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Critical behavior of one-particle spectral weights in the transverse Ising model

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We investigate the critical behavior of the spectral weight of a single quasiparticle, one of the key observables in experiment, for the particular case of the transverse Ising model. Series expansions are calculated for the linear chain and the square and simple cubic lattices. For the chain model, a conjectured exact result is discovered. For the square and simple cubic lattices, series analyses are used to estimate the critical exponents. The results agree with the general predictions of Sachdev [*Quantum Phase Transitions* (Cambridge University Press, Cambridge, England, 1999)].

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INTRODUCTION

There is currently much interest in quantum phase transitions in strongly correlated magnetic and/or electronic systems in condensed matter physics. The physics in the vicinity of such quantum critical points can be described via general scaling theories, independent of any particular microscopic model. Sachdev[1] has developed a scaling theory for the spectral weight (defined below), a quantity which can be measured experimentally, and thus provides a bridge between model calculations and real materials. Our goal here is to verify Sachdev's predictions for a particular quantum spin model, the Ising model in a transverse field. To the best of our knowledge, this is the first such microscopic verification of the scaling form.

A fundamental quantity to describe the dynamical properties of quantum magnets is the dynamical structure factor[2]

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

where the notation is standard, and the angular bracket denotes a thermal average or, at zero temperature, a ground state expectation value. As is well known, $S(\mathbf{k},\omega)$ can be related directly to the inelastic neutron scattering intensity, allowing a comparison between experiments on real materials and theoretical model calculations.

Integrating Eq. (1) over energy, we obtain the integrated or static structure factor,

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

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 Eq. (1) in the "spectral form" (valid for a discrete spectrum)

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

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

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

with

$$\Omega_{\Lambda}^{\beta}(\mathbf{k})=\frac{1}{\sqrt{N}}\sum_{i}\langle\psi_{\Lambda}|S_i^{\beta}|\psi_0\rangle e^{i\mathbf{k}\cdot\mathbf{r}_i}. \quad (5)$$

We consider only 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 $\mathbf{k}$. Near a quantum phase transition[1] these quantities are expected to show universal scaling properties, which can be derived from a field theoretic approach, independently of the details of a particular model. The spectral weight can be written, up to constant factors, as

$$S_{1p}(\mathbf{k})=\frac{A(\mathbf{k})}{E(\mathbf{k})} \quad (6)$$

where $A(\mathbf{k})$ is the "quasiparticle residue," i.e., the residue of the Green's function at the quasiparticle pole, and $E(\mathbf{k})$ is the quasiparticle energy at momentum $\mathbf{k}$. Near the critical point, these functions are expected to scale as

$$A(\mathbf{k})\sim(g_c-g)^{\eta\nu},$$

$$E(\mathbf{k_c})\sim(g_c-g)^{\nu}, \quad (7)$$

where g is a coupling or tuning parameter, $\mathbf{k_c}$ is the critical momentum at which the energy gap vanishes, and η,ν are the standard critical exponents. Then S_{1p} is expected to scale as

$$S_{1p}(\mathbf{k})\sim(g_c-g)^{\eta\nu},\quad \mathbf{k}\neq\mathbf{k_c};$$

$$S_{1p}(\mathbf{k_c})\sim(g_c-g)^{(\eta-1)\nu}. \quad (8)$$

Our aim is to confirm and demonstrate this scaling behavior for the transverse field Ising model

$$H=\sum_i(1-\sigma_i^z)-\lambda\sum_{\langle ij\rangle}\sigma_i^x\sigma_j^x, \quad (9)$$

where $\sigma_i^{\alpha}=2S_i^{\alpha}$ are Pauli operators and the second sum is over nearest-neighbor pairs. This model has a quantum phase transition at $\lambda=1$ in one dimension, and at some specific λ_c

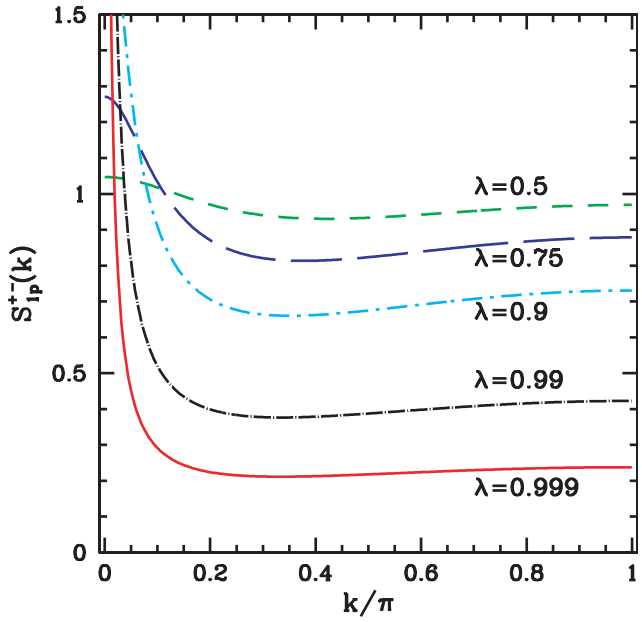

FIG. 1. (Color online) The one-particle spectral weight $S^{+-}_{1p}(k)$ for the linear chain model graphed against momentum k/π, for various couplings λ.

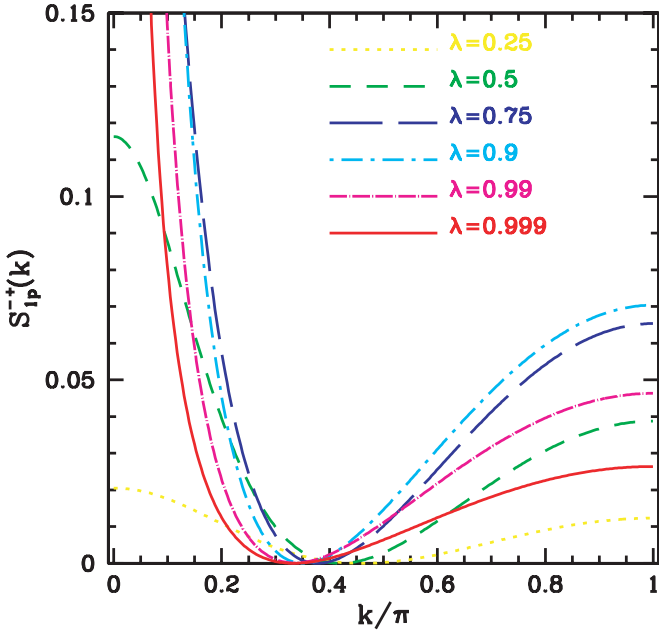

FIG. 2. (Color online) As Fig. 1, for the one-particle spectral weight $S^{-+}_{1p}(k)$.

for each higher-dimensional lattice. Our approach is to derive series expansions in λ for various one-particle spectral weights in the "disordered" phase $\lambda<\lambda_c$, via the linked-cluster techniques described by Oitmaa *et al.*,[3] and to analyze the series by standard methods to obtain the critical behavior.

LINEAR CHAIN

The transverse Ising chain model is exactly solvable, and expressions for the energy spectrum, magnetization, etc. have been given by Pfeuty.[4] We have computed series for the one-particle matrix elements $\Omega^{\pm}_{1p}(k)$ for this model up to order λ^{22}. The leading terms for $\Omega^{-}_{1p}(k)$ are given in Ref. 3; we can supply further coefficients on request.

While analyzing these series for their critical behavior, we realized that they could be represented *exactly*, up to the order calculated, by the closed form expressions,

$$\Omega^{\pm}_{1p}(k)=\frac{1}{2}(1-\lambda^2)^{1/8}\frac{[1\mp\Lambda(k)]}{\Lambda(k)^{1/2}}, \tag{10}$$

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

$$\Lambda(k)=E(k)/2=[1+\lambda^2-2\lambda\cos(k)]^{1/2}. \tag{11}$$

It is natural to conjecture that this result is exact to all orders.

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

$$S^{+-}_{1p}(k)=\frac{1}{4}(1-\lambda^2)^{1/4}\frac{[1+\Lambda(k)]^2}{\Lambda(k)}, \tag{12}$$

$$S^{-+}_{1p}(k)=\frac{1}{4}(1-\lambda^2)^{1/4}\frac{[1-\Lambda(k)]^2}{\Lambda(k)}, \tag{13}$$

$$S^{++}_{1p}(k)=S^{--}_{1p}(k)=\frac{1}{4}(1-\lambda^2)^{1/4}\frac{[1-\Lambda^2(k)]}{\Lambda(k)}. \tag{14}$$

These formulas give a very clear demonstration of the critical behavior expected theoretically. The quasiparticle residues for S^{-+}, S^{+-} are, respectively,

$$A(k)=\frac{1}{2}(1-\lambda^2)^{1/4}[1\mp\Lambda(k)]^2, \tag{15}$$

which vanish at the critical point $\lambda=1$ with exponent $1/4=\eta\nu$, as expected for the transverse Ising chain where $\eta=1/4$, $\nu=1$. At the critical momentum $k=0$, the energy gap is $2(1-\lambda)$, and vanishes with exponent $\nu=1$.

The behavior of $S^{+-}_{1p}(k)$ and $S^{-+}_{1p}(k)$ for several λ is shown in Figs. 1 and 2. We can see that both spectral weights slowly decrease towards zero as $\lambda\to1$, except at the point $k=0$ where they both diverge, just as we should expect. Note that $S^{-+}_{1p}(k)$ vanishes at $\lambda=2\cos(k)$.

The integrated one-particle structure factors are

$$\Phi_1=\frac{1}{\pi}\int_0^{\pi}S^{+-}_{1p}dk$$
$$=(1-\lambda^2)^{1/4}[(1+\lambda)E(m)+(1+\lambda)^{-1}K(m)+\pi]/(2\pi), \tag{16}$$

$$\Phi_2=\frac{1}{\pi}\int_0^{\pi}S^{-+}_{1p}dk$$
$$=(1-\lambda^2)^{1/4}[(1+\lambda)E(m)+(1+\lambda)^{-1}K(m)-\pi]/(2\pi), \tag{17}$$

where $m=4\lambda/(1+\lambda)^2$, and $K(m)$ and $E(m)$ are the complete elliptic integrals of the first and second kinds, respectively.[5]

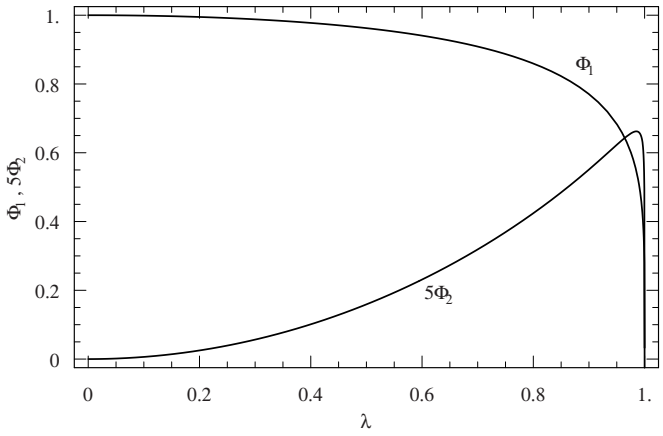

FIG. 3. The integrated one-particle structure factors Φ_1 and Φ_2 (corresponding to S^{+-}_{1p}, S^{-+}_{1p}, respectively) graphed as functions of coupling λ.

Their behavior is shown in Fig. 3, where we can see that Φ_2 has its maximum value at $\lambda=0.985\,12$, and when $\lambda=1$, both Φ_1 and Φ_2 vanish, despite the fact that S_{1p} diverges at $k=0$.

From Eq. (10), one can also show

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

$$S^{yy}_{1p}(k) = \tfrac{1}{4}(1-\lambda^2)^{1/4}\Lambda(k). \tag{18}$$

Note that whereas $S^{xx}_{1p}(k)$ diverges as $\{\lambda\to 1, k=0\}$, $S^{yy}_{1p}(k)$ does not.

By Fourier transforming, we obtain the one-particle contributions to the correlation functions [using Eq. (2)],

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

$$C^{yy}_{1p}(\delta) = (1-\lambda^2)^{1/4}\frac{1}{8\pi}\int_0^{2\pi} dk \cos(k\delta)\Lambda(k). \tag{19}$$

Now exact expressions for the one-particle contributions to the correlation functions in the two-dimensional (2D) classical Ising model have been obtained long ago by Wu, McCoy, Tracy, and Barouch.[6,7] Taking the anisotropic "Hamiltonian limit"[8,9] in which the classical Ising model reduces to the quantum Ising model (1), one can show that the expressions of Wu *et al.* reduce to Eq. (19) (details will be given elsewhere). This confirms that the results we have given are in fact exact.

SQUARE LATTICE

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 $\eta=0.0364(5)$, $\nu=0.6301(4)$, from various estimates.[10]

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 $\lambda\to-\lambda$. Correspondingly, there are symmetrical critical points at couplings $\lambda=\pm\lambda_c$, where λ_c has been estimated from series expansions[11] at 0.328 51(8), and from a finite-size scaling analysis[12] at 0.328 41(2).

We have computed series for the one-particle spectral weight $S^{xx}_{1p}(\mathbf{k})$ 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. The leading terms are

TABLE I. Pole and residue of N/M Dlog Padé approximants to S^{xx}_{1p} for the square lattice. Defective approximants are marked with an asterisk.

	$N-2/N$	$N-1/N$	N/N	$N+1/N$	$N+2/N$
			$k=(0,0)$		
$N=1$		0.4000(−0.8000)	0.2703(−0.3652)	0.3874(−1.0759)	0.2847(−0.3138)
$N=2$	0.2953(−0.4682)	0.3263(−0.5900)	0.3285(−0.6022)	0.3281(−0.5988)	0.3276(−0.5942)
$N=3$	0.3286(−0.6028)	0.3281(−0.5996)	0.3319(−0.5789)*	0.3278(−0.5969)	0.3282(−0.6017)
$N=4$	0.3238(−0.5113)*	0.3279(−0.5978)	0.3280(−0.5985)	0.3288(−0.6122)	0.3284(−0.6037)
$N=5$	0.3280(−0.5985)	0.3279(−0.5974)*	0.3282(−0.6016)	0.3283(−0.6035)	0.3284(−0.6036)
$N=6$	0.3283(−0.6019)	0.3284(−0.6059)	0.3284(−0.6053)	0.3284(−0.6050)	
$N=7$	0.3284(−0.6053)	0.3284(−0.6045)			
			$k=(\pi/2,\pi/2)$		
$N=2$		0.6030(0.5455)	0.6030(0.5455)	0.3428(0.0570)	0.3428(0.0570)
$N=3$	0.6030(0.5455)	0.6030(0.5455)	0.3428(0.0570)	0.3428(0.0570)	0.3586(0.0747)
$N=4$	0.4231(0.1781)	0.3579(0.0735)	0.3579(0.0735)	0.3521(0.0654)	0.3521(0.0654)
$N=5$	0.3579(0.0735)	0.3579(0.0735)	0.3521(0.0654)	0.3521(0.0654)	0.3425(0.0495)
$N=6$	0.3473(0.0576)	0.3407(0.0459)	0.3407(0.0459)	0.3390(0.0424)	
$N=7$	0.3407(0.0459)	0.3407(0.0459)			

$$E(\mathbf{k}) = 2 - 2\lambda(\cos k_x + \cos k_y) + \lambda^2[2 - (\cos k_x + \cos k_y)^2] + \lambda^3(\cos k_x + \cos k_y)[5 - 2(\cos k_x + \cos k_y)^2]/2 + \lambda^4[6 + 14(\cos k_x + \cos k_y)^2 - 5(\cos k_x + \cos k_y)^4]/4 + O(\lambda^5), \quad (20)$$

$$S^{xx}_{1p}(\mathbf{k}) = 1/4 + \lambda(\cos k_x + \cos k_y)/4 + \lambda^2\{12\cos(k_x)\cos(k_y) + 3[\cos(2k_x) + \cos(2k_y)]\}/16 + \frac{\lambda^3}{32}\{15(\cos k_x + \cos k_y) + 30[\cos(2k_x)\cos k_y + \cos k_x \cos(2k_y)] + 5[\cos(3k_x) + \cos(3k_y)]\} + O(\lambda^4) \quad (21)$$

(further terms can be supplied on request). Note that because the lattice is bipartite, both quantities are symmetric under the simultaneous transformations $\{\mathbf{k} \to \pi - \mathbf{k}, \lambda \to -\lambda\}$.

The results of a standard Dlog Padé analysis for $S^{xx}_{1p}(\mathbf{k})$ at $\mathbf{k}=(0,0)$ and $\mathbf{k}=(\pi/2,\pi/2)$ are shown in Table I. At $\mathbf{k}=(0,0)$, where the energy gap vanishes, Table I allows estimates $\lambda_c=0.3284(4)$ with exponent $-0.605(5)$, compared to the expected exponent $\nu(\eta-1)=-0.607$. At momentum $\mathbf{k}=(\pi/2,\pi/2)$, where the energy gap remains finite, we find $\lambda_c=0.34(3)$ with exponent 0.04(2) compared to the expected value $\nu\eta=+0.0229$. In the latter case, the exponent does not agree particularly well with the expected value, but this inaccuracy might easily be attributed to the weakness of this singularity. Complementary results follow for the antiferromagnetic singularity at $\lambda=-0.3284$, with exponent $\nu(\eta-1)$ at $\mathbf{k}=(\pi,\pi)$, and $\nu\eta$ at $\mathbf{k}=(\pi/2,\pi/2)$.

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]

We have computed series for the one-particle structure factor $S^{xx}_{1p}(\mathbf{k})$ and the quasiparticle energy $E(\mathbf{k})$ to orders λ^{10}. The critical point has been obtained previously[13] as $\lambda_c=0.19406(6)$. A Dlog Padé analysis of $S^{xx}_{1p}(\mathbf{k})$ at $\mathbf{k}=(0,0,0)$, where the energy gap vanishes, gives $\lambda_c=0.19406(8)$ with exponent $-0.54(1)$, while for another momentum, where the energy gap remains finite, we find $\lambda_c=0.22(3)$ with exponent 0.03(2). Allowing for logarithmic corrections, these agree reasonably well with the expected values.

CONCLUSION

In summary, then, we have shown that the one-particle spectral weights of the transverse Ising model satisfy the scaling behavior at a quantum phase transition as predicted by theory.[1] For the linear chain we obtain exact results; for the square and simple cubic lattices numerical estimates are obtained from series expansions. Further details will be published in a full length paper.

ACKNOWLEDGMENTS

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