van Hove singularity, persisting even at zero temperature because of zero point fluctuations, which is rounded out by the disorder in the chain. The result follows from (21) in entirely the same fashion as given above if q is expanded about 0 and q' about π. The results are

$$R_k=\sum_{\substack{m,n\neq 0\\ -\infty}}^{+\infty}\frac{\sqrt{J}}{4\xi^2}\frac{1}{(4J-\omega)\beta}\left(\frac{m^2+n^2}{4J-\omega}\right)^{3/2}m^{-2}\exp\{-\pi[J(m^2+n^2)/(4J-\omega)\xi^2]^{1/2}\}$$
$$\times\frac{1-\cos(\pi-k)\pi[J(n^2+m^2)/(4J-\omega)]^{1/2}}{\{(\pi-k)[J(n^2+m^2)/(4J-\omega)]^{1/2}+n+m\}^2} \tag{28}$$

for the ferromagnet as $\omega\to 4J$ (case (iii);

$$R_k=\sum_{\substack{m,n\neq 0\\ -\infty}}^{+\infty}\frac{\sqrt{J}}{4\xi^2}\frac{1}{4-\omega}\left(\frac{m^2+n^2}{4J-\omega}\right)^{1/2}\exp\{-\pi[J(m^2+n^2)/(4J-\omega)\xi^2]^{1/2}\}$$
$$\times\frac{1-\cos(\pi-k)\pi[J(n^2+m^2)/(4J-\omega)]^{1/2}}{\{(\pi-k)[J(n^2+m^2)/(4J-\omega)]^{1/2}+n+m\}^2} \tag{29}$$

for the XY chain as $\omega\to 4J$ and $h=0$ (case (iv)).

As stated above all these results can be written in the dynamic scaling form (2) using the appropriate scaling variables which for k and $\omega\to 0$ (case (i) and (ii)) are $a=k\xi$ and $b=\omega k^{-z}/J$. For $\omega\to 4J$ and $k\to\pi$ (case (iii) and (iv)) the corresponding variables are $c=(\pi-k)\xi$ and $d=[(4-\omega)/J]/(\pi-k)^{-z}$. In all four cases the exponent

z takes the value $z=2$ but the exponents η and the dynamic scaling functions F in (2) differ from case to case and are trivially obtained from the results (26)-(29):

(i) for the ferromagnet as $\omega \to 0$, η takes the value $\eta = 1$, and

$$F(a, b) = \frac{1}{4\beta J^2} \sum_{\substack{|m|>|n|\neq 0 \\ -\infty}}^{\infty} \frac{1}{n^2 m^2} (m^2 - n^2)^{5/2} \frac{\exp\{-\pi[(n^2-m^2)/ba^2]^{1/2}\}}{a^2 b^{5/2}} \times \frac{1-(-1)^{m+n} \cos k\pi[(n^2-m^2)/b]^{1/2}}{\{[(n^2-m^2)/b]^{1/2}+n+m\}^2} \tag{30}$$

(ii) for the XY chain at $h = J$ as $\omega \to 0$, η is $\eta = 3$, and

$$F(a, b) = \frac{\beta}{16} \sum_{\substack{|m|>|n|\neq 0 \\ -\infty}}^{\infty} (m^2 - n^2)^{1/2} \frac{\exp\{-\pi[(n^2-m^2)/ba^2]^{1/2}\}}{a^2 b^{1/2}} \times \frac{1-(-1)^{m+n} \cos k\pi[(n^2-m^2)/b]^{1/2}}{\{[(n^2-m^2)/b]^{1/2}+n+m\}^2} \tag{31}$$

(iii) for the ferromagnet as $\omega \to 4J$, $\eta = 1$ and

$$F(c, d) = \frac{1}{4\beta J^2} \sum_{\substack{m,n\neq 0 \\ -\infty}}^{\infty} \frac{(m^2+n^2)^{3/2}}{c^2 d^{5/2} m^2} \exp\{-\pi[(m^2+n^2)/dc^2]^{1/2}\} \times \frac{1-\cos \pi[(n^2+m^2)/d]^{1/2}}{\{[(n^2+m^2)/d]^{1/2}+n+m\}^2} \tag{32}$$

(iv) for the XY chain as $\omega \to 4J$, and $h = 0$, η becomes $\eta = 3$, and

$$F(c, d) = \sum_{\substack{m,n\neq 0 \\ -\infty}}^{\infty} (m^2+n^2)^{1/2} \exp\{-\pi[(m^2+n^2)/c^2 d]^{1/2}\} \times \frac{1-\cos \pi[(n^2+m^2)/d]^{1/2}}{\{[(n^2+m^2)/d]^{1/2}+n+m\}^2}. \tag{33}$$

Plots of these functions, and their interpretations, will be given in § 5.

4. The longitudinal density of states

In this section we show that the longitudinal density of states can be calculated using the same method as was used to calculate the full response function. The calculation is performed in the same limits as above. The density of states of a system is defined by the expression

$$\rho(\omega) = \sum_r \operatorname{Im} G_{rr}. \tag{34}$$

G_{rr} is easily found by putting $m = 0$ in (18). The trigonometric summation required is then just

$$\sum_{q,q'}^{\pi} \{\tfrac{1}{8}[\cos(q+q')(2r+x) + \cos(q-q')(2r+x)] + \tfrac{1}{4}[1 + (-1)^\alpha \cos q'(2r+x) + (-1)^\alpha \cos(2r+x)]\}. \tag{35}$$

As before we find only one term is important in the limits of interest leaving us with a much simplified expression:

$$\rho(\omega)=4\pi\int\frac{e^{-L/\xi}}{\xi}\sum_{q,q',r}\frac{1}{4L^2}\,dL\,\delta(\omega-\varepsilon_{q'}+\varepsilon_q)[n(q)-n(q')]. \tag{36}$$

Applying the same trick of reversing the order of summation and integration and again expanding occupation factors in the small frequency limit as was used above we obtain the following formulae for the density of states.

(i) Ferromagnet as $\omega\to 0$:

$$\rho(\omega)=\frac{\pi}{2\beta}\sum_{\substack{m>n\\1}}^{\infty}\frac{(m^2-n^2)^2}{n^2m^2}\frac{\exp\{-\pi[J(m^2-n^2)/\omega\xi^2]^{1/2}}{\omega^2\xi}. \tag{37}$$

(ii) XY chain at $h=J$ as $\omega\to 0$:

$$\rho(\omega)=\frac{\pi\beta}{8\xi}\sum_{\substack{m>n\\1}}^{\infty}\exp\{-\pi[J(m^2-n^2)/\omega\xi^2]^{1/2}\}. \tag{38}$$

(iii) Ferromagnet as $\omega\to 4J$:

$$\rho(\omega)=\frac{\pi}{2\xi\beta(4J-\omega)^2}\sum_{m,n=1}^{\infty}\frac{m^2+n^2}{m^2}\exp\{-\pi[J(m^2+n^2)/(4J-\omega)\xi^2]^{1/2}\}. \tag{39}$$

(iv) For the XY chain at $h=0$ as $\omega\to 4J$:

$$\rho(\omega)=\frac{\pi}{2\xi(4J-\omega)}\sum_{m,n=1}^{\infty}\exp\{-\pi[J(m^2+n^2)/(4J-\omega)\xi^2]^{1/2}\}. \tag{40}$$

Each of these results can be written in a dynamic scaling form

$$\rho(\omega)=\xi^{z+2-\eta}g(x) \tag{41}$$

where the scaling variable x for the density of states is $x=\omega\xi^z/J$ as $\omega\to 0$ and $x=[(4-\omega)/J]\xi^z$ as $\omega\to 4J$. The exponents z and η take the same values as before, but each $g(x)$ is now a new universal function trivially obtainable from (37)-(40).

5. Discussion of results

The results for both the average response and the density of states have been expressed in the form of sums over integers. These summations can be performed numerically and we give plots of the resulting scaling functions for the response in figures 1-5. In each case the graph is given for various values of the scaling variable $k\xi$ or $(\pi-k)\xi$, so that it is possible to see the crossover from a regime where chain lengths are long compared with typical wavelengths involved ($k\xi\gg 1$) or $(\pi-k)\xi\gg 1$) to a regime where the scattering is from segments short in comparison with the typical wavelengths ($k\xi\ll 1$ or $(\pi-k)\xi\ll 1$). In the first regime the response approaches that of a pure chain, which is strongly peaked about ω/Jk^2 or $[(4-\omega)/J]/(\pi-k)^2$ of order unity, except in case (ii); the sharp peaks arise from undamped boson or fermion pair contributions. In addition, in this regime of high $k\xi$ or $(\pi-k)\xi$ the response in cases (i), (iii) and (iv) shows an oscillatory structure at small ω/Jk^z or $[(4-\omega)/J]/(\pi-k)^2$ which is like that seen previously for the transverse response of diluted Heisenberg ferro- [8] and antiferromagnetic [11] chains where it arises because of the vanishing of the response

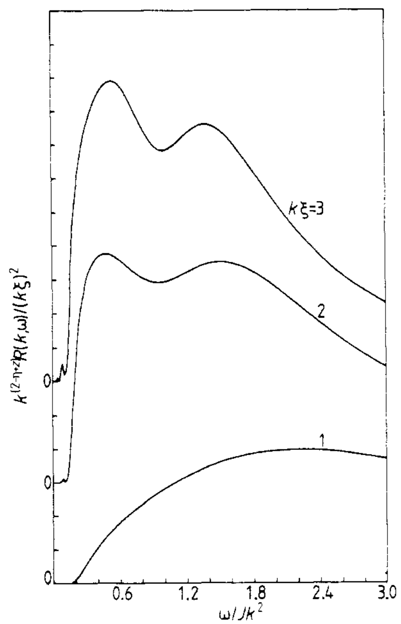

Figure 1. Scaling plot of longitudinal response function $R(k, \omega)$ for case (i) of the text, the diluted chain Heisenberg ferromagnet in the regime $\omega \to 0$, $k \to 0$, $\xi^{-1} \to 0$, where ξ is the percolation correlation length. The plot is against ω/Jk^2 for values of $k\xi$ ranging from 1-3.

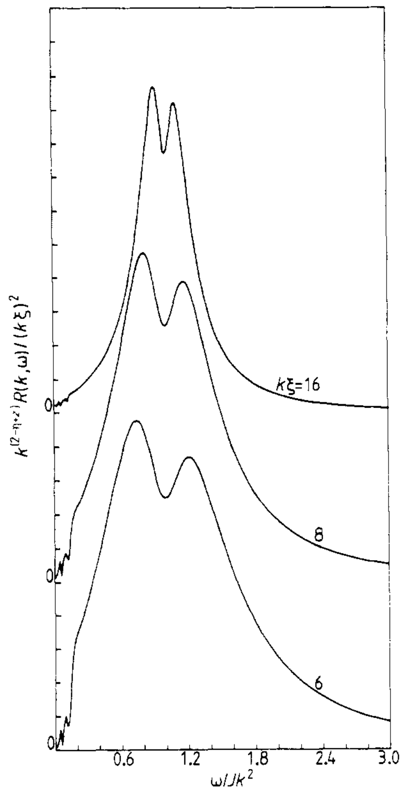

Figure 2. Scaling plot of longitudinal response function $R(k, \omega)$ for case (i) of the text, the diluted chain Heisenberg ferromagnet in the regime $\omega \to 0$, $k \to 0$, $\xi^{-1} \to 0$, where ξ is the percolation correlation length. The plot is against ω/Jk^2 for the values of $k\xi$ ranging from 6-16.

at values of the frequency for which there is zero coupling of internal wavefunction and kth Fourier component of external perturbation. As $k\xi$ or $(\pi - k)\xi$ decreases, the sharp structure of the response is broadened by finite lifetime effects due to scattering from the segment ends and eventually all the detail is lost with only a broad background remaining. The most important feature evident in this regime is the vanishing of the response at low frequencies. This actually occurs for all finite $k\xi$ (or $(\pi - k)\xi$) at sufficiently low frequency: as $\omega \to 0$ the response vanishes exponentially fast since the long chain segments required to support the low energy eigenstates become rare in the dilute system (see the exponential factors in (26)-(29)). Another example of the effect of the disorder being very strong at particular frequencies, even for very small concentrations of missing bonds, occurs at the strong peak in the nearly pure limit of case (i). For the pure system there is a non-integrable divergence of the response at the energy of the single-particle spin-wave peak (i.e. at $\omega = Jk^2$). This divergence is removed by any dilution which removes the lowest-lying eigenstates of the system. At any finite temperature these states become very highly populated because of the pole in the Bose occupation factors. This large population of low-lying eigenstates is what

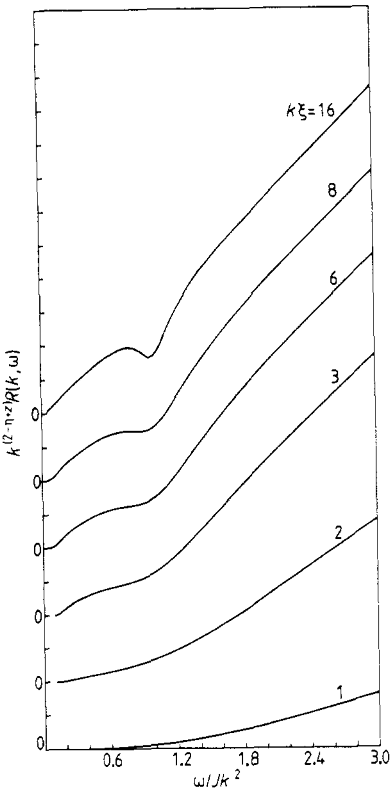

Figure 3. Scaling plot of longitudinal response function $R(k, \omega)$ for diluted quantum XY chain in the regime $\omega \to 0$, $k \to 0$, $\xi^{-1} \to 0$ (case (ii) of the text). The field takes the special value $h = J$.

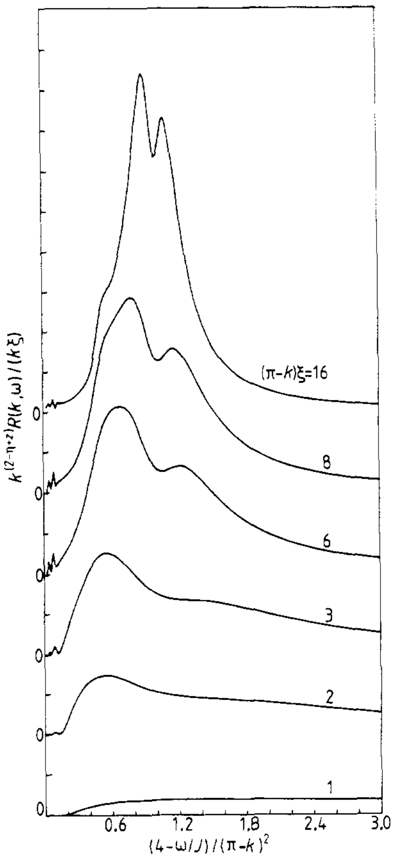

Figure 4. Scaling plot of longitudinal response function for diluted chain Heisenberg ferromagnet in the regime $\omega \to 4J$, $k \to \pi$, $\xi^{-1} \to 0$ (case (iii) of the text).

leads to strong scattering near this special energy. Similar effects occur near the pure limit of case (ii). The dilution also removes less singular divergences such as the square root Van Hove singularity in the Heisenberg and XY systems as $\omega \to 4J$.

The scaling functions g (defined in (41)) for the density of states are shown in figure 6 for all four cases, in terms of the appropriate scaling variable $\omega\xi^z/J$ or $[(4-\omega)/J]\xi^z$. For small values of this variable (i.e. for ω or $4J-\omega$ less than a crossover frequency $\omega^* \equiv J/\xi^2$) the same exponential decrease seen in the response occurs, and for the same reason. The exponential factors in (37)-(40) make this explicit. Above the crossover frequency the densities of states tend to the corresponding pure results. The crossover frequency ω^* corresponds to the lowest energy occurring in a segment of typical size (the percolation correlation length, ξ). It is interesting to note the sharp 'edges' which occur at the crossover frequency in the densities of states for the ferromagnet.

The dynamic exponent z is $z=2$ for all the cases considered. The exponent η takes a variety of values. That $\eta=1$ for the Heisenberg ferromagnet in case (i) $(k=0, \omega=0)$ is the usual static critical exponent of the critical (longitudinal) correlation

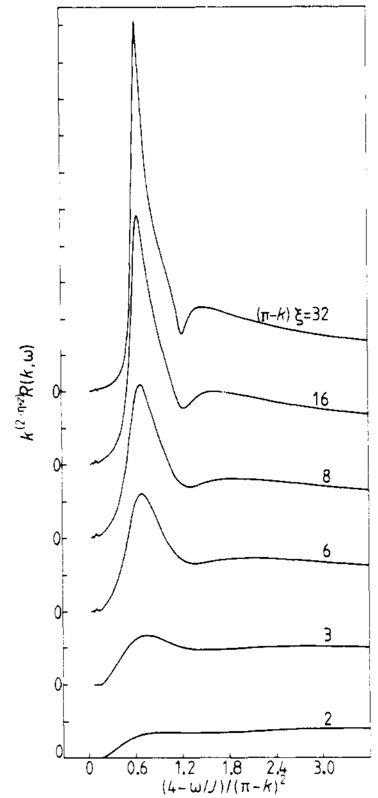

Figure 5. Scaling plot of longitudinal response function for diluted quantum XY chain at zero field in the regime $\omega\to 4J$, $k\to\pi$, $\xi^{-1}\to 0$ (case (iv) of the text).

of the pure system. Those for cases (iii) and (iv) relate to non-critical staggered correlations. The static longitudinal correlation functions of the pure quantum XY chain have however been treated generally [19] and from this work it is possible to extract the values of η for both case (ii) (long wavelength limit for the XY model at its quantum transition at $h=J$) and for case (iv) ($k\sim\pi$, i.e. staggered, limit for quantum XY model at $h=0$.) In both cases $\eta=3$, in agreement with our values for the dilute generalisation.

Because case (ii) corresponds to the critical point of a quantum model, and such models have higher-dimensional classical equivalents [20], our exact treatment of dilution in this case is equivalent to a treatment of striped randomness in a higher-dimensional classical model (cf for the Ising case, references [21, 22]).

No experimental investigations have yet been made with which to compare the results of this paper. The only experiments on critical dynamics of dilute chains so far carried out are on the antiferromagnet TMMC [12, 13]. Though we expect similar effects there in the longitudinal response and density of states to those predicted above (suppression of response coming from long wavelength excitations, crossover and scaling, etc) those effects appear to have been masked by incoherent scattering, and only the dominant features of the transverse response have been seen, which compare well with the theory developed for that case [11].

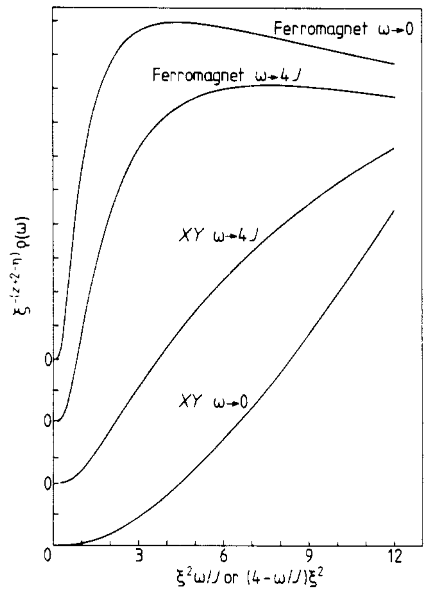

Figure 6. Scaling plot of longitudinal density of states for each of the following one-dimensional systems at weak dilution ($\xi^{-1} \to 0$): (i) ferromagnet as $\omega \to 0$; (ii) quantum XY chain at $h = J$ as $\omega \to 0$; (iii) ferromagnet as $\omega \to 4J$; (iv) quantum XY chain at zero field as $\omega \to 4J$.

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