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Gerhard Müller
University of Rhode Island, gmuller@uri.edu

Robert E. Shrock

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Wave-number-dependent susceptibilities of one-dimensional quantum spin models at zero temperature

Gerhard Müller
Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794
and Physics Department, University of Rhode Island, Kingston, Rhode Island 02881*

Robert E. Shrock
Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794
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We calculate the zero-temperature q-dependent susceptibilities of the one-dimensional, $S=\frac{1}{2}$, transverse Ising model at the critical magnetic field and of the isotropic XY model in zero field which have not been previously determined. Our method, which is based on a rigorous method of calculating dynamic correlation functions for these models, provides precise numerical values for the susceptibilities at wave numbers $q=k\pi/M$ for integral M and odd integral k, as well as exact analytic results for the dominant singularities at $q=0$ and $q=\pi$.

In a previous work,[1] henceforth referred to as I, we calculated precise numerical values for the zero-temperature staggered susceptibilities $(\overline{\chi}_{xx})_{\rm TI}$ and $(\overline{\chi}_{xx})_{XY}$ of the one-dimensional (1D), $S=\frac{1}{2}$, transverse Ising (TI) model at the critical magnetic field, and the 1D, $S=\frac{1}{2}$ isotropic XY model in zero field, specified, respectively, by the Hamiltonians

$$H_{\rm TI}=-J\sum_{l=1}^{N}(2S_l^xS_{l+1}^x+h_cS_l^z),\quad h_c=1 \tag{1}$$

and

$$H_{XY}=-J\sum_{l=1}^{N}(S_l^xS_{l+1}^x+S_l^yS_{l+1}^y) \tag{2}$$

in the thermodynamic limit $(N\to\infty)$, with $J>0$. For reasons of notational simplicity, we shall set $J\equiv 1$ henceforth.

The calculation reported in I relied on the important result[2] that the time-dependent correlation functions

$$\Xi_n(t)\equiv\langle S_0^\xi(t)S_n^\xi\rangle,\quad \xi=x,y \tag{3}$$

for the two models (1) and (2) at temperature $T=0$ can be expressed in terms of the solution $\sigma_n(z)$ of the nonlinear ordinary differential equation (ODE)

$$(z\sigma_n'')^2+4(z\sigma_n'-\sigma_n-n^2)[z\sigma_n'-\sigma_n+(\sigma_n')^2]=0 \tag{4}$$

with initial conditions as given before.[1,2] Specifically,

$$[X_n(t)]_{\rm TI}=[X_n(0)]_{\rm TI}\exp\left(-t^2/2+\int_0^{2t}dt'\sigma_n(it')/t'\right), \tag{5}$$

where

$$[X_n(0)]_{\rm TI}=\begin{cases}1 & \text{for } n=0\ ,\\ (2/\pi)^{|n|}\prod_{l=1}^{|n|}[1-(2l)^{-2}]^{l-|n|} & \text{for } n\neq 0\ ,\end{cases} \tag{6}$$

and for the remaining functions,

$$[Y_n(t)]_{\rm TI}=-\frac{d^2}{dt^2}[X_n(t)]_{\rm TI} \tag{7}$$

and

$$[X_n(t)]_{XY}=[Y_n(t)]_{XY}=\begin{cases}[X_{n/2}(t/2)]_{\rm TI}^2 & \text{for } n \text{ even}\ ,\\ [X_{(n-1)/2}(t/2)]_{\rm TI}[X_{(n+1)/2}(t/2)]_{\rm TI} & \text{for } n \text{ odd}\ .\end{cases} \tag{8}$$

Based on the above properties, asymptotic expansions (AE's) of these functions, applicable for large t and n, were calculated,[3] and a detailed numerical and analytic study of the frequency-dependent transverse autocorrelation functions $(n=0)$ was carried out.[4,5] The correlation functions $X_n(t)$ and $Y_n(t)$ for the models (1) and (2) are, in a sense, infinitely more complicated than the correlation function $Z_n(t)$, since after the Jordan-Wigner mapping to fermion operators, the former involve an infinite product of fermion operators, whereas the latter involves only a product of four operators. Thus, it is not surprising that in contrast to the functions $X_n(t)$ and $Y_n(t)$ studied in Refs. 1–5, $Z_n(t)$ is known in closed form for both the TI and XY models.[6]

The wave-number-dependent susceptibilities at $T=0$ can be expressed formally (letting q denote the wave number) as

$$\chi_{\xi\xi}(q)=\frac{1}{2}\sum_{n=-\infty}^{\infty}e^{-iqn}\int_0^\infty d\tau\,\Xi_n(-i\tau),\quad \xi=x,y,z \tag{9}$$

in terms of these correlation functions. Closed-form expressions are known for $[\chi_{zz}(q)]_{\rm TI}$, $[\chi_{yy}(q)]_{\rm TI}$, and $[\chi_{zz}(q)]_{XY}$; they are discussed in I. The calculation of the remaining two susceptibilities $[\chi_{xx}(q)]_{\rm TI}$ and $[\chi_{xx}(q)]_{XY}=[\chi_{yy}(q)]_{XY}$ is much more difficult. From exact results on the "spacelike" asymptotic expansions[3] (appropriately Wick rotated[1]) of the correlation functions $X_n(-i\tau)$, together with numerical solutions of the ODE (4) for arguments corresponding to n and τ in regimes where the AE's are not sufficiently accurate, precise numerical values for the staggered susceptibilities $(\bar{\chi}_{xx})_{\rm TI} \equiv [\chi_{xx}(q=\pi)]_{\rm TI}$ and $(\bar{\chi}_{xx})_{XY} \equiv [\chi_{xx}(q=\pi)]_{XY}$ were calculated in I.

In this Rapid Communication we use the same results for the functions $[X_n(-i\tau)]_{\rm TI}$ and $[X_n(-i\tau)]_{XY}$, respectively, in order to compute the corresponding wave-number-dependent susceptibilities $[\chi_{xx}(q)]_{\rm TI}$ and $[\chi_{xx}(q)]_{XY}$ at selected values of q. For an explicit calculation, it is obviously necessary to carry out the formal sum in (9) in such a way as to avoid divergent integrals. For wave numbers of the form $q=(k\pi/M)$, where k and M are integers and k is odd, this is achieved by rearranging terms as follows:

$$\chi_{xx}(k\pi/M) = -\sum_{n=1}^{\infty}\cos[(n-1)k\pi/M]C_{xx}(n,M) - \sum_{n=1}^{[M/2]}\cos(nk\pi/M)C_{xx}(n+1,M-2n) \; , \quad (10a)$$

where

$$C_{xx}(n,M) = \tfrac{1}{2}\int_0^{\infty} d\tau[X_{n-1+M}(-i\tau) - X_{n-1}(-i\tau)] \; , \quad (10b)$$

and $[M/2]$ denotes the integral part of $M/2$. The integrals $C_{xx}(n,M)$ are all finite, and the series in (10a) converges. Since the rational numbers form a topologically dense subset of the real numbers, it follows that, with arbitrary M and (odd) k, the set of wave numbers q contained in the above set of the form $q=k\pi/M$ are dense throughout the Brillouin zone. Thus, for the practical purpose of determining the susceptibilities, one can achieve arbitrarily high coverage of the Brillouin zone by taking sufficiently many values of k and M.

In I we derived large-(n,τ) AE's for the quantities $[C_{xx}(n,1)]_{\rm TI}$ and $[C_{xx}(n,1)]_{XY}$, using the AE's of the corresponding time-dependent correlation functions,[3] appropriately Wick rotated. The Wick-rotated forms (which connect smoothly to the spacelike AE's determined in Ref. 3) are

$$[X_n(-i\tau)]_{\rm TI} \sim \bar{A}(n^2+\tau^2)^{-1/8}\{1+2^{-6}(n^2+\tau^2)^{-3}(2\tau^4-5\tau^2n^2-n^4) - 3(2)^{-13}(n^2+\tau^2)^{-6}(108\tau^8-1500\tau^6n^2+1127\tau^4n^4+46\tau^2n^6+11n^8) + O([\max(|n|,\tau)]^{-6})\} \; , \quad (11)$$

and

$$[X_n(-i\tau)]_{XY} \sim 2^{1/2}(\bar{A})^2(n^2+\tau^2)^{-1/4}\{1+2^{-2}k_n(n^2+\tau^2)^{-2}(n^2-\tau^2)+2^{-3}(n^2+\tau^2)^{-3}(-n^4-5n^2\tau^2+2\tau^4) + 2^{-5}k_n(n^2+\tau^2)^{-5}(-8n^6-165n^4\tau^2+390n^2\tau^4-41\tau^6) + 2^{-7}(n^2+\tau^2)^{-6}(17n^8+74n^6\tau^2+1701n^4\tau^4-2260n^2\tau^6+164\tau^8) + O([\max(|n|,\tau)]^{-6})\} \; , \quad (12)$$

with $k_n = 2^{-1}[1-(-1)^n]$ and $A = 2^{1/12}\exp[3\zeta'(-1)]$. For small n and τ, where such large-(n,τ) expansions are manifestly inaccurate, we calculated the quantities $C_{xx}(n,1)$ numerically, using (10b), from the functions $X_n(-i\tau)$ as determined numerically via (5) from the solution of the ODE for small τ, and as represented by their AE's (11) and (12) for large enough τ. From these results, the staggered susceptibilities $\bar{\chi}_{xx} = \chi(q=\pi)$ were then evaluated in I using (10a).

Here we extend these earlier results and derive large-n AE's for the more general quantities $C_{xx}(n,M)$, with arbitrary M, from the same AE's of $X_n(-i\tau)$, viz., (11) and (12). The results have the following general structure:

$$[C_{xx}^{(\rm AE)}(n,M)]_{\rm TI} \sim -B_{\rm TI}M\sum_{m=0}^{\infty}a_m(M)n^{-(m+1/4)} \; , \quad (13a)$$

with

$$B_{\rm TI} = 2^{-1}(\bar{A})\pi^{1/2}\Gamma(\tfrac{5}{8})/\Gamma(\tfrac{1}{8}) \; , \quad (13b)$$

and

$$[C_{xx}^{(\rm AE)}(n,M)]_{XY} \sim -B_{XY}\sum_{m=0}^{\infty}[Mb_m(M) + (-1)^n c_m(M)]n^{-(m+1/4)} \; , \quad (14a)$$

with

$$B_{XY} = 2^{-1/2}(\bar{A})^2\pi^{1/2}\Gamma(\tfrac{3}{4})/\Gamma(\tfrac{1}{4}) \; . \quad (14b)$$

The coefficients $a_m(M)$, $b_m(M)$, and $c_m(M)$ which can be derived to the appropriate order from the AE's (11) and (12) are listed in Table I. For a given M and a given level of accuracy required in the final result, the values obtained from (13) or (14) can be used in (10a) if n exceeds some value, $n_0(M)$, which must be determined empirically. However, the values of $C_{xx}(n,M)$ for $0 \le n \le n_0(M)$ have to be determined using (10b) from a combination of numerical data and AE's of $X_n(-i\tau)$ via (10b). A detailed description of this procedure was given in I for the case $M=1$; it is essentially the same for general M and hence will not be repeated here.

With the same numerical data on $X_n(-i\tau)$ as was used in I, together with the new AE's (13) and (14) for the functions $C_{xx}(n,M)$, we can thus determine precise numerical values for the q-dependent susceptibilities $\chi_{xx}(q)$ for the TI and XY models by evaluating the respective sums (10a). For $k=M=1$, we expressed in I the series (10a) with the AE's (13) and (14) in terms of Riemann ζ and η functions, whose properties are well studied. However, for general k and M, the resultant series appear not to be expressible in terms of well-known functions. Consequently, we have evaluated them numerically, using standard numerical subaveraging algorithms to expedite convergence. The results of I for the case $k=M=1$ were utilized as checks on our general calculation.

We have carried out this calculation for $1 \le M \le 9$ and, for a given M, all odd k in the interval $1 \le k < M$. The

TABLE I. The coefficients $a_m(M)$ for $0 \le m \le 5$ and $b_m(M)$ and $c_m(M)$ for $0 \le m \le 4$ of the asymptotic expansions for the functions $C_{xx}(n,M)$.

$$a_0 = 1$$

$$a_1 = -\tfrac{1}{8}(M-2)$$

$$a_2 = \tfrac{5}{3264}(34M^2 - 102M + 79)$$

$$a_3 = -\tfrac{15}{8704}(M-2)(17M^2 - 34M + 11)$$

$$a_4 = \tfrac{13}{62808064}(92\,004M^4 - 460\,020M^3 + 712\,580M^2 - 297\,660M - 81\,689)$$

$$a_5 = -\tfrac{13}{29556736}(M-2)(30\,668M^4 - 122\,672M^3 + 110\,946M^2 + 23\,452M - 34\,785)$$

$$b_0 = 1$$

$$b_1 = -\tfrac{1}{4}(M-2)$$

$$b_2 = \tfrac{1}{40}(5M^2 - 15M + 9)$$

$$b_3 = -\tfrac{1}{64}(M-2)(5M^2 - 10M - 2)$$

$$b_4 = \tfrac{7}{141440}(1105M^4 - 5525M^3 + 6630M^2 + 2201M - 4452)$$

$$c_0 = 0$$

$$c_1 = \tfrac{1}{20}[1 - (-1)^M]$$

$$c_2 = \tfrac{3}{40}[1 + (-1)^M(M-1)]$$

$$c_3 = \tfrac{1}{7072}[(209 - (-1)^M(663M^2 - 1326M + 209)]$$

$$c_4 = -\tfrac{1}{14144}[1631 - (-1)^M(1547M^3 - 4641M^2 + 1463M + 1631)]$$

results for both the TI and the XY models are listed in Table II. We omit the entries for which k and M have a common divisor; although these contain no new information, they were useful for consistency tests. The estimated absolute error for all susceptibility values of Table II is $\lesssim 10^{-5}$.

Our new results for the susceptibilities $[\chi_{xx}(q)]_{\rm TI}$ and $[\chi_{xx}(q)]_{XY}$ are also plotted in Fig. 1. Smooth curves have been drawn through the two sets of circles representing the values given in Table II. Both curves diverge as $q \to 0$. The exact form of these divergences was determined in I from the respective leading terms of the AE's (11) and (12):

$$[\chi_{xx}(q)]_{\rm TI} \sim 2^{-1/4}(\bar{A})\cos(3\pi/8)\Gamma(\tfrac{7}{8})^2 q^{-7/4} \quad (15)$$

and

$$[\chi_{xx}(q)]_{XY} \sim 2^{-1/2}(\bar{A})^2\Gamma(\tfrac{3}{4})^2 q^{-3/4} \; . \quad (16)$$

In the vicinity of $q = \pi$, the two susceptibilities exhibit qualitatively different behavior. This is most easily seen in the magnified version of these parts of the curves, shown in the inset of Fig. 1. For the TI model, the structure of the AE (13) implies that $[\chi_{xx}(q)]_{\rm TI}$ is nonsingular at $q = \pi$. Reflection symmetry in the Brillouin zone then implies that this function approaches the point $q = \pi$ with a horizontal tangent. This behavior is, indeed, exhibited by the curve plotted in Fig. 1. In constrast, the terms in both the AE (12) and the AE (14), which are oscillatory in n, produce

TABLE II. The numerical values of the $T = 0$ susceptibilities $\chi_{xx}(q)$ for the TI and XY models at selected wave numbers of the form $q = k\pi/M$, where k and M are integers, and k is odd. The numbers are accurate to $\lesssim 1$ part in 10^5.

M	k	$[\chi_{xx}(k\pi/M)]_{\rm TI}$	$[\chi_{xx}(k\pi/M)]_{XY}$
1	1	0.070 593	0.075 566
2	1	0.131 07	0.215 62
3	1	0.242 48	0.389 83
4	1	0.389 02	0.603 18
4	3	0.081 342	0.127 22
5	1	0.567 18	0.848 86
5	3	0.103 11	0.168 28
6	1	0.774 92	1.122 73
6	5	0.075 115	0.112 19
7	1	1.010 79	1.421 95
7	3	0.163 94	0.268 72
7	5	0.085 078	0.134 94
8	1	1.273 65	1.744 41
8	3	0.201 17	0.326 94
8	5	0.098 196	0.159 55
8	7	0.073 089	0.105 61
9	1	1.562 59	2.088 45
9	5	0.113 65	0.186 48
9	7	0.078 910	0.121 82

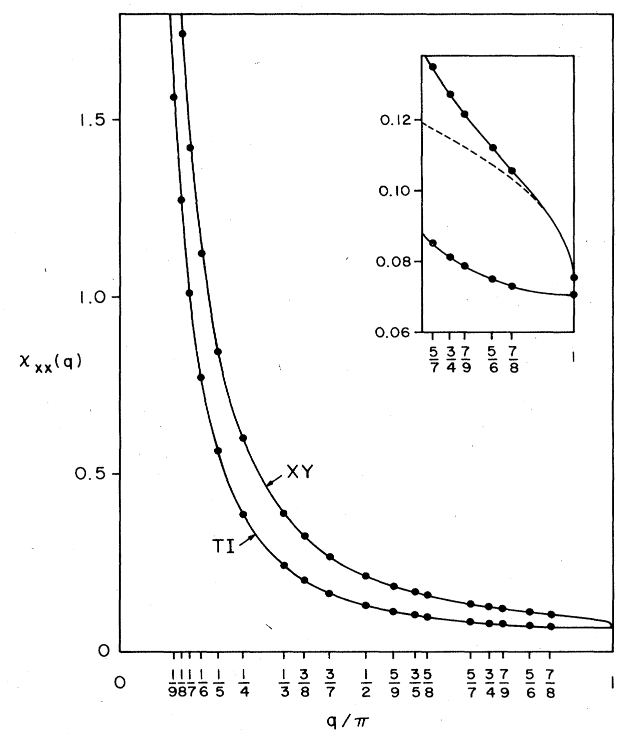

FIG. 1. The q-dependent susceptibilities $\chi_{xx}(q)$ of the TI and XY models at $T = 0$. The circles represent the numerical values given in Table II. The curves are drawn by simple interpolation and by the use of exact information on the singularity structure. The inset shows the part of the curves near $q = \pi$, with the scale on the vertical axis enlarged by a factor of 10.

singularities in $[\chi_{xx}(q)]_{XY}$ at $q=\pi$. We have determined the leading singularity to be a cusp of the following form:

$$[\chi_{xx}(q)]_{XY}-[\chi_{xx}(\pi)]_{XY} \sim 2^{-3/2}(5)^{-1}(\bar{A})^2\Gamma(\tfrac{3}{4})^2(\pi-q)^{1/2} \quad . \quad (17)$$

This is drawn as the dashed curve in the inset of Fig. 1 and agrees very well with the numerical results. Finally, we note that the singular behavior of $[\chi_{xx}(q)]_{XY}$ at $q=\pi$ may be responsible, at least in part, for the surprisingly poor predictions of extrapolated finite-chain calculations for the staggered susceptibility $[\chi_{xx}]_{XY}$, as discussed in I.

The present paper thus completes the determination of the zero-temperature, q-dependent susceptibilities $\chi_{\xi\xi}(q)$ of the 1D, $S=\frac{1}{2}$ transverse Ising model at the critical external magnetic field, and the 1D, $S=\frac{1}{2}$ isotropic XY model in zero field.

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*Present address.

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[6]See Ref. 5 for the explicit results and references to earlier work.