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Universal low-temperature properties of quantum and classical ferromagnetic chains

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We identify the critical theory controlling the universal, low-temperature, macroscopic properties of both quantum and classical ferromagnetic chains. The theory is the quantum mechanics of a single rotor. The mapping leads to an efficient method for computing scaling functions to high accuracy. [S0163-1829(96)52026-6]

A number of recent papers[1–5] have studied the finite temperature properties of ferromagnetic quantum spin chains. At low temperatures, macroscopic observables can be fully described by two dimensionful parameters which characterize the ground state. A convenient choice for these is the ground-state magnetization density M_0, and the ground-state spin stiffness ρ_s. Then the macroscopic properties of a quantum spin chain of length L, in the presence of an external magnetic field H, and at a temperature T are fully universal functions of the dimensionless ratios that can be formed out of these parameters. A convenient choice for these ratios is (recall that in $d=1$ ρ_s, has dimensions of energy $\times$ length)

$$r\equiv\rho_s M_0/T,\ \ h\equiv H/T,\ \ q\equiv\rho_s/(LT). \tag{1}$$

Here we have used units in which $\hbar=k_B=1$ and absorbed a factor of $g\mu_B$ into H (μ_B is the Bohr magneton). Thus, for instance, the temperature-dependent magnetization density obeys[5] $M=M_0\Phi_M(r,h,q)$ where Φ_M is a universal function. This, and other, universal functions will depend upon the boundary conditions on the chain: we will focus, for simplicity, on periodic boundary conditions, i.e., on spin rings. There is no method for computing Φ_M in complete generality—in this paper we shall show how to compute Φ_M efficiently in a limiting case when the quantum ring can be described by an effective classical model.

A convenient point for beginning discussion is the spin-wave expansion. This expansion is valid provided $r\gg 1$ (provided h is not too small), and it is quite easy to use standard methods to determine the leading term. For a ring we find

$$\Phi_M(r,h,q)=1-\frac{q}{r}\sum_n \frac{1}{\exp(4\pi^2n^2q^2/r+h)-1}\cdots, \tag{2}$$

where the sum is over all integers n. An interesting property of this expression emerges in the limit $r\rightarrow\infty$, $h\rightarrow 0$, but with

$$g\equiv rh=\rho_s M_0 H/T^2 \tag{3}$$

fixed; then we find $\Phi_M=1-(1/2\sqrt{g})\coth(\sqrt{g}/2q)$. The implication of recent works[3–5] is that this limit is nontrivial at each order in the spin-wave expansion, and that the resulting series has in fact properties of the *classical* ferromagnetic ring. Thus we may define the classical scaling function ϕ_M by

$$\phi_M(g,q)=\lim_{r\rightarrow\infty}\Phi_M(r,g/r,q). \tag{4}$$

Classical behavior emerges in this limit because the ferromagnetic correlation length becomes larger than the de Broglie wavelength of the spin waves.

One possible approach to the computation of the scaling function ϕ_M is to compute the magnetization of a nearest-neighbor, classical ferromagnetic chain, whose statistical mechanical properties were computed some time ago.[6–8] The scaling limit of classical solution was studied in recent work[3,4] and led, e.g., to the result $\phi_M(g,0)=(2/3)g-(44/135)g^3+\mathcal{O}(g^5)$—this result means that the usual linear susceptibility $\partial M/\partial H$ diverges as T^{-2} and that the third order nonlinear susceptibility $\partial^3 M/\partial H^3$ diverges as T^{-6}. However, the computations required to achieve this limited result were quite complicated. In this paper we shall develop an efficient method to computing the complete function $\phi_M(g,q)$ to essentially arbitrary accuracy. This will be done by a precise identification of the critical theory controlling this crossover function.

We begin by considering the partition function of a classical Heisenberg model in a uniform magnetic field:

$$Z=\int\exp\left(\sum_{i<j}\frac{J(i-j)}{T}\mathbf{n}_i\cdot\mathbf{n}_j+\frac{H}{T}\sum_{i=1}^{N}n_i^z\right)\prod_i d\mathbf{n}_i,$$

where the exchange constants $J(i)\geqslant 0$, $J(i)=J(N-i)$, the $\mathbf{n}_i$ are unit three-component vectors which are integrated over. The universal critical theory emerges when we take the continuum limit of this action. With a lattice spacing a, the continuum limit will be characterized by the values $M_0=1/a$, $L=Na$, and $\rho_s=a\Sigma_i i^2 J(i)$. Our results apply to all systems in which the summation in the definition of ρ_s is convergent—for $J(i)\sim i^{-q}$ this is the case for $q>3$. The continuum field theory which emerges by this method gives the partition function Z_c,

$$\int \mathcal{D}[\mathbf{n}]\exp\left[-\int_0^L \frac{\rho_s}{2T}\left(\frac{d\mathbf{n}(x)}{dx}\right)^2 - \frac{HM_0}{T}n^z(x)dx\right],$$

where the integral is now a functional integral over unit vector fields $\mathbf{n}(x)$ satisfying $\mathbf{n}(0)=\mathbf{n}(L)$. A key property of Z_c is that it is a finite field theory, free of ultraviolet divergences. This becomes clear when we reinterpret Z_c as the imaginary ''time'' (x) Feynman path integral for the quantum mechanics of a single particle with coordinate $\mathbf{n}(x)$ restricted to lie on a unit sphere: no discretization of time is required to define this problem. As a result, all observables are universal functions of the couplings in Z_c, and it is useful to now transform to dimensionless variables. We rescale spatial coordinates $y=Tx/\rho_s$, and obtain Z_c,

$$\int \mathcal{D}[\mathbf{n}]\exp\left[-\int_0^{1/q} \frac{1}{2}\left(\frac{d\mathbf{n}(y)}{dy}\right)^2 - gn^z(y)dy\right].$$

Subsequent computations are best carried out using the Hamiltonian, $\mathcal{H}$, of the quantum particle described by Z_c,

$$\mathcal{H}=\frac{\mathbf{L}^2}{2}-gn^z. \tag{5}$$

This describes a single *quantum rotor* with unit moment of inertia, angular momentum operator $\mathbf{L}$ (which obeys the usual commutation relations $[L^\alpha,L^\beta]=i\epsilon_{\alpha\beta\gamma}L^\gamma$), in the presence of a ''gravitational'' field g. There is no need to consider the radial motion as the length of $\mathbf{n}$ is constrained to unity. The logarithm of Z_c equals the free energy of the quantum system $\mathcal{H}$ at a ''temperature'' q; in the original spin ring, q is the ratio of correlation length at $H=0$ to length of the system. For other boundary conditions, Z_c will be given by appropriate propagators of $\mathcal{H}$.

We now consider eigenvalue equation $\mathcal{H}\psi=E\psi$. As $\mathcal{H}$ commutes with L^z, eigenstates are divided to subspaces of azimuthal quantum number $m=\ldots,-3,-2,-1,0,1,2,3,\ldots$. In spherical coordinates (θ,φ), ψ is given by $e^{im\varphi}u(\theta)$. At $g=0$ $u(\theta)$ is given by the associated Legendre polynomials $P_l^{|m|}(\cos\theta)$ and eigenstates of $\mathcal{H}$ are spherical harmonic states $|l,m\rangle$ with $l\geqslant|m|$. The matrix elements of $\mathcal{H}$ in this basis are

$$\langle l',m|\mathcal{H}|l,m\rangle=\frac{l(l+1)}{2}\delta_{ll'}-g\left(\delta_{l,l'+1}\sqrt{\frac{l^2-m^2}{4l^2-1}}+\delta_{l',l+1}\sqrt{\frac{l'^2-m^2}{4l'^2-1}}\right). \tag{6}$$

Notice that $\mathcal{H}$ is tridiagonal in each m subspace: this makes numerical diagonalization of $\mathcal{H}$ quite straightforward. The eigenvalues of Hamiltonian are given by $E_{m,n}(g)$, and $n=0,1,2,\ldots$, is the number of nodes of function $u(\theta)$. We also generated a power series expansion in g for the ground-state energy $E_{0,0}(g)$ using a symbolic manipulation program (Mathematica); this leads to the magnetization scaling function for the infinite ferromagnetic ring $\phi_M(g,0)=-dE_{0,0}(g)/dg$, for which we find (Fig. 1)

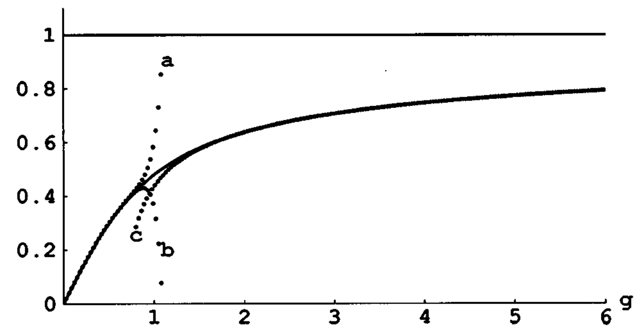

FIG. 1. The scaling function $\phi_M(g,0)$. Line a is expansion (7) up to g^{13} and line b is expansion up to g^{15}. Line c is the result of asymptotic expansion (8) up to $g^{-11/2}$ from $g=\infty$.

$$\phi_M(g,0)=\frac{2}{3}g-\frac{44}{135}g^3+\frac{752}{2835}g^5-\frac{465\,704}{1\,913\,625}g^7+\frac{356\,656}{1\,515\,591}g^9-\frac{707\,126\,486\,624}{3\,016\,973\,334\,375}g^{11}+\frac{1\,126\,858\,624}{4\,736\,221\,875}g^{13}-\frac{5\,083\,735\,857\,217\,648}{20\,771\,861\,407\,171\,875}g^{15}+\cdots. \tag{7}$$

All coefficients are rational numbers.

In the complementary large g limit, the particle spends most of its time near the ''north pole,'' and in its vicinity it experiences a harmonic oscillator potential well. It therefore pays to work now in the basis states of this harmonic oscillator and thereby generate a perturbation expansion valid

TABLE I. Expansion coefficients of $\phi_M(g,0)$ for small g expansion $\Sigma a_n g^{2n-1}$ and large g expansion $1-\frac{1}{2}g^{-1/2}+\Sigma b_n g^{-(n+2)/2}$.

n	a_n	b_n
1	0.666 666 666 666 666 67	-0.007 812 5
2	-0.325 925 925 925 925 93	-0.005 859 375
3	0.265 255 731 922 398 589	-0.004 852 294 921 875
4	-0.243 362 205 238 748 449	-0.004 531 860 351 562 5
5	0.235 324 701 717 019 961	-0.004 721 879 959 106 445 3
6	-0.234 382 743 316 652 222	-0.005 429 327 487 945 556 6
7	0.237 923 529 289 894 173	-0.006 830 555 852 502 584 5
8	-0.244 741 468 160 498 74	-0.009 339 863 900 095 224 4
9	0.254 229 904 051 448 52	-0.013 805 415 550 450 561 6
10	-0.266 079 264 257 003 861	-0.021 958 404 599 899 95
11	0.280 145 597 828 282 407	-0.037 433 421 774 196 063
12	-0.296 386 895 761 683 996	-0.068 149 719 593 456 837
13	0.314 829 857 750 047 932	-0.132 063 536 806 409 254
14	-0.335 551 676 759 620 67	-0.271 575 442 615 252 266
15	0.358 669 817 237 908 61	
16	-0.384 336 336 842 125 08	
17	0.412 734 951 469 368 57	
18	-0.444 079 858 077 944 98	
19	0.478 615 755 598 441 95	

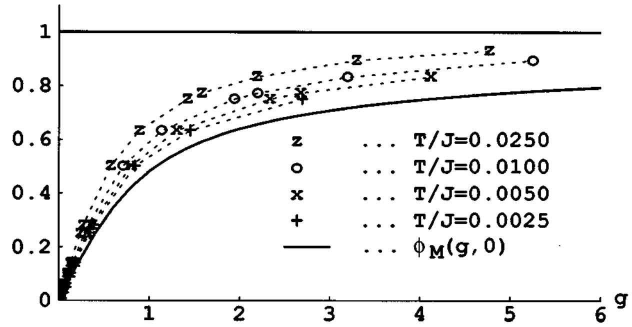

FIG. 2. Magnetization versus $g=JH/8T^2$ for spin-half and infinite-length ferromagnetic Heisenberg chain with nearest-neighbor exchange (9). As temperature goes down, the line approaches to the theoretical line $\phi_M(g,0)$.

for large g. Parametrizing $E=-g+\sqrt{g}\varepsilon$ and $u(\theta)=[\theta/\sin(\theta)]1/2f(g1/4\theta)$; *this gives us an eigenvalue equation for* f: $(h_0+h_1)f(z)=\varepsilon f(z)$ *with*

$$h_0=\frac{1}{2}\left(-\frac{1}{z}\frac{d}{dz}z\frac{d}{dz}+\frac{m^2}{z^2}+z^2\right),$$

$$h_1=2\sqrt{g}\left(\sin^2\frac{\theta}{2}-\frac{\theta^2}{4}\right)+\frac{1}{8\sqrt{g}}\left(\frac{1-4m^2}{\theta^2}-\frac{1-4m^2}{\sin^2\theta}-1\right),$$

where $z\equiv g^{1/4}\theta$. Notice that h_0 describes a two-dimensional harmonic oscillator in radial coordinates. Its eigenstates $|n\rangle, n\geqslant 0$ have energy $\varepsilon_0=2n+|m|+1$ and are represented by generalized Laguerre polynomials $z^{|m|}L^{|m|}_{n+|m|}(z^2)e^{-z^2/2}$. Further, notice that h_1 can be expanded as a series in positive integer powers of z^2, with all terms being small for large g. The matrix elements of h_1 in the $|n\rangle$ basis can be determined by repeated use of the identity $z^2|n\rangle=(2n+|m|+1)|n\rangle-\sqrt{n(n+|m|)}|n-1\rangle-\sqrt{(n+1)(n+|m|+1)}|n+1\rangle$. It now remains to diagonalize h in the $|n\rangle$ basis, which can be done order by order in $g^{-1/2}$ by Mathematica. Such a procedure was used to generate an expansion for the ground-state energy, $E_{0,0}(g)$ and hence for $\phi_M(g,0)$,

$$\phi_M(g,0)=1-\frac{g^{-1/2}}{2}-\frac{g^{-3/2}}{128}-\frac{3g^{-2}}{512}-\frac{159g^{-5/2}}{32\,768}-\frac{297g^{-3}}{65\,536}-\frac{19\,805g^{-7/2}}{4\,194\,304}-\frac{91\,089g^{-4}}{16\,777\,216}-\frac{14\,668\,507g^{-9/2}}{2\,147\,483\,648}-\frac{20\,057\,205g^{-5}}{2\,147\,483\,648}-\frac{3\,794\,803\,731g^{-11/2}}{274\,877\,906\,944}-\cdots. \quad (8)$$

Unlike the small g expansion, which has a finite radius of convergence, the large g expansion is only asymptotic. In particular, the large g limit loses topological information associated with tunneling paths which traverse the south pole—such paths will lead to ''instanton'' contributions which are exponentially small for large g. In Table I we give the higher order coefficients of these expansions.

For the quantum ferromagnetic Heisenberg ring with spin 1/2,

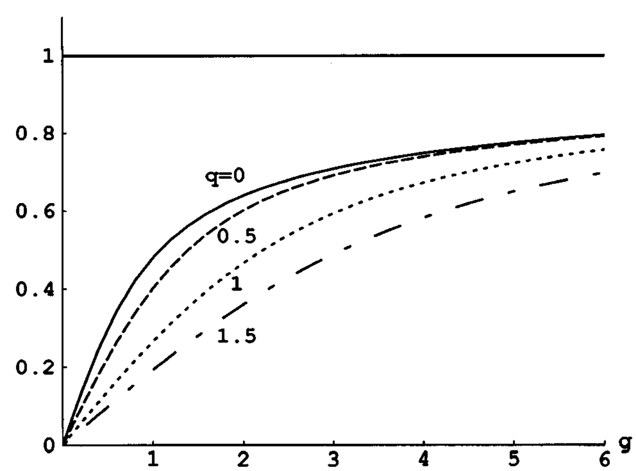

FIG. 3. Scaling function $\phi_M(g,q)$ for various values of q. Solid line is for $q=0$, dashed line is for $q=0.5$, dotted line is for $q=1.0$, and dashed chain line is for $q=1.5$.

TABLE II. Values of scaling function $\phi_M(g,q)$ for $q=0.0,0.5,1.0,1.5,2.0$.

$g\backslash q$	0	0.5	1.0	1.5	2.0
0.0	0.0	0.0	0.0	0.0	0.0
0.2	0.130 808	0.093 330	0.056 126	0.039 675	0.030 627
0.4	0.248 178	0.182 802	0.111 511	0.079 100	0.061 141
0.6	0.345 162	0.265 293	0.165 461	0.118 034	0.091 434
0.8	0.421 694	0.338 855	0.217 367	0.156 249	0.121 399
1.0	0.481 193	0.402 773	0.266 734	0.193 537	0.150 934
1.2	0.527 688	0.457 313	0.313 199	0.229 716	0.179 947
1.4	0.564 580	0.503 351	0.356 529	0.264 633	0.208 353
1.6	0.594 419	0.542 043	0.396 618	0.298 164	0.236 074
1.8	0.619 027	0.574 582	0.433 462	0.330 217	0.263 046
2.0	0.639 690	0.602 067	0.467 146	0.360 730	0.289 213
2.2	0.657 323	0.625 439	0.497 818	0.389 667	0.314 529
2.4	0.672 584	0.645 479	0.525 667	0.417 020	0.338 961
2.6	0.685 956	0.662 813	0.550 909	0.442 800	0.362 483
2.8	0.697 795	0.677 939	0.573 769	0.467 038	0.385 080
3.0	0.708 374	0.691 253	0.594 470	0.489 780	0.406 745
3.2	0.717 902	0.703 067	0.613 231	0.511 084	0.427 481
3.4	0.726 544	0.713 628	0.630 253	0.531 013	0.447 294
3.6	0.734 429	0.723 134	0.645 724	0.549 640	0.466 199
3.8	0.741 664	0.731 744	0.659 815	0.567 040	0.484 216
4.0	0.748 332	0.739 587	0.672 678	0.583 287	0.501 368
4.2	0.754 506	0.746 768	0.684 450	0.598 457	0.517 682
4.4	0.760 244	0.753 373	0.695 250	0.612 624	0.533 188
4.6	0.765 594	0.759 476	0.705 186	0.625 859	0.547 918
4.8	0.770 600	0.765 134	0.714 351	0.638 232	0.561 904
5.0	0.775 297	0.770 401	0.722 827	0.649 805	0.575 181
5.2	0.779 715	0.775 319	0.730 686	0.660 640	0.587 781
5.4	0.783 881	0.779 924	0.737 991	0.670 794	0.599 739
5.6	0.787 819	0.784 248	0.744 798	0.680 319	0.611 089
5.8	0.791 548	0.788 320	0.751 156	0.689 265	0.621 862
6.0	0.795 087	0.792 162	0.757 108	0.697 676	0.632 091

$$\mathcal{H}=-\sum_{k=1}^{N} J\mathbf{S}_k\cdot\mathbf{S}_{k+1}-H\sum_{k=1}^{N} S_k^z,$$

$$[S_l^\alpha,S_k^\beta]=i\,\delta_{lk}\epsilon_{\alpha\beta\gamma}S_l^\gamma, \tag{9}$$

we can calculate the magnetization at $N=\infty$ limit for given temperature and magnetic field using thermodynamic Bethe ansatz equations.[3] The magnetization still obeys the same limiting scaling function. The stiffness constant ρ_s is $Ja/4$ and M_0 is $1/2a$. In Fig. 2 we compare the magnetization as a function of $g=JH/8T^2$. As T goes down, the magnetization divided by M_0 approaches the scaling function $\phi_M(g,0)$, supporting the conclusion that the quantum ferromagnetic Heisenberg ring has the same magnetic scaling function with classical one.

In our scaling theory, the linear susceptibility $\partial M/\partial H$ of quantum ferromagnet diverges as T^{-2} at low temperature. Schlottmann[9] proposed the divergence of the type $T^{-2}/\ln(J/T)$ using the numerical analysis of thermodynamic Bethe ansatz equations. But later this was negated by the detailed investigations of thermodynamic Bethe ansatz equations.[10]

Next we consider the function $\phi_M(g,q)$ at $q>0$ (Fig. 3), which is important for the analysis of short rings. This is represented by the eigenvalues $E_{m,n}(g)$ of Hamiltonian (5),

$$\phi_M(g,q)=-\frac{\Sigma_m\Sigma_n E'_{m,n}(g)\exp[-E_{m,n}(g)/q]}{\Sigma_m\Sigma_n\exp[-E_{m,n}(g)/q]}. \tag{10}$$

For $q\ll 1$, ϕ_M is dominated by the ground state $m=n=0$. The energy gap to the second lowest eigenvalue at $m=\pm 1$, $n=0$ is more than 1. Then, deviations from $\phi_M(g,0)$ are exponentially small,

$$\phi_M(g,q)=\phi_M(g,0)+\mathcal{O}(e^{-1/q}),\quad q\ll 1. \tag{11}$$

In Table II we give the result of numerical calculation of $\phi_M(g,q)$. We calculate $E_{m,n}(g)$ and $E'_{m,n}(g)$ numerically by diagonalizing the tridiagonal matrices (6). Terms at very big n or m are not necessary because their contributions are exponentially small.

Finally, we note that the behavior of the scaling functions is also simple in the limit $q\gg 1$. The problem is now equivalent to a single *classical* rotor:

$$\phi_M(g,q)=\coth\frac{g}{q}-\frac{q}{g},\quad \frac{g}{q}=\frac{M_0HL}{T}. \tag{12}$$

This means that the system behaves as one big spin M_0L if the correlation length ρ_s/T is much longer than the system size L.

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