Universal low-temperature properties of quantum and classical ferromagnetic chains

Minoru Takahashi, Hiroaki Nakamura, and Subir Sachdev

Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106, Japan
Department of Physics, P.O. Box 208120, Yale University, New Haven, CT 06520-8120, USA

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.

A number of recent papers 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 $\rho_s$. 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 $\hbar$ is the Bohr magneton).

$$r \equiv \rho_s M_0 / T, \quad h \equiv H / T, \quad q \equiv \rho_s / (LT).$$

Here we have used units in which $\hbar = k_B = 1$ and absorbed a factor of $g \mu_B$ into $H$ ($\mu_B$ is the Bohr magneton). Thus, for instance, the temperature dependent magnetization density obeys $M = M_0 \Phi_M (r, h, q)$ where $\Phi_M$ 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 $\Phi_M$ in complete generality—in this paper we shall show how to compute $\Phi_M$ 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

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

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

$$g \equiv \rho_s M_0 H / T^2,$$

fixed; then we find $\Phi_M = 1 - (1/2 \sqrt{q}) \coth (\sqrt{q} / 2 q)$. The implication of recent works is that this limit is non-trivial 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 $\phi_M$ by

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

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 $\phi_M$ is to compute the magnetization of a nearest-neighbor, classical ferromagnetic chain, whose statistical mechanical properties were computed some time ago. The scaling limit of classical solution was studied in recent work, and led e.g. to the result $\phi_M (g, 0) = 2 g - \frac{3}{2} g^3 + O (g^5)$—this result means that the usual linear susceptibility $\partial M / \partial H$ diverges as $T^{-2}$ and that the third order non-linear 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 $J(i) \geq 0$ and $J(N-i)$, the $\mathbf{n}_i$ are unit 3-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 $M_0 = 1 / a$, $L = N a$, and $\rho_s = a \sum_i i^2 J(i)$. Our results apply to all systems in which the summation in the definition of $\rho_s$ 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 $Z_c$:...
\[ \int \mathcal{D}[\mathbf{n}] \exp \left( -\int_0^L \frac{\rho_s}{2T} \left( \frac{d\mathbf{n}(x)}{dx} \right)^2 - \frac{HM_0}{T} \mathbf{n}(x) \right) \],

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 re-interpret \( Z_c \) as the imaginary “time” \( (t) \) Feynman path integral for the quantum mechanics of a single particle with co-ordinate \( y \) variables. We rescale spatial co-ordinates and all observables are universal functions of the couplings in \( Z_c \), and it is useful to now transform to dimensionless variables. We rescale spatial co-ordinates \( y = \frac{T}{\rho_s}x \), and obtain \( Z_c \):

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

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

\[ \mathcal{H} = \frac{L^2}{2} - gn^z. \quad (5) \]

This describes a single quantum rotor with unit moment of inertia, angular momentum operator \( L \) (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 \( L^2 \), eigenstates are divided into subspaces of azimuthal quantum number \( m = \ldots, -3, -2, -1, 0, 1, 2, 3, \ldots \). In spherical co-ordinates \( (\theta, \varphi) \), \( \psi \) 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 \( l \geq |m| \).

The matrix elements of \( \mathcal{H} \) in this basis are

\[ <l', m|\mathcal{H}|l, m> = \frac{l(l+1)}{2} \delta_{l,l'} - g \left( \delta_{l,l'+1} \sqrt{\frac{l'^2 - m^2}{4l'^2 - 1}} + \delta_{l,l'+1} \sqrt{\frac{l'^2 - m^2}{4l'^2 - 1}} \right). \quad (6) \]

Notice that \( \mathcal{H} \) is tri-diagonal 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 \( q \) 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

\[ \phi_M(g,0) = \frac{2}{3} g - \frac{44}{135} g^3 + \frac{752}{2835} g^5 - \frac{465704}{1913625} g^7 + \frac{356656}{1515591} g^9 - \frac{707126486624}{3016973334375} g^{11} - \frac{1126858624}{4736221875} g^{13} - \frac{5083735857217648}{20771861407171875} g^{15} + \ldots \quad (7) \]

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

\[ h_0 = \frac{1}{2} \left( -\frac{1}{z} \frac{dz}{dz} \frac{d}{dz} + \frac{m^2}{z} + z^2 \right), \quad h_1 = \frac{2\sqrt{\delta}}{\sin^2 \theta} \left( \frac{\theta^2}{4} + \frac{1}{8} \frac{g}{\theta^2} \left( 1 - \frac{4m^2}{\sin^2 \theta} - 1 \right) \right), \]

where \( \varepsilon \equiv g^{1/4} \theta \). Notice that \( h_0 \) describes a two-dimensional harmonic oscillator in radial co-ordinates. Its eigenstates \( |n\rangle \), \( n \geq 0 \) have energy \( \varepsilon_0 = 2n + |m| + 1 \) and are represented by generalized Laguerre polynomials \( z^{|m|} L_{n+|m|}^{|m|} (z^2) e^{-z^2/2} \). 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 \( z^2 |n\rangle = (2n + |m| + 1) |n\rangle - \sqrt{m(n+|m|)} |n-1\rangle - \sqrt{(n+1)(n+|m|+1)} |n+1\rangle \). 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 \( \phi_M(g,0) \):

\[ \phi_M(g,0) = \frac{2}{3} + \frac{44}{135} g^3 + \frac{752}{2835} g^5 - \frac{465704}{1913625} g^7 + \frac{356656}{1515591} g^9 - \frac{707126486624}{3016973334375} g^{11} - \frac{1126858624}{4736221875} g^{13} - \frac{5083735857217648}{20771861407171875} g^{15} + \ldots \quad (8) \]

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 1 we give the higher order coefficients of these expansions.
For the quantum ferromagnetic Heisenberg ring with spin 1/2:

\[ \mathcal{H} = -\sum_{k=1}^{N} J S_k S_{k+1} - H \sum_{k=1}^{N} S_k^z, \]

\[ [S_k^+, S_k^z] = \delta_{kk'} \epsilon_{\alpha\beta\gamma} S_k^\alpha, \]

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 \( \rho_s \) is important for the analysis of short rings. This is represented by the eigenvalues \( E_{m,n}(g) \) of Hamiltonian [3]:

\[ \phi_M(g,q) = -\sum_m \sum_n E_{m,n}(g) \exp(-E_{m,n}(g)/q) / \sum_m \sum_n \exp(-E_{m,n}(g)/q). \]

For \( q \ll 1 \), \( \phi_M \) 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:

\[ \phi_M(g,q) = \phi_M(g,0) + \mathcal{O}(e^{-q}) \quad q \ll 1. \]

In Table 2 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 [3]. 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:

\[ \phi_M(g,q) = \coth \left( g - \frac{q}{g} \right) \frac{g}{q} = \frac{M_0 h L}{T}. \]

This means that the system behaves as one big spin \( M_0 L \) if the correlation length \( \rho_s/T \) is much longer than the system size \( L \).

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**TABLE I. Expansion coefficients of \( \phi_M(g,0) \) for small \( g \) expansion \( \sum a_n g^{2n-1} \) and large \( g \) expansion \( 1 - \frac{1}{2} g^{1/2} - \sum b_n g^{-(n+3)/2} \).**

| n   | \( a_n \)            | \( b_n \)            |
|-----|----------------------|----------------------|
| 1   | 0.66666666666666667  | -0.0078125            |
| 2   | -0.325925625625625625 | -0.005895737373737373 |
| 3   | 0.256255731922398589 | -0.004852294921875    |
| 4   | -0.2436120238748449  | -0.0045318603515625   |
| 5   | 0.235324701717019961 | -0.00472599591064453 |
| 6   | -0.23482773316652222 | -0.00542927487945566 |
| 7   | 0.2379325928994173   | -0.006805555852052845 |
| 8   | -0.2447146816049874  | -0.009398639000952244 |
| 9   | 0.2542299040544852   | -0.0138054155540505616 |
| 10  | -0.266079264257003861| -0.0219584054999899995 |
| 11  | 0.280145597828282407 | -0.03743421774196063 |
| 12  | -0.29638695761683996 | -0.06814971593456837 |
| 13  | 0.31482985775047932  | -0.1320653680409254 |
| 14  | -0.3355167679692607  | -0.2715754426152266 |
| 15  | 0.3586698172390861   |                      |
| 16  | -0.3843633684212508  |                      |
| 17  | 0.412734914693857    |                      |
| 18  | -0.4407985807794498  |                      |
| 19  | 0.47861575559844195  |                      |
TABLE II. Values of scaling function $\phi_M(g, q)$ for $q = 0, 0.5, 1.0, 1.5, 2.0$

| $g \times q$ | 0 | 0.5 | 1.0 | 1.5 | 2.0 |
|--------------|---|-----|-----|-----|-----|
| 0.0          | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.2          | 0.130808 | 0.093330 | 0.056126 | 0.039675 | 0.030627 |
| 0.4          | 0.248178 | 0.182802 | 0.111511 | 0.079100 | 0.061141 |
| 0.6          | 0.345162 | 0.265293 | 0.165461 | 0.118034 | 0.091434 |
| 0.8          | 0.421694 | 0.338855 | 0.217367 | 0.156249 | 0.121399 |
| 1.0          | 0.481193 | 0.402773 | 0.266734 | 0.193537 | 0.150934 |
| 1.2          | 0.527688 | 0.457313 | 0.313199 | 0.229716 | 0.179947 |
| 1.4          | 0.564580 | 0.503351 | 0.356529 | 0.264633 | 0.208353 |
| 1.6          | 0.594419 | 0.542043 | 0.396618 | 0.298164 | 0.236074 |
| 1.8          | 0.619027 | 0.574582 | 0.43462 | 0.330176 | 0.263046 |
| 2.0          | 0.639690 | 0.602067 | 0.467146 | 0.360730 | 0.289213 |
| 2.2          | 0.657323 | 0.625439 | 0.497818 | 0.398667 | 0.314529 |
| 2.4          | 0.672584 | 0.645479 | 0.525667 | 0.417020 | 0.338961 |
| 2.6          | 0.685956 | 0.662813 | 0.550909 | 0.442800 | 0.362483 |
| 2.8          | 0.697795 | 0.679393 | 0.573769 | 0.467038 | 0.385080 |
| 3.0          | 0.708374 | 0.691253 | 0.594470 | 0.489780 | 0.406745 |
| 3.2          | 0.719002 | 0.703067 | 0.613221 | 0.511084 | 0.427481 |
| 3.4          | 0.726544 | 0.713628 | 0.630253 | 0.531013 | 0.447294 |
| 3.6          | 0.734429 | 0.721314 | 0.645724 | 0.549640 | 0.466199 |
| 3.8          | 0.741664 | 0.731744 | 0.659815 | 0.567040 | 0.484216 |
| 4.0          | 0.748332 | 0.739587 | 0.672678 | 0.583287 | 0.501368 |
| 4.2          | 0.754506 | 0.746768 | 0.684450 | 0.598457 | 0.517682 |
| 4.4          | 0.760244 | 0.753373 | 0.695250 | 0.612624 | 0.533188 |
| 4.6          | 0.765594 | 0.759476 | 0.705186 | 0.625859 | 0.547918 |
| 4.8          | 0.770600 | 0.765134 | 0.714351 | 0.638232 | 0.561904 |
| 5.0          | 0.775297 | 0.770401 | 0.722827 | 0.649805 | 0.575181 |
| 5.2          | 0.779715 | 0.775319 | 0.730686 | 0.660640 | 0.587781 |
| 5.4          | 0.783881 | 0.779924 | 0.737991 | 0.670794 | 0.599739 |
| 5.6          | 0.787819 | 0.784248 | 0.744798 | 0.680319 | 0.610899 |
| 5.8          | 0.791548 | 0.788320 | 0.751156 | 0.689265 | 0.621862 |
| 6.0          | 0.795087 | 0.792162 | 0.757108 | 0.697676 | 0.632091 |

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

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

**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 $q = 1.5$. 