Order parameter statistics in the critical quantum Ising chain

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The probability distribution of the order parameter is expected to take a universal scaling form at a phase transition. In a spin system at a quantum critical point, this corresponds to universal statistics in the distribution of the total magnetization in the low-lying states. We obtain this scaling function exactly for the ground state and first excited state of the critical quantum Ising spin chain. This is achieved through a remarkable relation to the partition function of the anisotropic Kondo problem, which can be computed by exploiting the integrability of the system.

The concept of *universality* is central to our understanding of continuous phase transitions. Universal physical quantities at or near a transition in one system coincide with those in other systems that share a few key characteristics, including dimensionality and symmetry of the order parameter. Continuous transitions are therefore grouped naturally into *universality classes* of common critical behavior [1]. Familiar universal quantities include critical exponents that characterize the singular behavior of thermodynamic and response functions in the vicinity of the critical point. Although the amplitudes of these singularities are entirely system-dependent, certain *amplitude ratios* are universal [2].

A particularly natural family of universal amplitude ratios is formed from the volume-integrated order parameter M in a finite-size system by

$$\mathcal{A}_{2n} \equiv \frac{\langle M^{2n}\rangle}{\langle M^2\rangle^n} \ . \tag{1}$$

It is readily seen that the hypothesis of universality applied to this entire family is equivalent to the existence of a *universal scaling function* $f(X)$ defined by

$$f(X) \equiv sP(sX) \tag{2}$$

where $s^2 \equiv \langle M^2\rangle$ is the variance of the order parameter and $P(m)$ its probability distribution function. The existence of this scaling function relating the probability distribution for different system sizes is a consequence of hyperscaling, as emphasized in Ref. 3. Extensive numerical work has confirmed the universality of $sP(sX)$ [4, 5]. For the important benchmark of the two-dimensional classical Ising model, Ref. 6 is a useful guide to the literature as well as a tour-de-force numerical study.

The aim of this work is to remedy two striking deficiencies in our present understanding of order parameter distributions: the small number of analytical results and the scant attention that has been paid to *quantum* phase transitions. The study of order parameter fluctuations at quantum critical points, aside from being inherently interesting, is motivated by recent experiments in atomic physics, where the measurement of the full distribution of global fluctuating observables has become a reality [7, 8]. For the quantum Ising chain, we compute $P(m)$ exactly by relating its generating function to the partition function of a particular anisotropic Kondo problem. This remarkable relationship allows the application of the powerful analytic methods developed to solve this and other quantum impurity problems.

The quantum Ising chain, often referred to as the transverse-field Ising model, has Hamiltonian

$$H = -\sum_{i=1}^{L} \left[h\sigma_i^x + \sigma_i^z\sigma_{i+1}^z\right] \ . \tag{3}$$

For the moment, we impose periodic boundary conditions so that $\sigma_{L+1}^z \equiv \sigma_1^z$. The critical point of the model Eq. (3) is at $h = 1$, separating the ordered ($h < 1$) and disordered ($h > 1$) phases. The magnetization $M \equiv \sum_i \sigma_i^z/2$ does not commute with H, so eigenstates of H are typically sums over states with different eigenvalues of M. The distribution functions of the magnetization in the ground states for various boundary conditions were studied numerically in Ref. 9, and good scaling of $sP(sX)$ onto a universal curve was found for $L \gtrsim 16$. There are also analytical results for the distribution of the *transverse* magnetization $\sum_i \sigma_i^x$ [9, 10].

The magnetization distribution in a state $|\alpha\rangle$ is

$$P_\alpha(m) = \langle\alpha|\delta(m - M)|\alpha\rangle.$$

Rewriting the delta function as an integral gives

$$P_\alpha(m) = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-i\lambda m}\chi_\alpha(\lambda)$$

where $\chi_\alpha(\lambda) \equiv \langle\alpha|e^{i\lambda M}|\alpha\rangle$ is the generating function of the moments of the distribution. The flip operator $\mathcal{F} \equiv \prod_i \sigma_i^x$ commutes with the Hamiltonian, so the resulting $\mathbb{Z}_2$ symmetry requires that $P_\alpha(m) = P_\alpha(-m)$. A generalized Lee-Yang theorem shows that the generating function for the ground state has the factorization [11]

$$\chi_0(\lambda) = \prod_p \left(1 - \frac{\lambda^2}{E_p}\right) \tag{4}$$

for real positive $\{E_p\}$. The even cumulants, given by the coefficients of the expansion of $\ln \chi_0(\lambda)$, are then

$$\langle M^{2n}\rangle_c = (-1)^{n-1}\frac{(2n)!}{n}\sum_p (E_p)^{-n}$$

and therefore alternate in sign.

In the scaling limit, the sum in the operator M can be replaced with an integral $M = \int_0^L dx\, \sigma(x)$, where $\sigma(x)$ is the standard Ising quantum field. Expectation values in the ground state can be computed in the path-integral picture by taking Euclidean spacetime to be a very long cylinder of circumference L; the long cylinder means that in the Hamiltonian picture the system is projected onto its ground state. The path integral for the generating function for the ground state is then precisely the partition function of the 2d classical Ising model with an imaginary magnetic field along a defect line wrapping around the cylinder. In this path integral, we are free to exchange the roles of space and time so that the new Euclidean "time" direction τ is periodic. Since all the operators in χ_0 were originally at the same time, this exchange puts them all at the same spatial position. Thus in this new picture, χ_0 describes the continuum limit of infinitely-long Ising chain at temperature $1/L$ and an imaginary magnetic field $i\lambda$ at point 0. The underlying lattice Hamiltonian is that of the quantum Ising chain (3) on an infinite line, so that the sum runs from $i = -\infty$ to ∞. The generating function is simply

$$\chi_0(\lambda) = \mathrm{tr}\ \left[e^{-HL}\mathcal{T}\, e^{i\lambda\int_0^L d\tau\, \sigma_0^z(\tau)}\right] \qquad (5)$$

where $\mathcal{T}$ represents time-ordering and the (Euclidean) time dependence of the operator denotes the Heisenberg picture: $\sigma_0^z(\tau) = e^{H\tau}\sigma_0^z e^{-H\tau}$.

Writing χ_0 as (5) allows us to compute it exactly at the critical point. We first relate χ_0 to the partition function of a famous quantum impurity model, the anisotropic Kondo problem [12]. We then apply the methods of integrability to compute $\chi_0(\lambda)$ and hence $P_0(m)$.

There are two ways of showing why the Kondo problem arises. The first is quite direct. At the critical point $h = 1$, the trace in Eq. (5) can be expressed as an expectation value in the critical Ising field theory. We then can expand in λ and use the known spin correlation functions in the field theory to write integral expressions for the moments. The integrals for the term order λ^{2n} term are over values of $0 < \tau_j < L$, but because spin correlations are independent of the ordering of the τ_j, we can multiply by $(2n)!$ and order them $0 < \tau_1 < \cdots \tau_{2n} < L$. This allows us to exploit a result for critical Ising correlators when all spin fields lie on a cycle of a cylinder [13]:

$$\langle\sigma(0,\tau_{2n})\cdots\sigma(0,\tau_1)\rangle \propto \prod_{i>j}^{2n}\left[\sin\left(\pi\frac{\tau_i-\tau_j}{L}\right)\right]^{(-)^{i+j}2g} \qquad (6)$$

where $g = 1/8$, the scaling dimension of the spin field. This formula is valid only when the τ_j are ordered. Keeping track of the constants in front of (6) shows $\chi_0(\lambda)$ is a function of the dimensionless quantity $z \equiv \lambda(2\pi a)^{1/8}L^{7/8}$, which establishes the system size independence of the amplitude ratios Eq. (1) and the scaling form of the order parameter distribution (Eq. (2)) for this model, with $s \propto a^{1/8}L^{7/8}$.

The correspondence with the Kondo problem is now apparent. $\chi_0(\lambda)$ takes the form of the partition function at imaginary fugacity iz of a Coulomb gas on a ring. The gas consists of positive and negative charges with logarithmic interactions; because of the $(-1)^{i+j}$ in (6) the signs of the charges required to alternate in space. This is precisely the Anderson-Yuval expansion for the partition function $\mathcal{Z}_K$ of the Kondo model, describing the interaction of a spin-1/2 impurity with a Fermi gas [12]. The expansion in z is a perturbative expansion in the spin-flip part of the Hamiltonian, with alternation in signs of charges arising from the two spin states of the impurity. In the Kondo problem g parametrizes the anisotropy (in spin space) of the interaction. Thus we have shown that

$$\chi_0(\lambda) = \frac{1}{2}\mathcal{Z}_K(iz), \qquad (7)$$

with $g = 1/8$. A very similar result was derived for the chiral version of this problem, describing a point contact in a $p+ip$ superconductor [14], and is in accord with the results for the boundary entropy of the Ising model with a defect magnetic field [15, 16].

An illuminating way of rederiving Eq. (7) is to use boundary conformal field theory. Expanding Eq. (5) in λ and using the time ordering gives

$$\chi_0(\lambda) = \sum_{n=0}^{\infty}(i\lambda)^{2n}\int_0^L d\tau_n\int_0^{\tau_n} d\tau_{n-1}\cdots\int_0^{\tau_2} d\tau_1 \mathrm{tr}\left[e^{-H(L-\tau_{2n})}\sigma_0^z e^{-H(\tau_{2n}-\tau_{2n-1})}\sigma_0^z\cdots\sigma_0^z e^{-H(\tau_2-\tau_1)}\sigma_0^z e^{-H\tau_1}\right] \qquad (8)$$

Since $\sigma^z\sigma^x\sigma^z = -\sigma_x$, the effect of the boundary magnetic field is to flip the sign of the transverse field h at

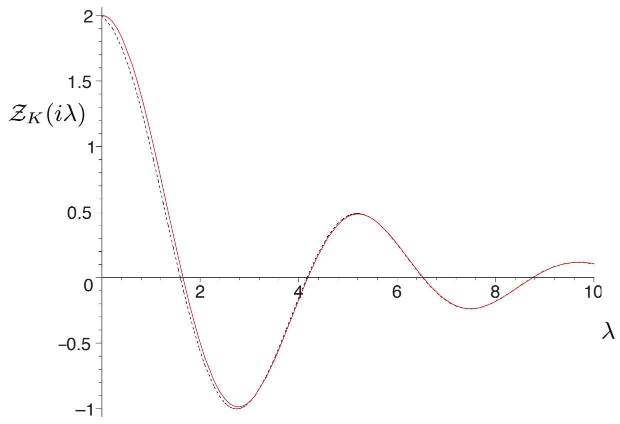

FIG. 1: $\mathcal{Z}_K(i\lambda)$ at g=1/8 and (dashed) its approximation (10)

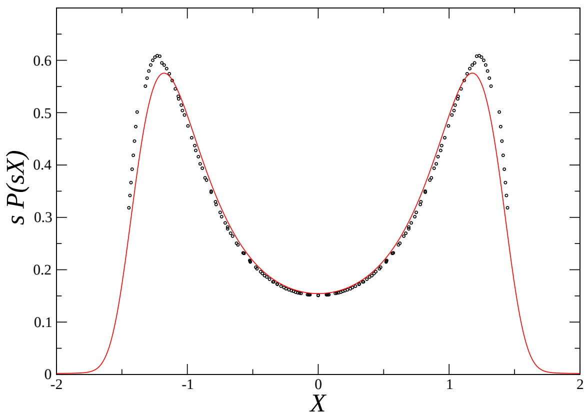

FIG. 2: Dots show numerical data for $sP(sX)$ for the ground state of the critical Ising chain for $L = 16-23$. The continuous line is the scaling function $f_0(X)$ for the ground state, the Fourier transform of $\mathcal{Z}_K(iz)$.

site zero for *every other* interval between insertions of σ_0^z. This means we can effectively treat h as being time-dependent, i.e. $h(\tau) = h\prod_{j=1}^{2n} \mathrm{sgn}(\tau_j - \tau)$. The Ising spin chain has only nearest-neighbor interactions, so we can "fold" the theory in half at site 0, turning the defect into a boundary. The continuum analog of $\sigma_0^z(\tau)$ is then a *boundary-condition-changing operator* $\mathcal{B}(\tau)$ [17]. Here, inserting $\mathcal{B}(\tau_j)$ at an instant τ_j toggles between two different critical boundary conditions. The bosonization analysis of Ref. [15] allows us to show that $\mathcal{B}(\tau)$ is identical to the spin-flip operator in the anisotropic Kondo model. This follows from two key facts about $\mathcal{B}(\tau)$: it has dimension 1/8, and inserting it simply toggles back and forth between two Dirichlet-type boundary conditions on the boson, corresponding to fixed values $\varphi = \pi/4$ and $\varphi = 3\pi/4$ of the boson field. A free boson calculation immediately yields Eq. (6) with $2g = \Delta\varphi^2/\pi^2 = 1/4$.

We now find $\chi_0(\lambda)$, its asymptotics, and its moments. There are three distinct ways of evaluating the partition function $\mathcal{Z}_K(iz)$, all of which work to high numerical accuracy. One way is to use the thermodynamic Bethe ansatz [18, 19], the second is to use series expansions [19, 20], and the third is to compute the spectral determinant of an associated ordinary differential equation [21, 22]. We have used the latter two approaches, both of course giving the same result, displayed in Fig. 1 along with a very accurate asymptotic expression to be discussed below. In accord with the generalized Lee-Yang theorem mentioned earlier, the zeroes $\mathcal{Z}_K(iz)$ occur at real z. In fact, the set $\{E_p\}$ appearing in Eq. (4) are just the eigenvalues of the spectral problem.

The scaled distribution function $sP(sX)$ is obtained by (numerically) taking the Fourier transform of $\mathcal{Z}_K(iz)$, and shown in Fig. 2. We have tested our predictions by exact diagonalization of the lattice Hamiltonian Eq. (3) for $L = 16-23$ using the ALPS libraries [23, 24]. We find excellent agreement, with the numerical results getting closer to the exact curve as L is increased.

We find accurate approximations for the scaling functions and exact values of the moments by utilizing the functional relation between the partition functions of the Kondo and the boundary sine-Gordon models [19, 25, 26]

$$\mathcal{Z}_K(2i\sin(\pi g)z) = \frac{\mathcal{Z}_{BSG}(e^{i\pi g}z) + \mathcal{Z}_{BSG}(e^{-i\pi g}z)}{\mathcal{Z}_{\mathrm{BSG}}(z)} \quad (9)$$

Both partition functions have similar Coulomb-gas expansions, but $\mathcal{Z}_{BSG}$ is given in terms of *unordered* charges. The asymptotic expression for $\mathcal{Z}_{BSG}(z)$, valid for large z in a region near the positive real axis is [19]

$$\mathcal{Z}_{BSG}(z) \approx \exp\left(\frac{\sqrt{\pi}\,\Gamma(\alpha/\pi)}{\Gamma(\frac{1}{2}-\frac{\alpha}{\pi})}\left(\frac{z}{\Gamma(g)}\right)^{1/(1-g)}\right)$$

where $\alpha = \pi g/(2-2g)$. (In the differential equation approach [21, 22], this expression arises from the WKB approximation.) Plugging this into (9) gives

$$\mathcal{Z}_K(i\lambda) \approx 2\cos\left[\cos(\alpha)\,(m_0\lambda)^{\frac{1}{1-g}}\right] e^{-\sin(\alpha)\,(m_0\lambda)^{1/(1-g)}} \quad (10)$$

where

$$m_0 = \left(\frac{2\sqrt{\pi}\,\Gamma(\frac{1}{2}-\frac{\alpha}{\pi})}{\Gamma(1-\frac{\alpha}{\pi})}\right)^{1-g} \frac{\Gamma(1-g)}{2\pi}\ .$$

As $\lambda \to \infty$ along the real axis, this falls off as an oscillating exponential. Even though this asymptotic expression in principle holds only at large λ, when $g = 1/8$ it is a quite accurate approximation. It is plotted along with the exact expression in Fig. 1. Taking the Fourier transform of the asymptotic expression, one finds

$$P_0(m) \approx \frac{2\pi(1-g)}{m_0}\sum_{k=0}^{\infty}\frac{1}{(2k)!\,\Gamma((2k+1)g-2k)}\left(\frac{m}{m_0}\right)^{2k}$$

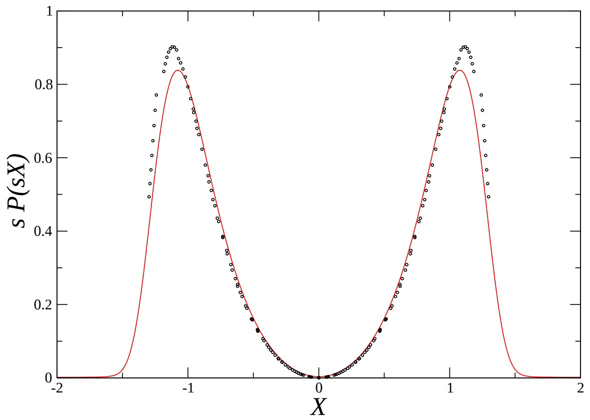

FIG. 3: Comparison of numerical and analytical results for the first excited state scaling function $f_1(X)$.

while a stationary phase approximation to the Fourier integral gives $f_0(X \to \infty) \propto X^{-1+1/2g} \exp\left(-cX^{1/g}\right)$ with $c = g[m_0/(1-g)]^{1-1/g}$.

The moments of the distribution are related to $\mathcal{Z}_K$ by $\langle M^{2n} \rangle \propto (2n)! K_{2n}/2$, where

$$\mathcal{Z}_K(z) = 2+\sum_{n=1}^{\infty} K_{2n} z^{2n}, \qquad \mathcal{Z}_{BSG}(z) = 1+\sum_{n=1}^{\infty} B_{2n} z^{2n} .$$

The universal amplitude ratios are therefore

$$\mathcal{A}_{2n} = \frac{(2n)!}{2} \frac{K_{2n}}{(K_2)^n}$$

The B_{2n} have explicit series expressions [20] which allow accurate numerical evaluation; the K_{2n} are then found in terms of the B_{2m} with $m \le n$ using Eq. (9). The first two ratios are exactly $\mathcal{A}_4 = 1.43138\ldots$ and $\mathcal{A}_6 = 2.35464\ldots$, while from exact diagonalization we find

L	16	17	18	19	20	21	22	23
$\mathcal{A}_4$	1.390	1.393	1.395	1.396	1.398	1.399	1.401	1.402
$\mathcal{A}_6$	2.163	2.173	2.182	2.190	2.198	2.204	2.211	2.216

This method can be extended to the computation of the distribution function for excited states as well. The lowest-lying excited state can be viewed as the ground state of a periodic Ising system with an antiferromagnetic defect. In the Hamiltonian formulation of the field theory, this excited state is given by acting on the ground state with the spin field, so the generating function for the moments of the first excited state is given by inserting spin fields $\sigma(x = +\infty, \tau)$ and $\sigma(x = -\infty, \tau)$ into the correlator (6). These insertions amount to setting $p = 1/4$ in the conventions of [20] or $p = 1/8$ in [25]. The resulting scaling function $f_1(X)$ of the first excited state is shown in Fig. 3. It is quite different from $f_0(X)$, illustrating the importance of different boundary conditions.

In conclusion, we have shown how the quantum critical distribution of the order parameter in the universality class of the Ising chain may be calculated analytically using a remarkable map to the Kondo problem.

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