One-particle dispersion and spectral weights in the transverse Ising model

C. J. Hamer, J. Oitmaa, and Weihong Zheng

School of Physics, University of New South Wales, Sydney, New South Wales 2052, Australia

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The one-particle contribution to the dynamical structure factor is explored for the simple case of the transverse Ising model, using series expansion methods. The critical behavior of the spectral weight is found to conform with the general predictions of Sachdev. For the linear chain, exact results are obtained, and confirmed by correspondence with exactly known results for the correlation functions of the quantum *XY* model in one dimension. In higher dimensions, series are calculated for the triangular, square, and simple cubic lattices, and numerical estimates for the critical exponents are found to agree with expectations, within errors.

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I. INTRODUCTION

Quantum phase transitions in strongly correlated magnetic or electronic systems in condensed matter physics are currently a topic of great interest.¹ Physics in the vicinity of such quantum critical points can be described in terms of general scaling theories and effective Lagrangians, independently of the details of any particular microscopic model. Quantum critical points are thought to play an important role in many low-temperature phenomena, such as heavy-fermion superconductors, "high-temperature" superconductors, organic conductors, and related compounds.

For quantum magnets, the dynamical structure factor is an important quantity which is proportional to the inelastic neutron scattering intensity, and thus allows a direct comparison between experiments on real materials and theoretical model calculations. At low energies, the structure factor is often dominated by a single quasiparticle excitation, which can provide crucial information about the dynamics of the system.

Sachdev¹ has developed a scaling theory for the spectral weight of a single quasiparticle in the vicinity of a quantum phase transition. In this paper, we use series expansion techniques to study the one-particle spectral weight for a particular quantum spin model, the Ising model in a transverse field. This is a very simple model, often used as a paradigm for quantum spin models in general. We will show that the critical behavior of the one-particle spectral weight conforms very well with the general predictions of Sachdev.¹ Many of the results were announced previously in an earlier Rapid Communication[.2](#page-9-1)

The dynamical structure factor is 3

$$
S^{\alpha\beta}(\mathbf{k},\omega) = \frac{1}{2\pi N} \sum_{i,j} \int_{-\infty}^{\infty} dt \ e^{i[\omega t + \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)]} \langle S_j^{\alpha}(t) S_i^{\beta}(0) \rangle \quad (1)
$$

where $S_j^{\alpha}(t)$ denotes a component of the spin operator at site *j* and time *t*, while the angular brackets denote a thermal average or, at zero temperature, a ground-state expectation value. Integrating ([1](#page-0-0)) over energy, we obtain the integrated or static structure factor

$$
S^{\alpha\beta}(\mathbf{k}) = \frac{1}{N} \sum_{i,j} e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle S_j^{\alpha} S_i^{\beta} \rangle
$$
 (2)

which is just the Fourier transform of the spin-spin correlation function.

At low temperatures the major contribution to $S(\mathbf{k}, \omega)$ will often come from low-energy quasiparticle excitations. It is then useful to write (1) (1) (1) in the "spectral form" (valid for a discrete spectrum)

$$
S^{\alpha\beta}(\mathbf{k},\omega) = \sum_{\Lambda} \delta(\omega + E_0 - E_{\Lambda}) S^{\alpha\beta}_{\Lambda}(\mathbf{k}), \tag{3}
$$

where the sum is over all eigenstates with energies E_{Λ} , and the "spectral weights" $S_{\Lambda}^{\alpha\beta}(\mathbf{k})$ are given by

$$
S_{\Lambda}^{\alpha\beta}(\mathbf{k}) = \Omega_{\Lambda}^{\alpha^*}(\mathbf{k})\Omega_{\Lambda}^{\beta}(\mathbf{k})
$$
 (4)

with

$$
\Omega_{\Lambda}^{\beta}(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{i} \langle \psi_{\Lambda} | S_{i}^{\beta} | \psi_{0} \rangle e^{i\mathbf{k} \cdot \mathbf{r}_{i}}.
$$
 (5)

We restrict ourselves to the zero-temperature case.

Henceforth we consider only the "one-particle" spectral weights $S_{1p}(\mathbf{k})$, referring to a state of a single quasiparticle with momentum **k**. Near a quantum phase transition at some coupling $g = g_c$ this quantity is expected to show universal scaling properties, which can be derived from a field theoretic approach, independently of the details of a particular model.

Sachdev, $¹$ for instance, discusses the scaling properties of</sup> the dynamic susceptibility χ (**k**, ω), which at zero temperature is related to the structure factor by

$$
S(\mathbf{k}, \omega) = \frac{1}{\pi} \operatorname{Im} \{ \chi(\mathbf{k}, \omega) \}
$$
 (6)

note that our definition of the structure factor differs from Sachdev's by a constant factor). Assuming relativistic invariance of the effective field theory, which applies to many, though not all, models, the dynamic susceptibility in the vicinity of a quasiparticle pole is expected to have the form

$$
\chi(\mathbf{k}, \omega) = \frac{A}{c^2 \mathbf{k}^2 + \Delta^2 - (\omega + i\epsilon)^2} + \cdots
$$
 (7)

where ϵ is a positive infinitesimal, *c* the quasiparticle velocity, Δ the quasiparticle energy gap, and *A* the quasiparticle residue.

Let

$$
E(\mathbf{k}) = \sqrt{c^2 \mathbf{k}^2 + \Delta^2};\tag{8}
$$

then from Eqs. (6) (6) (6) and (7) (7) (7) we find

$$
S_{1p}(\mathbf{k}, \omega) = \frac{A}{2E(\mathbf{k})} \delta(\omega - E(\mathbf{k})).
$$
 (9)

Hence we are led to define

$$
S_{1p}(\mathbf{k}) = \frac{A(\mathbf{k})}{2E(\mathbf{k})}
$$
 (10)

where $A(\mathbf{k})$ is the residue function: strictly speaking, the quasiparticle residue is then $A(\mathbf{k})$ at $\mathbf{k} = 0$.

The expected scaling behavior of these functions can be derived¹ using the renormalization group. For instance, at the critical point a correlation function $\langle \phi_i(r_1) \phi_i(r_2) \rangle \propto |r_1|$ $-r_2$ ^{$-2x_i$}, where

$$
x_i = d - y_i \tag{11}
$$

[Ref. [4,](#page-9-3) Eq. (3.55)], with x_i the scaling dimension and y_i the renormalization group eigenvalue corresponding to operator ϕ_i , and *d* the number of dimensions. Thus the scaling dimension of the spin-spin correlation function

$$
C^{\alpha\beta}(j-i) = \langle S_i^{\alpha} S_j^{\beta} \rangle \tag{12}
$$

is

$$
\dim[C] = 2(d - y_h) \tag{13}
$$

where d is the number of space-time dimensions and y_h is the renormalization group magnetic eigenvalue, and so from Eqs. (1) (1) (1) and (6) (6) (6)

$$
\dim[\chi] = d - 2y_h = -2 + \eta \tag{14}
$$

using the identity

$$
\eta = 2 + d - 2y_h; \tag{15}
$$

and finally

$$
\dim[A] = \eta. \tag{16}
$$

The scaling behavior of the residue as a function of coupling in the vicinity of the critical point can be inferred from that of the correlation length $\xi \sim (g_c - g)^{-\nu}$ [Ref. [4,](#page-9-3) Eq. (3.50)], and hence as one approaches the quantum phase transition point the quasiparticle residue is expected to scale as

$$
A \sim (g_c - g)^{\eta \nu}, \quad g \to g_{c-}.\tag{17}
$$

Since the energy gap scales as

$$
E(\mathbf{k} = \mathbf{0}) \sim (g_c - g)^{\nu},\tag{18}
$$

then the spectral weight

$$
S_{1p}(\mathbf{k} = \mathbf{0}) \sim (g_c - g)^{(\eta - 1)\nu}.
$$
 (19)

Our aim is to confirm and demonstrate this scaling behavior for the transverse field Ising model. In the disordered phase, the Hamiltonian for the model can be written as

$$
H = \sum_{i} (1 - \sigma_i^z) - \lambda \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x \tag{20}
$$

where $\sigma_i^{\alpha} = 2S_i^{\alpha}$ are Pauli operators and the second sum is over nearest neighbor pairs; while in the ordered phase, the Hamiltonian can be represented in the modified form

$$
H = \sum_{\langle ij \rangle} (1 - \sigma_i^z \sigma_j^z) - x \sum_i \sigma_i^x \tag{21}
$$

where $x=1/\lambda$. This model has a quantum phase transition at $\lambda = 1$ in one dimension, and at some specific λ_c for each higher-dimensional lattice.

Our approach is to derive series expansions in λ for various one-particle spectral weights in the disordered phase λ $\langle \lambda_c, \rangle$ using the linked-cluster techniques reviewed by Oitmaa *et al.*, [5](#page-9-4) and to analyze the series by standard methods to obtain the critical behavior. We also derive series for the one-particle dispersion in both ordered and disordered phases. Note that in the ordered phase the one-particle state belongs to the same sector as the ground state, and so the linked-cluster expansion with the traditional similarity $transformation⁷$ fails, as it allows an excitation to annihilate from one site and reappear on another far away, violating the assumptions necessary for the cluster expansion to hold. To generate a successful linked-cluster expansion, one must use the multiblock orthogonality transformation introduced in Ref. [8.](#page-9-6) Indeed, we find that with proper orthogonalization the linked-cluster property holds in this case. At the critical point λ_c , we find that the one-particle dispersions estimated from both phases agree.

In Sec. II of the paper, we discuss the model on a onedimensional lattice, the transverse Ising chain. Analysis of the series leads us to an exact result for the one-particle structure factors, which provides an explicit demonstration of the critical behavior predicted by Sachdev.¹ In Sec. III we discuss two-dimensional versions of the model, on the square and triangular lattices, and in Sec. IV we treat a threedimensional version, on the simple cubic lattice. Here no exact results are available, but the numerical evidence is again in good agreement with the predictions of Sachdev.¹ Graphs are given to illustrate the behavior of the structure factors in each case.

II. THE LINEAR CHAIN

The transverse Ising chain model is exactly solvable, and expressions for the energy spectrum, magnetization, etc. have been given by Pfeuty.⁶

A. Numerical results

We have computed series for the one-particle matrix elements $\Omega_{1p}^{\pm}(k)$ for this model up to order λ^{22} . The leadingorder terms are

$$
\Omega_{1p}^{-}(k) = 1 - \frac{\lambda^2}{16} - \frac{47\lambda^4}{1024} - \frac{513\lambda^6}{16384} + \left(\frac{\lambda^3}{16} + \frac{\lambda^5}{64}\right)\cos(k) \n+ \left(\frac{\lambda^2}{16} + \frac{9\lambda^4}{256} + \frac{315\lambda^6}{32768}\right)\cos(2k) + \left(\frac{\lambda^3}{16} + \frac{13\lambda^5}{512}\right)\cos(3k) + \left(\frac{59\lambda^4}{1024} + \frac{329\lambda^6}{16384}\right)\cos(4k) \n+ \frac{27\lambda^5 \cos(5k)}{512} + \frac{1589\lambda^6 \cos(6k)}{32768} + O(\lambda^7),
$$
\n(22)

$$
\Omega_{1p}^{+}(k) = \frac{\lambda^{4}}{128} + \frac{9\lambda^{6}}{2048} + \left(\frac{\lambda}{2} - \frac{3\lambda^{3}}{64} - \frac{33\lambda^{5}}{2048}\right) \cos(k)
$$

+
$$
\left(\frac{\lambda^{2}}{4} - \frac{\lambda^{4}}{64} - \frac{35\lambda^{6}}{8192}\right) \cos(2k) + \left(\frac{11\lambda^{3}}{64} - \frac{29\lambda^{5}}{4096}\right) \cos(3k) + \left(\frac{17\lambda^{4}}{128} - \frac{7\lambda^{6}}{2048}\right) \cos(4k)
$$

+
$$
\frac{447\lambda^{5} \cos(5k)}{4096} + \frac{763\lambda^{6} \cos(6k)}{8192} + O(\lambda^{7}).
$$
 (23)

We can supply further coefficients on request.

We then set out to perform a standard *D*log Padé analysis of the series for $\Omega^{\pm}_{1p}(\hat{k})$. That is, we computed series in λ for the logarithmic derivative

$$
D\Omega_{1p}^{\pm}(k,\lambda) = \frac{d\Omega_{1p}^{\pm}(k,\lambda)/d\lambda}{\Omega_{1p}^{\pm}(k,\lambda)}
$$
(24)

and computed the poles and residues of Padé approximants to $D\Omega^{\pm}_{1p}(k,\lambda)$, giving direct estimates of the critical point and critical exponents.⁹ For $k=0$, it immediately became apparent that some pole-residue pairs were turning up exactly and consistently at all orders. For $\Omega_{1p}^{-}(k=0,\lambda)$, we found the following: a pole at $\lambda = 1$ with critical index $-3/8$, a pole at 2 with critical index 1, and a pole at -1 with critical index $1/8$, and so the matrix element can be represented exactly, up to the order calculated, by the closed form expression

$$
\Omega_{1p}^{-}(k=0,\lambda) = (1-\lambda)^{-3/8}(2-\lambda)(1+\lambda)^{1/8}/2. \qquad (25)
$$

For $\Omega_{1p}^+(k=0,\lambda)$, we found a pole at $\lambda = 1$ with critical index $-3/8$, and a pole at -1 with critical index 1/8, and so the matrix element can be represented exactly by

$$
\Omega_{1p}^{+}(k=0,\lambda) = \lambda (1-\lambda)^{-3/8} (1+\lambda)^{1/8} / 2. \tag{26}
$$

After further investigation, we then realized that the series for general *k* could be represented exactly, up to the order calculated, by the closed form expressions

$$
\Omega_{1p}^{\pm}(k) = \frac{1}{2} (1 - \lambda^2)^{1/8} \frac{[1 \mp \Lambda(k)]}{\Lambda(k)^{1/2}} \tag{27}
$$

where $\Lambda(k)$ is just half the one-particle energy $E(k)$:

$$
\Lambda(k) = E(k)/2 = [1 + \lambda^2 - 2\lambda \cos(k)]^{1/2}.
$$
 (28)

It is natural to conjecture that this result is exact to all orders, and indeed we justify this below.

One can now write down any desired spectral weight $S_{1p}^{\alpha\beta}(k)$, e.g.,

$$
S_{1p}^{+-}(k) = \frac{1}{4}(1 - \lambda^2)^{1/4} \frac{[1 + \Lambda(k)]^2}{\Lambda(k)},
$$
 (29)

$$
S_{1p}^{-+}(k) = \frac{1}{4}(1 - \lambda^2)^{1/4} \frac{[1 - \Lambda(k)]^2}{\Lambda(k)},
$$
 (30)

$$
S_{1p}^{++}(k) = S_{1p}^{-}(k) = \frac{1}{4} (1 - \lambda^2)^{1/4} \frac{[1 - \Lambda^2(k)]}{\Lambda(k)}.
$$
 (31)

These formulas give a very clear demonstration of the critical behavior expected theoretically. The quasiparticle residue functions for *S*−+, *S*+− are, respectively,

$$
A(k) = (1 - \lambda^2)^{1/4} [1 \pm \Lambda(k)]^2,
$$
 (32)

which vanish at the critical point $\lambda = 1$ with exponent 1/4 $=\eta v$, as expected for the transverse Ising chain where η $=1/4$, ν =1. At the critical momentum k =0, the energy gap is $2(1-\lambda)$, and vanishes as $\lambda \rightarrow 1$ with exponent $\nu = 1.6$ $\nu = 1.6$ Note that the residue function vanishes at $\lambda = 1$ for all k, not just $k=0$. It is not clear whether this feature will generalize to other models.

From Eqs. (27) (27) (27) , one can also show

$$
S_{1p}^{xx}(k) = \frac{(1 - \lambda^2)^{1/4}}{4\Lambda(k)},
$$

\n
$$
S_{1p}^{yy}(k) = \frac{1}{4}(1 - \lambda^2)^{1/4}\Lambda(k).
$$
\n(33)

Thus the quasiparticle residue for the dominant spectral weight S^{xx} at $k=0$ is

$$
A = (1 - \lambda^2)^{1/4} \sim [2(1 - \lambda)]^{1/4}, \quad \lambda \to 1,
$$
 (34)

in agreement with Sachdev's result, $\frac{1}{1}$ after one takes into account differing normalization factors in our definitions. Note that whereas $S_{1p}^{xx}(k)$ diverges as $\{\lambda \rightarrow 1, k=0\}$, $S_{1p}^{yy}(k)$ does not. It appears that *Syy* decouples from the one-particle state at the critical point.

By Fourier transforming, we obtain the one-particle contributions to the correlation functions

$$
C^{\alpha\alpha}(n) = \langle S_0^{\alpha} S_n^{\alpha} \rangle_0 \tag{35}
$$

[using Eq. (2) (2) (2)] as

$$
C_{1p}^{xx}(n) = (1 - \lambda^2)^{1/4} \frac{1}{8\pi} \int_0^{2\pi} dk \frac{\cos(kn)}{\Lambda(k)},
$$

$$
C_{1p}^{yy}(n) = (1 - \lambda^2)^{1/4} \frac{1}{8\pi} \int_0^{2\pi} dk \cos(kn) \Lambda(k).
$$
 (36)

Now multiparticle expansions for correlation functions have been discussed in the case of the two-dimensional (2D) classical Ising model by several authors. $10-14$ $10-14$ For the related quantum *XY* model in one space dimension, corresponding results have been obtained by Vaidya and Tracy.¹⁵ The transverse Ising model is merely a special case of the model considered by them; and so it turns out that Eqs. (36) (36) (36) are merely the leading terms in multiparticle expansions already derived by Vaidya and Tracy (Sec. 2.2 of Ref. [15](#page-9-11) for $t=0$, $\gamma \rightarrow 1$, and $h = 1/\lambda$). This confirms that our results are indeed exact.

III. TWO-DIMENSIONAL MODELS

Next, we use series methods to study the two-dimensional version of the model on the triangular and square lattices.

 $\overline{}$

The transverse Ising model in $(2+1)$ dimensions lies in the universality class of the 3D classical Ising model, and so its critical exponents are expected to be $\eta = 0.0364(5)$, v $= 0.6301(4)$, from various estimates.¹⁶

A. The triangular lattice

The critical point for the transverse Ising model on the triangular lattice has been estimated from series expansions as $\lambda_c = 0.20972(7)$ by Hamer and Guttmann¹⁷ and λ_c $= 0.209$ 72(2) by He *et al.*^{[18](#page-9-14)}

We have computed series in the disordered phase for the one-particle structure factors $S_{1p}^{xx}(\mathbf{k})$ and $S_{1p}^{yy}(\mathbf{k})$ and the quasiparticle energy $E(\mathbf{k})$ to order λ^{12} . The calculation involved a list of 4 140 438 clusters, consisting of up to 13 sites. We also computed a series in the ordered phase for the oneparticle dispersion $E(\mathbf{k})$ to order x^{16} ; this calculation involving a list of 8469 clusters, consisting of up to nine sites. Consistent with the symmetry of the triangular lattice, the series for all quantities computed here can be expressed in the general form

$$
\sum_{r=0}^{\infty} \lambda^{r} \sum_{m,n} c_{r,m,n} \left[\cos\left(\frac{m}{2}k_{x}\right) \cos\left(\frac{n\sqrt{3}}{2}k_{y}\right) + \cos[k_{y}\sqrt{3}(m+n)/4] \cos[k_{x}(m-3n)/4] + \cos[k_{y}\sqrt{3}(m-n)/4] \cos[k_{x}(m+3n)/4] \right] / 3 \quad (37)
$$

where *m* and *n* are integer, λ is the expansion parameter, and $c_{r,m,n}$ are the series coefficients. The leading-order terms for the the quasiparticle energy $E(\mathbf{k})$ and spectral weights $S_{1p}^{xx}(\mathbf{k})$ and $S_{1p}^{yy}(\mathbf{k})$ in the disordered phase are

$$
E(\mathbf{k}) = 2 - 2\lambda [\cos(k_x) + 2 \cos(k_x/2)\cos(\sqrt{3}k_y/2)]
$$

+
$$
\frac{\lambda^2}{2} \left[3 - 2 \cos(k_x) - \cos(2k_x) - 4 \cos\left(\frac{k_x}{2}\right) \right]
$$

$$
\times \cos\left(\frac{\sqrt{3}k_y}{2}\right) - 4 \cos\left(\frac{3k_x}{2}\right)\cos\left(\frac{\sqrt{3}k_y}{2}\right) - 2 \cos(\sqrt{3}k_y)
$$

-
$$
2 \cos(k_x)\cos(\sqrt{3}k_y) + O(\lambda^3),
$$
 (38)

$$
S_{1p}^{xx}(\mathbf{k}) = \frac{1}{4} + \frac{\lambda}{4} \Bigg[\cos(k_x) + 2 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right) \Bigg] + \frac{\lambda^2}{16} \Bigg[6 \cos(k_x) + 3 \cos(2k_x) + 12 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right) + 12 \cos\left(\frac{3k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right) + 6 \cos(\sqrt{3}k_y) + 6 \cos(k_x) \cos(\sqrt{3}k_y) \Bigg] + O(\lambda^3), \quad (39)
$$

FIG. 1. One-particle excitation energies $E(\mathbf{k})$ along highsymmetry cuts through the Brillouin zone for the triangular lattice with couplings $\lambda = 0.15, 0.209$ 72, 0.25.

$$
S_{1p}^{yy}(\mathbf{k}) = \frac{1}{4} - \frac{\lambda}{4} \Bigg[\cos(k_x) + 2 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right) \Bigg] - \frac{\lambda^2}{16} \Bigg[2 \cos(k_x) + \cos(2k_x) + 4 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right) + 4 \cos\left(\frac{3k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right) + 2 \cos(\sqrt{3}k_y) + 2 \cos(k_x) \cos(\sqrt{3}k_y) \Bigg] + O(\lambda^3).
$$
 (40)

In the ordered phase, the leading-order terms for the quasiparticle dispersion $E(\mathbf{k})$ are

$$
E(\mathbf{k}) = 12 - \frac{x^2}{12} [1 + \cos(k_x) + 2 \cos(k_x/2) \cos(\sqrt{3}k_y/2)]
$$

$$
- \frac{x^4}{13824} \Bigg[7 + 16 \cos(k_x) + \cos(2k_x)
$$

$$
+ 32 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right) + 4 \cos\left(\frac{3k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right)
$$

$$
+ 2 \cos(\sqrt{3}k_y) + 2 \cos(k_x) \cos(\sqrt{3}k_y) + O(x^6). \quad (41)
$$

The full series is available upon request. The full series at momenta $\mathbf{k} = (0,0), (4\pi/3,0),$ and $(\pi, \pi/\sqrt{3})$ are given in Table [I.](#page-3-0) The series for the minimum energy $E(\mathbf{k})$ at **k** $=(0,0)$ agrees with results of previous calculations^{18[,21](#page-9-15)} using different techniques.

The dispersion along high-symmetry cuts through the Brillouin zone for the system with couplings $\lambda = 0.15$, 0.209 72, and 0.25 is shown in Fig. [1.](#page-4-0) At the critical point λ_c = 0.209 72, the results obtained from both ordered and disordered expansions are the same, indicating a second-order transition. For a first-order transition, the dispersions obtained at the critical point from the two different expansions

TABLE II. Pole and residue of *N/M D*log Padé approximants to S_{1p}^{xx} for the triangular lattice. Defective approximants are labeled with an asterisk.

\boldsymbol{N}	$(N-2)/N$	$(N-1)/N$	N/N	$(N+1)/N$	$(N+2)/N$
			S_{1p}^{xx} at $k=(0,0)$		
1		$0.2222(-0.6667)$	$0.2069(-0.5779)$	$0.2101(-0.6055)$	$0.2083(-0.584457)$
\overline{c}	$0.2078(-0.5855)$	$0.2096(-0.5992)$	$0.2090(-0.5932)$	$0.2092(-0.5958)$	$0.2094(-0.599522)$
3	$0.2090(-0.5940)$	$0.2091(-0.5954)$	$0.2113(-0.6885)$	$0.2097(-0.6065)$	$0.2096(-0.603142)$
$\overline{4}$	$0.2087(-0.5931)^{*}$	$0.2097(-0.6060)$	$0.2095(-0.5999)$	$0.2096(-0.6035)$	$0.2096(-0.602915)^{*}$
5	$0.2096(-0.6016)$	$0.2096(-0.6034)$	$0.2097(-0.6049)$	$0.2097(-0.6047)$	
6	$0.2097(-0.6060)$	$0.2097(-0.6047)$			
			S_{1p}^{xx} at $k = (4\pi/3, 0)$		
1				0.4706(0.9379)	0.1801(0.020109)
\overline{c}	0.4082(0.3062)	0.2679(0.1210)	0.2523(0.0988)	0.2416(0.0815)	0.2376(0.074489)
3	0.2499(0.0945)	0.2278(0.0548)	0.2347(0.0683)	0.2291(0.0549)	0.2202(0.032590)
4	0.2345(0.0678)	0.2325(0.0636)	0.2130(0.0186)	0.2163(0.0243)	0.2164(0.024506)
5	$0.1975(0.0049)^{*}$	0.2165(0.0247)	0.2164(0.0245)	0.2163(0.0243)	
6	0.2164(0.0245)	0.2165(0.0247)			
			S_{1p}^{xx} at $k=(\pi, \pi/\sqrt{3})$		
1		0.4000(0.4000)	0.5263(0.6925)	0.1792(0.0274)	0.2577(0.116856)
$\overline{\mathbf{c}}$	0.6667(2.0000)	0.4171(0.4200)	0.2395(0.0824)	0.2399(0.0830)	0.2340(0.071712)
3	0.2847(0.1690)	0.2399(0.0830)	0.2395(0.0824)	0.2280(0.0580)	0.2266(0.054014)
4	0.2351(0.0739)	0.2250(0.0499)	0.2267(0.0545)	$0.2287(0.0595)^*$	0.2182(0.030235)
5	0.2266(0.0542)	0.2256(0.0513)	0.2207(0.0375)	0.2170(0.0273)	
6	0.2182(0.0303)	0.2154(0.0230)			
			S_{1p}^{yy} at $k=(0,0)$		
1		0.1818(0.5455)	0.2222(0.8148)	0.2089(0.6765)	0.2128(0.7292)
$\overline{\mathbf{c}}$	0.2389(1.0445)	0.2121(0.7164)	0.2119(0.7144)	0.2111(0.7025)	0.2107(0.6955)
3	0.2119(0.7144)	$0.2121(0.7166)^*$	0.2105(0.6924)	0.2093(0.6513)	0.2101(0.6808)
$\overline{4}$	0.2106(0.6946)	0.2100(0.6794)	0.2100(0.6792)	0.2100(0.6784)	$0.2106(0.6824)$ *
5	0.2100(0.6792)	$0.2100(0.6795)^*$	$0.2100(0.6794)^*$	0.2099(0.6735)	
6	$0.2100(0.6794)^*$	$0.2100(0.6795)^*$			
			S_{1p}^{yy} at $k = (4\pi/3, 0)$		
$\overline{\mathbf{c}}$	$-0.2500(0.0000)^*$	0.2184(0.0333)	0.2473(0.0515)	0.2414(0.0463)	0.2384(0.0432)
3	0.2497(0.0537)	0.2423(0.0472)	0.2355(0.0394)	0.2144(0.0120)	0.2086(0.0079)
4	0.2375(0.0422)	0.2195(0.0172)	0.2082(0.0077)	0.2109(0.0094)	0.2281(0.0414)
5	0.2092(0.0083)	0.2116(0.0099)	0.2197(0.0196)	0.2174(0.0160)	
6	0.2498(0.0561)	0.2175(0.0161)			
			S_{1p}^{yy} at $k=(\pi, \pi/\sqrt{3})$		
$\mathbf{1}$		$-2.0000(2.0000)$	0.1176(0.0069)	0.3400(0.1670)	0.2258(0.0325)
$\overline{\mathbf{c}}$	$-0.0556(0.0000)^*$	$0.5714(4.5714)^*$	0.2578(0.0606)	0.2300(0.0356)	$0.2481(0.0116)^*$
3	0.2127(0.0251)	0.2339(0.0392)	0.2333(0.0387)	0.2320(0.0373)	0.2309(0.0361)
$\overline{4}$	0.2333(0.0387)	$0.2341(0.0393)^{*}$	0.2264(0.0295)	$0.2030(0.0039)^*$	$0.2099(0.0076)^*$
5	0.2283(0.0326)	$0.2130(0.0102)^{*}$	$0.2092(0.0071)^*$	$0.2111(0.0086)$ [*]	
6	$0.2093(0.0072)^{*}$	$0.2102(0.0079)^*$			

would be expected to differ, and so this is a good way to distinguish between second-order and weakly first-order transitions.

The results of a standard *D*log Padé analysis of the series for S_{1p}^{xx} and S_{1p}^{yy} are shown in Table [II.](#page-5-0) At $\mathbf{k}=(0,0)$, where the energy gap vanishes at the critical point, the table for S_{1p}^{xx} allows estimates $\lambda_c = 0.2097(2)$ and for the critical index

 $-0.605(4)$, compared to the expected value $\nu(\eta-1)$ = −0.607. For S_{1p}^{yy} , the estimate for the critical point is λ_c $= 0.210(1)$ with critical index 0.67, very close to the value $\nu(\eta+1)$ =0.65. Just as in one dimension, *S*^{*yy*} appears to decouple from the single-particle state at the critical point, and vary proportionally to two extra powers of the energy gap. At $k = (4\pi/3, 0)$ and $(\pi, \pi/\sqrt{3})$, where the energy gap remains

FIG. 2. (Color online) $S_{1p}^{xx}(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for the triangular lattice with couplings λ $= 0.05, 0.1, 0.15, 0.2, 0.2097.$

finite, the corresponding estimates are λ_c = 0.21 with index +0.02, versus the expected index $\nu \eta = +0.0229$. Thus the critical indices agree with the expected values, within errors, at least for the dominant spectral weight *Sxx*.

Estimates for S_{1p}^{xx} and S_{1p}^{yy} along high-symmetry cuts through the Brillouin zone for the system with couplings λ $= 0.05, 0.1, 0.15, 0.2,$ $= 0.05, 0.1, 0.15, 0.2,$ $= 0.05, 0.1, 0.15, 0.2,$ and 0.2097 are given in Figs. 2 and [3,](#page-6-1) where for $\lambda = 0.2$ and 0.2097, we have biased the critical point λ_c = 0.209 72 with critical index $\nu \eta$ = + 0.0229. We can see from these figures that even for $\lambda = 0.2097$, which is very close to the critical point $\lambda_c = 0.209$ 72, S_{1p}^{xx} and S_{1p}^{yy} are still far from zero, reflecting the tiny value of the critical index in this case.

FIG. 3. (Color online) $S_{1p}^{yy}(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for the triangular lattice with couplings λ $= 0.05, 0.1, 0.15, 0.2, 0.2097.$

FIG. 4. One-particle excitation energies $E(\mathbf{k})$ along highsymmetry cuts through the Brillouin zone for the square lattice with couplings $\lambda = 0.2, 0.328, 41, 0.4$.

B. The square lattice

The square lattice is bipartite, and hence one finds that the Hamiltonian is symmetric under a spin rotation by π about the *z* axis on the *B* sublattice, followed by a coupling inversion $\lambda \rightarrow -\lambda$. Correspondingly, there are symmetrical critical points at couplings $\lambda = \pm \lambda_c$, where λ_c has been estimated from series expansions¹⁸ at 0.328 51(8), and from a finitesize scaling analysis¹⁹ at 0.328 41(2).

We have computed series in the disordered phase for the one-particle structure factors $S_{1p}^{xx}(\mathbf{k})$ and $S_{1p}^{yy}(\mathbf{k})$ and the quasiparticle energy $E(\mathbf{k})$ to order λ^{14} . The calculation involved a list of 4 654 284 clusters, consisting of up to 15 sites. We also computed a series in the ordered phase for the oneparticle dispersion $E(\mathbf{k})$ to order x^{18} , this calculation involving a list of 6473 clusters consisting of up to ten sites. The series are available upon request. The series for the minimum energy $E(\mathbf{k})$ at $\mathbf{k}=(0,0)$ agrees with results of previous calculations.^{18,[21](#page-9-15)} All series are symmetric under the simultaneous transformations $\{k \rightarrow π - k, \lambda \rightarrow -\lambda\}.$

The series are analyzed in the same way as for the triangular lattice. The dispersion along high-symmetry cuts through the Brillouin zone for the system with couplings λ $= 0.2$, 0.328 41, and 0.4 is shown in Fig. [4.](#page-6-2) Again the results obtained from both ordered and disordered expansions agree well at the critical point.

For S_{1p}^{xx} and S_{1p}^{yy} , our *D*log Padé analysis shows similar results to those of the triangular lattice. At $\mathbf{k} = (0,0)$, where the energy gap vanishes, the critical indices for S_{1p}^{xx} and S_{1p}^{yy} are consistent with the expected values $\nu(\eta-1)$ and $\nu(\eta)$ $+1$), respectively, while away from $\mathbf{k}=(0,0)$, where the energy gap remains finite, the critical index is consistent with the expected value $\nu \eta = +0.0229$. The estimated critical point is also consistent with $\lambda = 0.328\,41(2)$, as discussed in our previous paper.² The results for S_{1p}^{xx} and S_{1p}^{yy} along highsymmetry cuts through the Brillouin zone for the system with couplings $\lambda = 0.1, 0.2, 0.3, 0.328$, and 0.3284 are given in Figs. [5](#page-7-0) and [6,](#page-7-1) where for $\lambda = 0.328$ and 0.3284, we have

FIG. 5. (Color online) $S_{1p}^{xx}(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for the square lattice with couplings λ = 0.1, 0.2, 0.3, 0.328, 0.3284.

biased the critical point to λ_c =0.328 41 with critical index $\nu \eta = +0.0229$ in our analysis. Again, we can see from these figures that even for $\lambda = 0.3284$, which is very close to the critical point, S_{1p}^{xx} and S_{1p}^{yy} are still far from zero.

IV. THE SIMPLE CUBIC LATTICE

The transverse Ising model in $(3+1)$ dimensions lies in the universality class of the 4D classical Ising model, where we expect the mean-field exponents $\eta=0$, $\nu=1/2$, modulo logarithmic corrections.¹ The critical point has been obtained previously²⁰ as $\lambda_c = 0.194\,06(6)$.

We have computed series in the disordered phase for the one-particle structure factors $S_{1p}^{xx}(\mathbf{k})$ and $S_{1p}^{yy}(\mathbf{k})$ and the quasiparticle energy $E(\mathbf{k})$ to order λ^{10} . This calculation involved

FIG. 6. (Color online) $S_{1p}^{yy}(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for the square lattice with couplings λ $= 0.1, 0.2, 0.3, 0.328, 0.3284.$

FIG. 7. One-particle excitation energies $E(\mathbf{k})$ along highsymmetry cuts through the Brillouin zone for the simple cubic lattice with couplings $\lambda = 0.15, 0.19406, 0.25$.

a list of 1 487 597 clusters, consisting of up to 11 sites. We also computed a series in the ordered phase for the oneparticle dispersion $E(\mathbf{k})$ to order x^{16} , this calculation involving a list of 29 977 clusters, consisting of up to nine sites. The series for the minimum quasiparticle energy at **k** $(0,0,0)$ in both ordered and disordered phases agrees with results of a previous calculation.²⁰

In Fig. [7,](#page-7-2) we show the dispersion along high-symmetry cuts through the Brillouin zone for the system with couplings $\lambda = 0.15$, 0.194 06, and 0.25. At the critical point λ_c = 0.194 06, the results obtained from both ordered and disordered expansions are the same.

The results of a standard *D*log Padé analysis of the series S_{1p}^{xx} for a few different momenta are shown in Table [III.](#page-8-0) The analysis of $S_{1p}^{xx}(\mathbf{k})$ at $\mathbf{k}=(0,0,0)$, where the energy gap vanishes, gives $\lambda_c = 0.194\,06(8)$ with exponent $-0.54(1)$, while for $S_{1p}^{yy}(\mathbf{k})$ at $\mathbf{k}=(0,0,0)$, the estimate of the critical point is $\lambda_c = 0.194(4)$ with exponent 0.55(3). Away from **k** = (0,0,0), where the energy gap remains finite, we find $\lambda_c = 0.22(3)$ with exponent 0.03(2) for both $S_{1p}^{xx}(\mathbf{k})$ and $S_{1p}^{yy}(\mathbf{k})$. Allowing for logarithmic corrections, these estimates agree reasonably well with the expected values. Figures [8](#page-8-1) and [9](#page-8-2) show S_{1p}^{xx} and S_{1p}^{yy} , respectively, for high-symmetry cuts through the Brillouin zone at selected couplings on the cubic lattice.

V. DISCUSSION

This paper expands on a previous shorter communication² showing that the one-particle spectral weights of the transverse Ising model exhibit scaling behaviour at a quantum phase transition as predicted by the general theory of Sachdev.¹ Our approach is to calculate high-order series expansions for the spectral weights in the disordered phase for the model in one, two, and three dimensions, and then estimate the critical exponents at the quantum phase transition using standard methods.⁹

TABLE III. Pole and residue of N/M Dlog Padé approximants to S_{1p}^{xx} for the simple cubic lattice. Defective approximants are labeled with an asterisk.

N	$(N-2)/N$	$(N-1)/N$	N/N	$(N+1)/N$	$(N+2)/N$				
	S_{1p}^{xx} at $k=(0,0,00)$								
1		$0.2222(-0.6667)$	$0.1765(-0.4204)$	$0.2069(-0.677519)$	$0.184045(-0.424236)$				
$\overline{2}$	$0.1831(-0.4671)$	$0.1940(-0.5384)$	$0.1935(-0.5333)$	$0.1941(-0.540212)$	$0.194060(-0.540008)$				
3	$0.1935(-0.5335)$	$0.1938(-0.5363)$	$0.1941(-0.5400)$	$0.1941(-0.540176)$	$0.194082(-0.540331)$				
$\overline{4}$	$0.1941(-0.5402)$	$0.1941(-0.5411)$	$0.1941(-0.5403)$	$0.1941(-0.540228)$					
5	$0.1941(-0.5404)$	$0.1941(-0.5398)$							
	S_{1p}^{xx} at $k=(\pi,0,0)$								
1		$-0.4000(0.4000)$	0.3846(0.3698)	0.1405(0.018043)	0.918969(32.984939)				
$\overline{2}$	$-0.0980(0.0000)$ [*]	0.1701(0.0377)	0.2552(0.1418)	0.2968(0.252687)	0.278523(0.184754)				
3	$-0.4161(0.2521)^{*}$	0.3068(0.2997)	0.2845(0.2083)	$0.1112(0.000097)^{*}$	0.217318(0.034256)				
$\overline{4}$	0.2729(0.1652)	0.1775(0.0062)	0.2411(0.0846)	0.2097(0.024458)					
5	0.2328(0.0636)	0.2186(0.0373)							
	S_{1p}^{xx} at $k=(\pi,\pi,0)$								
1		0.4000(0.4000)	$-0.3846(0.3698)$	$-0.1405(0.018043)$	$-0.918969(32.984939)^{*}$				
$\overline{2}$	$0.0980(0.0000)$ [*]	$-0.1701(0.0377)$	0.1587(0.0081)	0.2308(0.038903)	0.259588(0.070606)				
3	0.4161(0.2521)	0.2215(0.0316)	0.2947(0.1805)	0.2399(0.046140)	0.224405(0.030751)				
$\overline{4}$	0.2478(0.0535)	0.2340(0.0400)	0.2289(0.0354)	0.2218(0.028131)					
5	0.2272(0.0336)	0.2085(0.0140)							
	S_{1p}^{xx} at $k=(\pi,\pi,\pi)$								
1	0.0000(0.0000)	$-0.2222(-0.6667)$	$-0.1765(-0.4204)$	$-0.2069(-0.677519)$	$-0.184045(-0.424236)$				
$\overline{2}$	$-0.1831(-0.4671)$	0.2829(0.0638)	0.2621(0.0514)	0.2353(0.033838)	0.234556(0.033327)				
3	0.2615(0.0510)	0.1540(0.0020)	0.2345(0.0333)	0.2355(0.033945)	0.238215(0.035366)				
$\overline{4}$	0.2338(0.0327)	0.2311(0.0304)	0.2381(0.0353)	0.2346(0.033524)					
5	0.2356(0.0338)	0.2194(0.0197)							

For the linear chain model, the series results led us to conjecture exact results for the one-particle spectral weights in the disordered phase. $²$ As it turns out, corresponding exact</sup> expressions for the correlation functions, which are the Fou-

FIG. 8. (Color online) $S_{1p}^{xx}(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for the simple cubic lattice with couplings λ $= 0.1, 0.15,$ and 0.19.

rier transforms of these spectral weights, have already been derived by Vaidya and $Tracy$,¹⁵ providing proof of the conjecture.

In the related 2D classical Ising model, a great deal of

FIG. 9. (Color online) $S_{1p}^{yy}(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for the simple cubic lattice with couplings λ $= 0.1, 0.5,$ and 0.19.

work has been done in studying two-particle and higher multiparticle contributions to the correlation functions and the dynamic susceptibility, as reviewed by Orrick *et al.*[10](#page-9-9) It has been shown that each individual term in the susceptibility is differentiably finite, i.e., satisfies a system of differential equations of finite order. The total susceptibility is not *D*-finite, however, and seems to display a natural boundary at $|s|=1$ in the complex $s = \sinh 2K$ plane (for the isotropic model). Presumably, analogous results will apply for the 1D quantum model.

In higher dimensions, our study was purely numerical. We have calculated series for the spectral weights on the triangular, square, and simple cubic lattices. We have then employed standard *D*log Padé techniques to estimate their critical exponents at the phase transition. In each case, the dominant component S^{xx} diverges at $k=0$ with the exponent $\eta(\nu-1)$, as predicted by Sachdev.¹ The component *S^{yy}*, however, decouples from the one-particle state at the transition point, and vanishes at $k=0$ with exponent $\eta(\nu+1)$, in all dimensions, proportional to an extra factor of the square of

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the one-particle energy gap. Away from $k=0$, both spectral weights vanish with exponent $\eta \nu$, as expected. It would be very interesting to compare the predicted spectral weights with experiments on some real materials belonging to the transverse Ising class.

We also find at the critical point that the one-particle dispersions obtained from both ordered and disordered expansions are the same, indicating a second-order transition. We believe that this is a good way to distinguish between second-order and weakly first-order transitions.

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