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Dynamic structure factor of the transverse Ising model

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Abstract. We report the first analytic study of *real time and frequency dependent* behaviour at $T = \infty$ of the 2D square lattice transverse Ising model. Our study, along with known results in the 1D case, in the mean field or ∞D case and in other studies, helps understand the experimentally obtained longitudinal dynamic structure factor of the induced moment ferromagnet $LiTbF_4$ studied by Youngblood *et al*, and is consistent with the studies of Kötzler *et al*.

1. Introduction

The transverse Ising model was originally proposed by Blinc and by de Gennes [1] to describe the order parameter motion in hydrogen bonded ferroelectrics. It is one of the simplest quantum spin models with non-trivial spin dynamics. It turns out, however, that there is no understanding of quantum spin dynamics in this model in finite dimensions $D > 1$. The spin dynamics in the $D = 1$ case is solvable at temperatures $T = 0$ and at $T = \infty$. Some studies on the spin dynamics of this model in the mean field limit, i.e., at $D = \infty$, have also been carried out. We shall return to these points later.

The Hamiltonian for the transverse Ising model is given by:

$$H = -(1/2)\sum_{\delta} J_\delta S_r^z S_{r+\delta}^z - (\Gamma/2)\sum_{r} S_r^x. \tag{1}$$

In equation (1), Γ describes the crystal field splitting of the ground state doublet into two non-magnetic singlets in ferromagnets such as $LiTbF_4$ [2, 3] and the tunnelling frequency of the protons in their double-well potentials while opposing the ordering effect of the interaction J_δ in ferroelectrics such as KH_2PO_4 (KDP), and $S = \frac{1}{2}$. The longitudinal dynamic structure factor, i.e., the Fourier transform of the total zz component of the normalized dynamical spin correlations, is defined as follows,

$$S^{zz}(k,\omega) = (1/\pi)\int_0^\infty \langle S_z(-k,0), S_z(k,t)\rangle \cos(\omega t)\,dt / \langle S^z(-k,0), S^z(k,0)\rangle. \tag{2}$$

The angular brackets in equation (2) denote canonical ensemble averages. The longitudinal dynamics of this model has been carefully studied experimentally by Youngblood *et al* [2] and by Kötzler *et al* [3]. The latter [3] have pointed out that the dynamical behaviour of this model can be well described by a certain phenomenological *relaxation coupled oscillator* model [3]. However, it is fair to say that an understanding of the dynamical behaviour of the transverse Ising model in $D = 2, 3$ based on the *actual quantum spin dynamics* of the model is still lacking in spite of rather extensive work on this model. Given that this is

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among the simplest model Hamiltonians for studying quantum spin dynamics, it would be highly desirable to understand the experimental results based on an analytic study of the longitudinal dynamics in a transverse Ising Hamiltonian. That is precisely the focus of this work.

This paper is organised as follows. We discuss the known results and the open questions on the dynamics of the transverse Ising model that motivate this study in section 2. Section 3 details the formalism used to carry out this study. The calculations and the results are presented in section 4. Section 5 summarizes this work.

2. Motivation for the study

It is well known that the partition function for the 1D nearest-neighbour transverse Ising model was first exactly evaluated by Lieb and coworkers in 1961 [4]. These authors showed that the 1D transverse Ising model can be mapped onto a gas of *non-interacting* fermions, which is a solvable problem. The transverse and logitudinal dynamics of the 1D nearest-neighbour transverse Ising model has been studied by several authors at $T = \infty$ [5, 6] and at $T = 0$ (Lee and Kobayashi's work in [6]).

Not surprisingly, the static and dynamical behaviour of the ∞D transverse Ising model has also been well studied by several authors such as Pytte and Thomas, Stinchcombe and others [7]. In addition, an approximate 3D study of the longitudinal dynamics of the nearest-neighbour transverse Ising model on the simple cubic lattice has been carried out using both the three-pole approximation method and the mean field approximation method (to calculate the necessary static correlations) by Tommet and Huber [8]. The entire subject was reviewed some ten years ago by Dumont [9].

In the ∞D limit at $T = \infty$, it is theoretically well established and intuitively transparent that for the limiting case of weak (strong) transverse magnetic field Γ compared to $\langle J_\delta^2\rangle^{1/2}$, the longitudinal dynamic structure factor will show a peak at $\omega = 0$ ($\omega = \Gamma/2$) [8]. Thus, the weak-field limit exhibits no longitudinal dynamics, i.e., δ function peak at $\omega = 0$, and the strong-field limit leads to a picture in which N independent spins precess about the field $\Gamma/2$ [8]. The dynamic structure factor, however, is more interesting when $\Gamma \approx \langle J_\delta^2\rangle^{1/2}$, that is when the field strength and the ferromagnetic coupling are competitive.

Experiments with real 3D systems show that in the neighbourhood of $\omega \approx \Gamma/2$, for $\Gamma \approx J/2$ the dynamic structure factor, which exhibits a broad central peak, possesses a rather long tail [2, 3]. In theoretical studies with $D > 1$, this regime is inaccessible via standard perturbative approaches and hence the study of the dynamics of the transverse Ising model in this regime in all finite $D > 1$ has remained a challenge. The study of the behaviour of the dynamic structure factor in this competitive regime (to be precise, at $\Gamma = J/2$) at $T = \infty$ at $D > 1$ is the primary objective of this work. It turns out that the results are not strongly sensitive to the precise value of Γ as long as $\Gamma \sim J/2$ [10]. Hence, as we shall see, our theoretical calculations can be directly compared with the experimental data in [2].

In addition to our calculations [10], it is experimentally observed that for the transverse Ising model, lowering of temperature leaves the dynamic structure factor approximately invariant [2, 3]. This observation suggests that the physics of the system at $T = \infty$ is probably an acceptable description for the entire paramagnetic regime. Such evidence is also present in studies on a related system, that of the dynamics of a classical oscillator in a double-well potential in contact with a heat bath at temperatures $\approx$ barrier height [11].

It is well known that in 1D, the relaxation function $\langle S_r^z(t)S_r^z\rangle$ for $\Gamma = J/2$ is exactly a Gaussian and the dynamic structure factor is approximately a Gaussian at $T = \infty$, where J

is the nearest-neighbour Ising coupling [8, 5, 6]. It is not surprising that an exact calculation is possible in 1D. After all, in 1D the transverse Ising model can be mapped to a gas of non-interacting fermions [4].

The same quantity, quite understandably, becomes prohibitively difficult to estimate analytically in 2D when any mapping to the fermionic picture yields a system of *interacting* fermions. We have, however, managed to estimate the dynamic structure factor analytically in 2D using the highly successful recurrence relations method [12, 13] (the 1D treatment via this method appears in the work of Florencio and Lee in [6]) in conjunction with the newly developed and powerful direct summation method [14, 15] for studying dynamical correlations. Our 2D calculations reveal a dynamic structure factor with the characteristics mentioned above and experimentally observed for $LiTbF_4$, which has a 3D tetragonal lattice. Since the essential difference between the 2D and 3D models at $T = \infty$ lies in the different coordination numbers of the two systems and in the increased lattice connectivity in 3D [16], we conjecture that the general properties of the relaxation function in the $T = \infty$ dynamics will be marginally affected as one goes from 2D to 3D. In other words, the overall qualitative features of the dynamic structure factor should only weakly depend on the lattice dimensionality for $D > 1$ at $T = \infty$ in the transverse Ising model. Therefore, we expect that our 2D calculations should lead to some understanding of the dynamic structure factor in $LiTbF_4$ in the paramagnetic phase. As we shall see later, this expectation indeed comes through.

Based on a calculation of the first two moments of the shape function in the simple cubic lattice, and comparison between analytical calculations and numerical simulations for a $S = 1$ transverse Ising chain, Tommët and Huber [8] have pointed out that at $T = \infty$, the shape function and hence the dynamic structure factor are most likely *nearly* independent of k. Therefore, one can replace the total spin zz correlations in equation (2) by $4N\langle S_r^z(t)S_r^z(0)\rangle$ at $T = \infty$ and still expect to get quantitatively meaningful results should the Tommet–Huber hypothesis be approximately true. As we shall see, our results compare well with experiments and hence give further evidence in favour of the Tommet–Huber hypothesis for the transverse Ising model [8]. We will therefore focus on a calculation of the tagged spin dynamical correlation for the remainder of this paper.

3. The formalism

The calculation of the tagged spin relaxation function for a square lattice is accomplished as follows. Using the recurrence relations method [12, 13] we first write the time evolving spin operator $S_r^z(t)$ as an orthogonal expansion in a Hilbert space $\mathcal{S}$ defined by some suitably chosen scalar product. A reasonable choice of the scalar product is the Kubo scalar product which is nothing other than the susceptibility formula [12]. The reader may note that the Kubo scalar product becomes the fluctuation formula in the $T = \infty$ limit. This simplification, which trivializes the calculation of the static correlations at $T = \infty$, is one of the reasons why the study of spin dynamics at $T = \infty$ is easier to carry out than doing the same at $T = 0$. Thus, we begin by writing

$$S_r^z(t) = \sum_{\mu=0}^{d-1} f_\mu a_\mu(t) \tag{3}$$

where f_μ and $a_\mu(t)$ are orthogonal basis vectors (defining the Hilbert space $\mathcal{S}$) and their time dependent coefficients, respectively, in $\mathcal{S}$. The orthogonality of the f_μ are realized through the Kubo scalar product as mentioned above.

Thus, upon choosing a f_0, one can exploit the Kubo scalar product to determine f_1 and the higher f_μ. In general, the choice of the Kubo scalar product leads to a simple recurrence relation (RR I) for the f_μ (given the choice of f_0) given by

$$f_{\mu+1} = \mathrm{i}[H, f_\mu] + \Delta_\mu f_{\mu-1} \tag{4}$$

where $\Delta_\mu = (f_\mu, f_\mu)/(f_{\mu-1}, f_{\mu-1})$, are the ratios of the 'length squared' of the basis vectors in the space $\mathcal{S}$ ($\hbar \equiv 1$). Thus, the Δ_μ carry information about the geometrical properties of $\mathcal{S}$. Since equation (4) above must satisfy the Heisenberg equation of motion, it turns out that there must also be a recurrence relation for the $a_\mu(t)$. This recurrence relation, RR II is given by

$$\Delta_{\mu+1} a_{\mu+1} = -\mathrm{d}a_\mu/\mathrm{d}t + a_{\mu-1}. \tag{5}$$

A more convenient way of writing RR II is by taking a Laplace transform of RR II. One can show [12] that the Laplace transformed version of equation (5) can be bent into an expression for $a_0(z)$ in terms of a continued fraction. The reader may note that the structure of the continued fraction obtained from equation (5) is sensitive to the choice of the scalar product. Thus, a choice of a different scalar product will yield a continued fraction which is structurally different and hence could be easier or more difficult to solve [13]. Typically, it turns out that $d \to \infty$ in equation (3) and the expression for $a_0(z)$ is an infinite continued fraction [14, 15, 17]. The following is an expression for $a_0(z)$:

$$a_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cdots \cfrac{\Delta_r}{z + \cdots \text{ to } \infty}}}}}. \tag{6}$$

Realizing the fact that $a_0(t) = 4\langle S_r^z(t) S_r^z \rangle$ at $T = \infty$, it follows that the necessary information for computation of the Laplace transformed relaxation function given in equation (6) above is contained in $\{\Delta_\mu\}$. The following summarizes the calculations leading to an estimation of Δ_μ and the subsequent evaluation of our relaxation function, $a_0(t)$, and of the dynamic structure factor $S(\boldsymbol{k}, \omega)$ (where superscript zz has been supressed).

The evaluation of the continued fraction in equation (6) is non-trivial. Typically, for most interesting problems, the continued fraction in equation (6) is not exactly solvable. It turns out that it may be possible to numerically obtain the distribution of poles in equation (6) when it is not exactly solvable. This is accomplished via the direct summation method [14, 15]. This method is discussed in detail elsewhere [15]. We therefore summarize the basic idea behind the direct summation method.

It turns out that typically $\Delta_\mu \sim \mu^\alpha$, where $0 \leqslant \alpha \leqslant 2$ for most many-body quantum spin systems [18]. If $\alpha < 2$, then any infinite continued fraction can be replaced by a finite continued fraction with a large number of levels. The accuracy to which the poles of the infinite continued fraction can be estimated obviously improves when a larger number of levels are kept in the truncated continued fraction. It is rather straightforward to estimate continued fractions with as many as 10^6 levels. Thus, for most many-body quantum spin systems, it is possible to replace infinite continued fractions by finite continued fractions. The direct summation method then provides a simple recipe for evaluating these finite continued fractions efficiently with minimum round-off error. It also provides a simple and powerful algorithm to evaluate the inverse Laplace transform of the evaluated continued fraction. This inverse Laplace transformed function is the relaxation function under study.

It may be noted that, to our knowledge, the following is the first calculation of dynamical correlations of spin operators in a 2D quantum spin system at high temperatures which does not resort to the mean field approximation or related approximation techniques but rather approaches the real time dynamics problem directly, to the extent feasible via the state of the art symbolic manipulation algorithms, on the real space lattice [19].

4. Calculations and results

Let us take δ_x and δ_y (see equation (1)) to equal unity in our square lattice, i.e., we have nearest-neighbour Ising interactions. Let us also impose toroidal boundary conditions on our system. Thus, $f_0 = S_r^z$ and $f_1 = -(\Gamma/2)S_r^y$. The terms in f_2 are obtained using RR I with $\Delta_1 = \Gamma^2/4$ and involve strings of two-spin operators involving the nearest-neighbour sites of the spin at r. Likewise, f_3 involves strings of three-spin operators with the spin operators of the rth site, its nearest and second-nearest neighbours, and so on for the higher f_μ. The sequence of f_μ quickly becomes extremely complicated. Thus, the expression for f_6, which is the highest order to which we have carried out rigorous calculations, already contains about 1500 terms. The efforts required to obtain higher f_μ grow exponentially and are therefore truly formidable [10]. It turns out, however, that the Δ_μ, which are the ratios of the lengths squared of the basis vectors, are more tractable quantities. For the special case of $\Gamma = J/2$ with $\Gamma = 2$ K and $J = 4$ K in equation (1), these are,

$$\Delta_1 = 1 \qquad \Delta_2 = 4 \qquad \Delta_3 = 7$$
$$\Delta_4 = \tfrac{72}{7} \qquad \Delta_5 = \tfrac{253}{21} \qquad \Delta_6 = 354\,074/21\,252 \tag{7}$$

and so on. It may be noted that our choice of Γ and J is consistent with those in [2] where $\Gamma = 2.68$ K and $J \approx 4$ K.

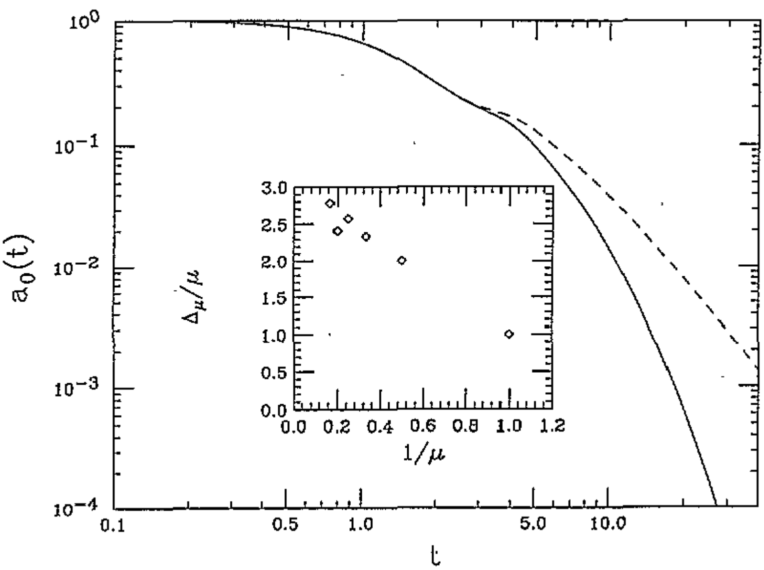

Figure 1. Log–log plot of the relaxation function using '$1/\mu$' (solid) and '$1/\sqrt{\mu}$' (dashed) schemes (see text) at $T = \infty$. Window shows plot of Δ_μ/μ against $1/\mu$.

The problem now is to estimate the infinite continued fraction in equation (6) with the knowledge of the first few recurrants above [20]. Although these are just a few of an infinite set, a plot of Δ_μ/μ versus $1/\mu$ (see figure 1 inset) already reveals an important general feature of Δ_μ as a function of μ, i.e., an overall *linear pattern with oscillations around linearity* [21]. It is well known that an infinite continued fraction with linear Δ_μ, which occurs in the 1D transverse Ising model problem for $\Gamma = J/2$, is exactly solvable and yields a Gaussian relaxation function [6, 15]. In addition, approximately linear behaviour of Δ_μ has also been obtained in other simple quantum spin dynamics problems yielding a variety of relaxation functions [22]. Note, however, that the deviations from linearity in Δ_4, Δ_5, Δ_6 indicate that the relaxation function will be different from a Gaussian case [15]. Let us focus on how the behaviour of Δ_μ for $\mu > 6$ can affect the long-time behaviour of the relaxation function. The following aspect of the study relies on the recently developed direct summation method of calculating dynamical correlations using continued fractions [14, 15].

We have explored several extrapolation schemes to approximately describe Δ_μ for $\mu > 6$ based on available information. The following describes some of the schemes we have tried for even and odd μ, respectively,

$$\Delta_\mu = 3\mu - 2 + \phi(\mu)0.67 \tag{8}$$

$$\Delta_\mu = 3(\mu - 1) - \phi(\mu) \tag{9}$$

where $\phi(\mu)$ is a parameter that describes the amplitude of the oscillations of Δ_μ about linearity. There are several obvious possibilities for $\phi(\mu)$, namely, (i) the oscillations can increase with μ, (ii) the oscillations can remain constant, and (iii) the oscillations can decrease with μ. We will argue that (i) is not to be expected on physical grounds because if the oscillations are to continue to increase, $a_0(z)$ will (a) eventually *tend to truncate* [15] or (b) for sufficiently rapidly growing oscillations Δ_μ will eventually become less than zero if the overall linear growth rate of Δ_μ must be respected. Possibility (ia) is physically less appealing as it would imply that the infinite continued fraction tends to self-truncate and hence the excitation tends to localize in real space [15]. (ib) is physically unreasonable because the Δ_μ are, by definition, positive definite quantities. Thus, $\phi(\mu)$ must either satisfy (ii) or (iii). We have carried out extensive calculations using the coefficient of $\phi(\mu) = 0.67$ for even μ and -1.0 for odd μ to explore option (ii). We have also studied the cases with $\phi(\mu) = 1/(\mu - 4)$ for even μ and $\phi(\mu) = 1/(\mu - 5)$ for odd μ and $\phi(\mu) = 1/\sqrt{\mu - 4}$ and $\phi(\mu) = 1/\sqrt{\mu - 5}$ for even and odd μ, respectively of option (iii). The constants 0.67 and -1.0 in even and odd μ cases of ϕ are arrived at by using the deviations of Δ_4, Δ_5 and Δ_6, respectively, from the straight line $\Delta_\mu = 3\mu - 2$.

It is important to note that for option (ii) to be physically reasonable, one must find that the Δ_μ will oscillate around linearity with constant amplitude for all $\mu > 3$ for $\Gamma = J/2$. Observe that Δ_μ are functions of multipoint static correlations of our system. Thus, at infinite distances from site r, one might expect that the Δ_μ, which are the ratios of sums of large numbers of static correlations entering from each of the allowed strings of spin operators in the f_μ versus those from $f_{\mu-1}$, will go to ∞ (although special cases to the contrary are known [15]). While our calculations suggest that $\Delta_\mu \to \infty$ as $\mu \to \infty$, they do not give any indication to expect that Δ_μ will oscillate uniformly about linearity for all μ. In fact, a Padé analysis [10] of the expression using the exact Δ_1–Δ_6 for the relaxation function, $4\langle S_r^z(t)S_r^z\rangle$, reveals that the oscillations in Δ_μ should decrease as in option (iii) above. The decay of the oscillations as predicted by Padé analysis of the relaxation function, $a_0(t)$, is consistent with the $1/\mu$ type decay hypothesis invoked above. We therefore use the data from the solid line in figure 1 to compute the dynamic structure factor in figure 2 and ignore the results obtained using the $1/\sqrt{\mu}$ type decay hypothesis (described via the dashed line) in figure 1.

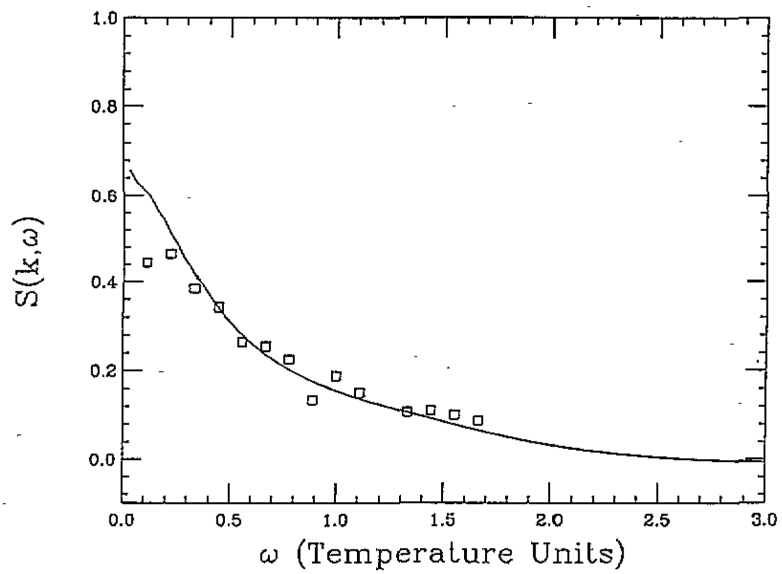

Figure 2. Dynamic structure factor. Solid, theory, using '$1/\mu$' scheme; squares experiments of Youngblood *et al* [2].

Upon taking a Fourier transform of the dynamical correlation we find a spectrum that exhibits a broad central peak centred at $\omega = 0$ without any obvious side peaks or shoulders but, instead, a smoothly decaying $S(\boldsymbol{k}, \omega)$ between $1.0 \leqslant \omega \leqslant 2.0$, i.e., between energy transfers of 0.09 meV and 0.17 meV (i.e., $1.0 < \omega < 2.0$ in temperature units) or so in $S(\boldsymbol{k}, \omega)$ as seen in the experiments of Youngblood *et al* as shown in figure 2. The reader may note that in reproducing the experimental data in [2] we have manually estimated the positions of the data points from the data in figure 2 (open circles) of [2]. The errors in the data are roughly commensurate with the same in our plots and hence, for our purposes, the data reproduced in figure 2 are adequate. Clearly, the agreement between theory and experiment is significant except for one data point at $\omega \approx 0.01$. Based upon the dynamic structure factor obtained exactly in 1D and in the mean field analysis we suspect that the experimental data point at $\omega \approx 0.01$, if accurate, could be representative of the rather low T (≈ 4 K) of the actual system which possesses a 3D tetragonal lattice structure (as opposed to our 2D quadratic lattice structure). To understand the disagreement between the experimental data and the theoretical prediction at $\omega \approx 0.01$ let us note that we have made three important assumptions in this study. First, we have assumed that the Tommet–Huber hypothesis is valid for the 2D system, second, we have assumed that the Δ_μ in (8, 9) are correct as $\mu \to \infty$, and third, our results at $T \to \infty$ adequately represent the behaviour of the relaxation function at $T > T_c$. In general, however, our results are significantly closer to the experimental data when compared with the three-pole approximation based results of Tommet and Huber and the mean field based results of Stinchcombe and others which find a 'peak' near $\omega/\Gamma = \frac{1}{2}$, i.e., at 1 K.

Our results can also be successfully compared with the work of Kötzler *et al* [3] who measured the dissipative part of the dynamic susceptibility $\chi''(\omega)$ (see the inset in figure 1 in [3]). The connection between $S(\omega)$ and $\chi''(\mathrm{i}\omega)$ is given by [23]

$$S(\omega) = \frac{1}{\pi} \frac{\coth(\omega\beta/2)}{\exp(\omega\beta) + 1} \chi''(\mathrm{i}\omega) \tag{10}$$

where we have set $\hbar \equiv 1$ as mentioned earlier.

5. Summary

We know that the dynamic structure factor is a Gaussian in the 1D case [6]. It is also known that the same quantity exhibits a distinct peak at $\omega = \Gamma/2$ in the ∞D case [8]. It is therefore intuitively reasonable that the 3D case might exhibit a tendency of suppression of the quasielastic central peak and one of enhancement in magnitude of $S(\boldsymbol{k}, \omega)$ in the neighbourhood of $\omega = \Gamma/2$. The validation of this conjecture will be addressed elsewhere [10].

To summarize, we have presented a calculation of the dynamic structure factor of the 2D transverse Ising model at $T = \infty$ via the recurrence relations method. In addition, we have exploited the direct summation method and the Tommet–Huber hypothesis for calculation of the dynamic structure factor of the transverse Ising model. We have also compared our results with experimental data for a 3D transverse Ising model at $T > T_c$. Our study reveals details of the propagation of excitations in real space in the 2D transverse Ising model and our calculation of the dynamic structure factor compares favourably with experimental data without ours having to invoke any free parameters in the study.

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