

Quantum phase transitions and conserved charges

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(November 30, 1993)

Abstract

The constraints on the scaling properties of conserved charge densities in the vicinity of a zero temperature (T), second-order quantum phase transition are studied. We introduce a generalized Wilson ratio, characterizing the non-linear response to an external field, H , coupling to any conserved charge, and argue that it is a completely universal function of H/T : this is illustrated by computations on model systems. We also note implications for transitions where the order parameter is a conserved charge (as in a $T = 0$ ferromagnet-paramagnet transition).

cond-mat/9312018 4 Dec 93

I. INTRODUCTION

There has been some interest in the theory of zero temperature quantum phase transitions in condensed matter systems for a few years now [1], particularly in the context of metal-insulator transitions [2]. However, the recent proliferation of experimental systems in which such transitions may be observed has led to a surge in theoretical work. Transitions of interest include the superconductor-insulator transition in thin films [3], the transition between the plateaus in the quantum hall effect [4], and a variety of magnetic order-disorder transitions in the cuprate compounds [5], metal-semiconductor composites [6], and heavy-fermion [7,8] systems.

In this paper we will examine some special properties, in the vicinity of second-order quantum transitions, associated with “conserved charges”, *i.e.* observables which commute with the Hamiltonian. Related issues have been discussed recently by other investigators [9,10], with their focus being on the $T = 0$ properties of the currents associated with conserved charge. We will study here the unusual and remarkable properties of fluctuations of conserved charges themselves in the finite-temperature *quantum-critical* [11,5,12,13] region near the quantum phase transition.

The quantum-critical region was introduced by Chakravarty *et. al* [11] in the context of the two-dimensional quantum sigma model. An analogous region can in fact be defined in the vicinity of *any* second-order quantum phase transition, as the region where $k_B T$ is significantly larger than any energy scale which measures deviations of the coupling constants from their zero temperature critical values. Note that, somewhat counter-intuitively, the quantum-critical region occurs at high temperatures; of course, the temperature cannot be so large that it becomes of the order of some high-energy cutoff in the system. At short distance/time scales the system displays the scale-invariant properties of some zero temperature critical point; at larger scales, the critical fluctuations are quenched by thermal effects in a universal manner described in Ref. [5,13]. Because $k_B T$ is large, the thermal quenching occurs *before* the deviations of the couplings from their ground-state critical values have had a chance to take effect. Thus, in the quantum-critical region, the dominant behavior of the system is described at *all* scales by the zero temperature critical point and its universal response to a finite temperature. Further, the only effect of a finite temperature is to impose a finite length $\hbar/(k_B T)$ along the imaginary time direction on the quantum field-theory of the zero-temperature critical-point; the temperature response of the critical point can thus be described by the principles of finite-size scaling [11,5,12,13].

This paper will examine the non-linear, finite temperature response of a system in the quantum-critical region to an external field which couples to a conserved charge. Our motivation to examine this issue comes primarily from quantum spin systems [12,13] and heavy-fermion alloys [7,8], although we will attempt to phrase our discussion as generally as possible. After some general discussion on conserved charges and their scaling properties in Sections II and III, we will present illustrative calculations on a number of model systems (Section IV).

Strictly speaking, the considerations of this paper will use only some modest assumptions about the zero temperature critical point. In particular we will only require that it be gapless with a power-law singularity in the density of low-energy excitations. One can imagine, particularly in random quantum systems, that this condition may be satisfied

even by systems which are strictly not at a scale-invariant critical point. We expect that our results will apply to such systems too. However, for definiteness, we will continue to phrase our discussion in the language of second-order quantum phase transitions.

In Section V, we will consider a special application of our results to the case where the conserved charge is itself the order parameter of the transition: the most familiar example of this is the ferromagnet-paramagnet transition in a Fermi liquid. We will show that the existing treatment of this transition [1] is fundamentally incomplete, and will indicate the restrictions any correct theory must satisfy; we will, however, not provide such a theory here.

II. GENERAL CONSIDERATIONS

This section will discuss the general constraints that are imposed on correlators of conserved charges and currents. These constraints are perhaps most familiar in the particle physics context of ‘current algebra’ [14]. We will review these ideas here in a formulation designed to address quantum phase transitions in condensed matter systems. Moreover, in the latter context, our point of view is different from previous ones [9,10], and it therefore appears worthwhile to present the complete argument in its full generality. Consider, then, the partition function, Z , of the system of interest in the vicinity of the quantum phase transition:

$$Z = \int_{\phi_a(\tau+L_\tau)=\phi_a(\tau)} \mathcal{D}\phi_a \exp\left(-\frac{1}{\hbar} \int d\tau \mathcal{L}[\phi_a]\right). \quad (2.1)$$

The Lagrangian \mathcal{L} is a functional of a set of fields ϕ_a which are assumed to be bosonic for simplicity - the extension to fermionic fields is straightforward. The fields depend implicitly on the d spatial co-ordinates x and the imaginary time co-ordinate τ . All allowed configurations are periodic in τ , with period

$$L_\tau \equiv \frac{\hbar}{k_B T}, \quad (2.2)$$

where T is the absolute temperature. We will find it more convenient to think of τ running from $-\infty$ to ∞ with the constraint on the periodicity of the fields, rather than, as is conventionally done, restricting attention to the fundamental domain $0 < \tau < L_\tau$.

Let us now assume that \mathcal{L} is invariant (upto a total time derivative), under some spacetime-*independent* symmetry transformation of the fields ϕ^a . In its infinitesimal form, this transformation can be written as

$$\phi_a \rightarrow \phi_a + i\eta_\alpha F_{ab}^\alpha \phi_b \quad (2.3)$$

where the η_α are the infinitesimal, dimensionless, parameters specifying the transformation and the F^α are the generators of the Lie algebra associated with the symmetry. These generators will satisfy a commutation relation of the form

$$[F^\alpha, F^\beta] = i f_{\alpha\beta\gamma} F^\gamma \quad (2.4)$$

where the $f_{\alpha\beta\gamma}$ are the structure constants of the Lie algebra.

We now use the usual Noether argument to identify the charges and currents. Make the transformation (2.3) on \mathcal{L} , but with the η_α spacetime-*dependent*. In general, any variation in the action under this transformation, will depend, to linear order, on the derivatives of the η_α . We therefore have for small η_α (and again upto a total time derivative)

$$\mathcal{L} \rightarrow \mathcal{L} + i\hbar \int d^d x \partial_\mu \eta_\alpha q_{\mu\alpha}(x, \tau) \quad (2.5)$$

where the index μ extends over the $d + 1$ spacetime co-ordinates. The co-efficients, $q_{\tau\alpha}$ of $\partial_\tau \eta_\alpha$ are, of course, the conserved charge densities associated with the symmetry under consideration, while the $q_{x\alpha}$ are the associated currents. (At this point, it is conventional in some field theory books to identify the $q_{\mu\alpha}$ with $\phi_a F_{ab}^\alpha \delta\mathcal{L}/\delta(\partial_\mu \phi_b)$; we caution the reader that this latter form fails for the coherent state path integral of quantum spins - the definition (2.5) is more generally valid.)

We are interested in the special constraints that apply to correlation functions of the $q_{\mu\alpha}$. To this end, we place the system in external fields $A_{\mu\alpha}$ which couple to the $q_{\mu\alpha}$; the correlation functions can then be obtained by taking appropriate functional derivatives w.r.t the $A_{\mu\alpha}$. While it is sufficient to simply add a linear coupling $A_{\mu\alpha} q_{\mu\alpha}$ to \mathcal{L} to achieve this, we will find that this approach is not the most convenient in deriving the Ward identities. The following approach is found to be the most direct: Generalize the Lagrangian $\mathcal{L}[\phi_a]$ to the field-dependent $\mathcal{L}[\phi_a, A_{\mu\alpha}]$ and evaluate

$$Z(A_{\mu\alpha}) = \int_{\phi_a(\tau+L\tau)=\phi_a(\tau)} \mathcal{D}\phi_a \exp\left(-\frac{1}{\hbar} \int d\tau \mathcal{L}[\phi_a, A_{\mu\alpha}]\right). \quad (2.6)$$

The new $\mathcal{L}[\phi_a, A_{\mu\alpha}]$ is chosen such that it is invariant (upto total time derivatives) under spacetime-*dependent* transformations of the form (2.3) accompanied by the following transformation of the $A_{\mu\alpha}$

$$A_{\mu\alpha} \rightarrow A_{\mu\alpha} + \partial_\mu \eta_\alpha - f_{\alpha\beta\gamma} \eta_\beta A_{\mu\gamma} \quad (2.7)$$

In other words, we have promoted the global symmetry to a gauge symmetry, and the $A_{\mu\alpha}$ are the non-abelian gauge connections.

Let us now examine a few simple examples of the above construction.

1. Non-relativistic electrons in a magnetic field

Non-relativistic spin-1/2 electrons, $c_a(x, \tau)$ ($a = \uparrow, \downarrow$), in an external magnetic field $H = \eta_{\alpha\beta\gamma} \partial a_\gamma / \partial x_\beta$ ($\alpha, \beta, \gamma = 1, 2, 3$) are described by the following Lagrangian

$$\mathcal{L} = \int d^d x \left[\hbar c_a^\dagger \frac{\partial c_a}{\partial \tau} - \frac{gH_\alpha}{2} c_a^\dagger \sigma_{ab}^\alpha c_b - \frac{\hbar^2}{2m} \left| \left(\frac{\partial}{\partial x_\alpha} - ia_\alpha \right) c_a \right|^2 + \dots \right] \quad (2.8)$$

where the ellipses indicate terms without any derivatives, the σ^α are Pauli matrices, and g is the gyromagnetic coupling. The paramagnetic and diamagnetic couplings of the field

to the electrons play totally distinct roles in the present symmetry analysis. There are two distinct conserved charges - the total number and total spin of the electrons. The first is associated with the $U(1)$ symmetry

$$c_a \rightarrow c_a + i\eta c_a. \quad (2.9)$$

Upon gauging this symmetry we see that the a_α are the spatial components of the A_μ fields introduced above

$$a_\alpha \rightarrow a_\alpha + \frac{\partial\eta}{\partial x_\alpha} \quad (2.10)$$

The second is the spin-rotation symmetry

$$c_a \rightarrow c_a + i\frac{\eta_\alpha}{2}\sigma_{ab}^\alpha c_b \quad (2.11)$$

which when gauged leads to the transformation

$$gH_\alpha \rightarrow gH_\alpha - \frac{i}{\hbar}\partial_\tau\eta_\alpha - g\varepsilon_{\alpha\beta\gamma}\eta_\beta H_\gamma, \quad (2.12)$$

on the magnetic field (ε is the totally antisymmetric tensor). Thus igH_α/\hbar is the τ -component of the non-abelian $SU(2)$ gauge field, $A_{\mu\alpha}$, associated with the $SU(2)$ spin-rotation invariance. Note that $A_{\tau\alpha}$ is purely imaginary. We shall mainly focus on the consequences of this second symmetry in this paper.

2. $O(3)$ sigma model

This model is a popular long-wavelength description of low-lying spin excitations in an insulating antiferromagnet. In the presence of an external magnetic field H_α , the Lagrangian takes the form [15]

$$\mathcal{L} = \frac{1}{2g} \int d^d x \left[\frac{1}{c^2} \left(\partial_\tau n_a - \frac{ig}{\hbar} \varepsilon_{\alpha ab} H_\alpha n_b \right)^2 + (\partial_x n_a)^2 \right] \quad (2.13)$$

where n_a is a 3-component, real, unit-vector representing the local orientation of the antiferromagnetic order parameter. \mathcal{L} is invariant under an $O(3)$ symmetry under which

$$n_a \rightarrow n_a - \eta_\alpha \varepsilon_{\alpha ab} n_b, \quad (2.14)$$

while H_α continues to transform as in (2.12) and thus igH_α/\hbar is the τ -component of a $O(3)$ non-abelian gauge field.

3. Quantum spins

The symmetry analysis of the path-integral of quantum spin systems is somewhat more subtle, but our general discussion has been phrased carefully to include this case. As was first shown by Haldane [16], the path integral of any quantum spin Hamiltonian involves the Lagrangian

$$\mathcal{L} = i\hbar S \sum_j W_b(\Omega_{aj}) \frac{d\Omega_{bj}}{d\tau} + \mathcal{H}(\Omega_{aj}) \quad (2.15)$$

where S is the half-integral/integral magnitude of the spin, the Ω_{aj} are unit 3-vectors on sites j representing the instantaneous orientation of the spin, and W_a is any function satisfying

$$\varepsilon_{abc} \frac{\partial}{\partial \Omega_b} W_c = \Omega_a \quad (2.16)$$

(we have momentarily dropped the site index j). The Hamiltonian \mathcal{H} does not involve any time derivatives, and is spin-rotation invariant. Let us now make a space-independent, but time-dependent rotation of all the spins

$$\Omega_a \rightarrow \Omega_a - \eta_c(\tau) \varepsilon_{cab} \Omega_b, \quad (2.17)$$

Inserting this into \mathcal{L} , using (2.16) and the unit-length constraint on Ω , simple manipulations show that, upto a total time derivative,

$$\mathcal{L} \rightarrow \mathcal{L} + i\hbar S \frac{d\eta_a}{d\tau} \cdot \sum_j \Omega_{aj} \quad (2.18)$$

By our prescription (2.5) this identifies $S \sum_j \Omega_{aj}$ as the conserved total spin. In the presence of a magnetic field the action is clearly

$$\mathcal{L} = i\hbar S \sum_j W_b(\Omega_{aj}) \frac{d\Omega_{bj}}{d\tau} - gH_a \sum_j \Omega_{aj} + \mathcal{H}(\Omega_{aj}) \quad (2.19)$$

This is now invariant under time-dependent gauge transformations with H_a transforming as in (2.12). Note that the ‘rule’ of replacing derivatives with covariant derivatives does not hold in this case - our formulation is however still valid.

We now return to the general considerations. We will consider first the Ward identities satisfied by correlators of the conserved charges and currents. This will be followed by a discussion of properties of the system in a time-independent external field.

A. Ward Identities

An important property of the functional $Z(A_{\mu\alpha})$ in (2.6) is that

$$Z(A_{\mu\alpha}) = Z(A_{\mu\alpha} + \partial_\mu \eta_\alpha - f_{\alpha\beta\gamma} \eta_\beta A_{\mu\gamma}) \quad (2.20)$$

for any spacetime dependent gauge transformation η_α such that (2.3) is consistent with the boundary conditions $\phi_a(\tau + L_\tau) = \phi_a(\tau)$. (This follows from performing (2.3) on the ϕ_a dummy variables of integration, followed by (2.7), which leaves the action invariant.) We expand (2.20) to linear order in η and obtain the key Ward identity

$$\partial_\mu \frac{\delta Z(A_{\mu\alpha})}{\delta A_{\mu\alpha}(x, \tau)} = f_{\alpha\beta\gamma} A_{\mu\gamma}(x, \tau) \frac{\delta Z(A_{\mu\alpha})}{\delta A_{\mu\beta}(x, \tau)} \quad (2.21)$$

The left-hand-side of this equation is simply the divergence of the conserved charge and currents. The right-hand side is the analog of the ‘streaming’ or ‘Poisson-bracket’ terms [17] in the theory of the dynamics of classical phase transitions; this term dictates that the conserved charge undergoes a uniform precession under the presence of the external field.

In the following we will mostly be interested in constraints on correlators of the conserved charges $q_{\tau\alpha}$ under conditions in which only the τ component of the $A_{\mu\alpha}$ is non-zero. By integrating (2.21) over all space we can obtain a constraint on these correlators

$$\int d^d x \partial_\tau \frac{\delta Z(A_{\tau\alpha}, A_{x\alpha} = 0)}{\delta A_{\tau\alpha}(x, \tau)} = \int d^d x f_{\alpha\beta\gamma} A_{\tau\gamma}(x, \tau) \frac{\delta Z(A_{\tau\alpha}, A_{x\alpha} = 0)}{\delta A_{\tau\beta}(x, \tau)} \quad (2.22)$$

A particularly useful consequence of (2.22) is the constraints it places on two and three-point functions of the conserved charges. If we make the expansion (restricting, for simplicity, to a translationally invariant system)

$$\begin{aligned} \mathcal{F}(A_{\tau\alpha}, A_{x\alpha} = 0) &= \int d^d q d\omega G(q, \omega) A_{\tau\alpha}(q, \omega) A_{\tau\alpha}(-q, -\omega) + \\ &\int d^d q_1 d^d q_2 d\omega_1 d\omega_2 \Gamma^{\alpha\beta\gamma}(q_1, q_2, \omega_1, \omega_2) A_{\tau\alpha}(q_1, \omega_1) A_{\tau\beta}(q_2, \omega_2) A_{\tau\gamma}(-q_1 - q_2, -\omega_1 - \omega_2) \\ &+ \dots \end{aligned} \quad (2.23)$$

where the q_i and ω_i are momenta and frequencies and \mathcal{F} is the free energy density, we see from (2.22) that

$$3i(\omega_1 + \omega_2) \Gamma^{\alpha\beta\gamma}(q, -q, \omega_1, \omega_2) = f^{\alpha\beta\gamma} (G(q, \omega_1) - G(q, \omega_2)) \quad (2.24)$$

This identity will be useful to us later in our study of ferromagnets.

B. Time-independent, uniform, external field

We will consider explicitly only the case of a time-independent, uniform, $A_{\tau\alpha}$ field; the spatial components $A_{x\alpha}$ will be taken to be zero. As was clear from the examples considered above, the $A_{\tau\alpha}$ corresponds to an *imaginary* external magnetic field in spin systems. To emphasize this we will use the notation

$$A_{\tau\alpha} \equiv \frac{igH_\alpha}{\hbar}. \quad (2.25)$$

As in Section II A we attempt to ‘gauge away’ the field dependence of $Z(H_\alpha) \equiv Z(A_{\tau\alpha}, A_{x\alpha} = 0)$ for the case of a time-independent H_α . From (2.7) it appears that we should choose

$$\frac{d\eta_\alpha}{d\tau} = i \frac{gH_\alpha}{\hbar} \quad (2.26)$$

(a generalized Josephson equation). However the corresponding transformation (2.3) on the ϕ_a necessarily modifies the boundary conditions. We have therefore

$$Z(H_\alpha) = \int_{\phi_a(\tau+L_\tau)=\phi_a(\tau)+i(igH_\alpha L_\tau/\hbar)F_{ab}^\alpha \phi_b(\tau)} \mathcal{D}\phi_a \exp\left(\frac{1}{\hbar} \int d\tau \mathcal{L}[\phi_a]\right). \quad (2.27)$$

Thus the *sole* effect of the field H_α is to put a twist in the periodic boundary conditions on ϕ by an *imaginary* angle $igHL_\tau/\hbar$.

III. SCALING PROPERTIES NEAR QUANTUM PHASE TRANSITIONS

We will focus almost all our subsequent attention in the ‘quantum-critical region’ [11,5,12,13] where $k_B T$ is much greater than any intrinsic low-energy scale associated with the deviation of the ground state from criticality (we must of course not make $k_B T$ so large that it becomes comparable to ultraviolet cutoff’s in the system). In this region, the leading T dependence of all observables is specified by properties of the $T = 0$ critical point. In the following, we will therefore neglect the deviation of the ground state from criticality, although the extension to including its consequences are quite straightforward. Also, we will mostly consider the case of a uniform, time-independent field $A_{\tau\alpha} \neq 0$, $A_{x\alpha} = 0$, and refer to the external field using (2.25).

We consider the properties of the the free-energy density $\mathcal{F} = -(\hbar/(L_\tau V)) \log Z = -(k_B T/V) \log Z$ (V is the spatial volume of the system which is assumed to be infinite) as a function of T and H . Consider first the case $H = 0$, and T close to 0. The only effect of a finite T is in the imposition of a periodicity in ϕ with period L_τ on the critical, scale-invariant theory at $T = 0$, $H = 0$. The hypothesis of finite-size scaling [18] predicts the following temperature dependence in \mathcal{F}

$$\mathcal{F}(T, H = 0) = \mathcal{F}(0, 0) - c_1 T^p \quad (3.1)$$

There is no general expression for the exponent p , or the constant c_1 . However, if the system is below its upper critical dimension, the hyperscaling hypothesis [18] states that the scaling dimension of \mathcal{F} is identical to its naive engineering dimension: this yields

$$p = 1 + \frac{d}{z} \quad (3.2)$$

The 1 contribution is due to the $1/L_\tau$ prefactor in the definition of \mathcal{F} , and the remaining d/z contribution is from the $1/V$. The dynamic-critical exponent z expresses the anisotropic scaling between space and time directions. The pre-factor c_1 in (3.1) is in general non-universal. For the special case of a relativistic field theory we have $z = 1$ and the c_a becomes universally related to the velocity of the low-lying excitations; in this case in $d = 1$ the number c_1 is closely related to the central charge of the conformal field theory describing the critical point.

Now consider the effect of a time-independent external field H . From (2.27) the *only* effect of H is a twist in the τ boundary conditions on the system. The excitations responding to the change in the boundary conditions will be precisely the same low-energy modes which led to a size (T) dependence of \mathcal{F} in (3.1): the only effect of a finite H should therefore be a modification of the term proportional to c_1 in (3.1). Furthermore, as the twist is a long-wavelength effect, the modification of c_1 should be ‘universal’ (*i.e.* independent of all microscopic details) function of the ‘angle’ of the twist $igHL_\tau/\hbar$. Alternatively, this is simply the statement that all finite-size scaling corrections are universal functions of ‘geometrical’ properties of the sample like aspect ratios, shape, nature of boundary conditions etc. The fact that the angle of the twist is imaginary should not be too disturbing - the process of analytic continuation commutes with all scaling arguments, and one can just lift the scaling forms from those of real twists. We have therefore

$$\mathcal{F}(T, H) = \mathcal{F}(0, 0) - c_2 T^p \Omega\left(\frac{gH}{k_B T}\right) \quad (3.3)$$

where $c_1 = c_2 \Omega(0)$. The value of $\Omega(0)$ will be chosen at our convenience, but the function $\Omega(r)$ is otherwise universal (we use $r = gH/(k_B T)$ below). Note in particular that the argument of the scaling function is precisely $gH/k_B T$ and there are no arbitrary scale factors in the argument. There is no guarantee that the function $\Omega(r)$ is analytic for finite, positive values of r . In particular, some systems may undergo a phase transition at a finite H , which will then correspond to a (universal) singularity in $\Omega(r)$; we will see an example of this in the model calculations below.

The form of (3.3) implies immediately that the scaling dimension of H (or equivalently $A_{\tau\alpha}$) is precisely the same as that of T . In other words, under a scaling transformation which rescales spatial lengths by a factor s

$$A'_{\tau\alpha}(x', \tau') = s^z A_{\tau\alpha}(x, \tau) \quad (3.4)$$

where $x' = x/s$ and $\tau' = \tau/s^z$. Exactly parallel arguments can be made for the spatial components of the $A_{\mu\alpha}$ by thinking about the properties of the system in a geometry which is finite in the spatial directions, but infinite along the time direction - this will yield the scaling dimension of $A_{x\alpha}$:

$$A'_{x\alpha}(x', \tau') = s A_{x\alpha}(x, \tau) \quad (3.5)$$

We emphasize that that none of the results (3.3), (3.4) or (3.5) rely upon the validity of hyperscaling.

In the presence of hyperscaling, one can go further, and also deduce the scaling dimensions of the conserved charges and currents. The $q_{\mu\alpha}$ and the $A_{\mu\alpha}$ are conjugate variables and their product should therefore have the same scaling dimension as the free energy (which is $z + d$). We have therefore

$$q'_{\tau\alpha}(x', \tau') = s^d q_{\tau\alpha}(x, \tau) \quad q'_{x\alpha}(x', \tau') = s^{d+z-1} q_{x\alpha}(x, \tau) \quad (3.6)$$

only if hyperscaling is valid.

A number of strong experimental consequences now follow from (3.3). We can immediately obtain scaling forms for the ‘magnetization’ $M = -\partial\mathcal{F}/\partial H$ and the specific heat $C_V = -T\partial^2\mathcal{F}/\partial T^2$:

$$\frac{M}{H} = \frac{c_2 g^2}{k_B^2} T^{p-2} \Omega_M \left(\frac{gH}{k_B T} \right) \quad ; \quad C_V = c_2 T^{p-1} \Omega_C \left(\frac{gH}{k_B T} \right) \quad (3.7)$$

where the universal functions Ω_M, Ω_C are both simply related to linear combinations of Ω and its derivatives. Notice that it is the same non-universal number c_2 which appears in both M/H and C_V , and there are no other non-universal quantities; the only choice that had to be made was in the value of $\Omega(0)$. All dependence on this choice, and hence c_2 , can be eliminated by considering the dimensionless generalized Wilson ratio, W

$$W \equiv \frac{k_B^2 T}{g^2} \frac{M/H}{C_V} = \Omega_W \left(\frac{gH}{k_B T} \right) \quad (3.8)$$

which is a fully universal function of H/T . We emphasize that the universality of W did not rely on hyperscaling. Experimental measurements of this ratio can thus provide us with strong tests of various theoretical scenarios, and also determine if different experimental systems are in the same universality class. We note that the universality of the Wilson ratio as $H \rightarrow 0$ has also been noted recently for the incremental thermodynamic response of impurities in Fermi liquids [19]: these models map onto boundary critical phenomena, whereas we have been considering the bulk response of a macroscopic critical system.

IV. MODEL CALCULATIONS

We will now illustrate the general principles described above by model calculations on a number of systems. We begin with the simplest realization in the theory of Luttinger liquids; in this case the function $\Omega_W(r)$ will turn out to be independent of r . None of the remaining models will have this property. We follow this by a second simple system - a dilute fermi gas - which also satisfies the scaling ansatzes. We will then examine a simple phenomenological model of a very complicated system - the Bhatt-Lee [20] model of random quantum antiferromagnets. Finally we will present a self-contained analysis of a truly interacting system: the $O(N)$ sigma model, whose main applicability is to the low-energy properties of clean, quantum antiferromagnets.

A. Luttinger Liquids

We begin by presenting the simplest illustration of our results in the Luttinger liquid theory of the low temperature properties of a dense one-dimensional gas of spin-1/2 fermions. In this case we are considering a whole critical phase, rather than a critical point.

The low energy action of the Luttinger liquid can be expressed in terms of two dimensionless scalar fields, $\theta_\rho, \theta_\sigma$

$$\mathcal{L} = \frac{\hbar}{2\pi} \int dx \left[K_\rho \left(u_\rho (\partial_x \theta_\rho)^2 + \frac{1}{u_\rho} (\partial_\tau \theta_\rho)^2 \right) + K_\sigma \left(u_\sigma (\partial_x \theta_\sigma)^2 + \frac{1}{u_\sigma} (\partial_\tau \theta_\sigma)^2 \right) \right] \quad (4.1)$$

where u_ρ , u_σ are the charge and spin excitation velocities, and K_ρ , K_σ are dimensionless couplings which determine the exponents of the Luttinger liquid; we have used here the notation of Ref. [21]. Spin rotation invariance requires $K_\sigma = 1$.

In the presence of an external magnetic field coupling via the Zeeman term to the spin-1/2 fermions, \mathcal{L} gets modified by the replacement $\partial_\tau\theta_\sigma \rightarrow \partial_\tau\theta_\sigma - igH/(\sqrt{2}\hbar)$. Computing the action of the free field theory \mathcal{L} at finite temperature is now completely straightforward. We get

$$\mathcal{F}(H, T) = -\frac{K_\sigma}{4\pi\hbar u_\sigma}(gH)^2 + \frac{k_B T}{2} \sum_{\omega_n} \int \frac{dk}{2\pi} \left(\log(\omega_n^2 + u_\sigma^2 k^2) + \log(\omega_n^2 + u_\rho^2 k^2) \right) \quad (4.2)$$

Note that the H dependence of \mathcal{F} is rather simple and has decoupled completely from its T dependence: this is a special feature of the present model. The frequency summations and integrals can be performed exactly and yield a result consistent with (3.3) which is:

$$\begin{aligned} \mathcal{F}(H, T) &= \mathcal{F}(0, 0) - \frac{(k_B T)^2}{\hbar u_\sigma} \Omega\left(\frac{gH}{k_B T}\right) \\ \Omega(r) &= \frac{\pi}{6} \left(1 + \frac{u_\sigma}{u_\rho}\right) + \frac{K_\sigma}{4\pi} r^2 \end{aligned} \quad (4.3)$$

The scaling properties of the magnetization and the specific heat now follow. In particular, we obtain for the generalized Wilson ratio

$$\Omega_W(r) = \frac{3K_\sigma}{2\pi^2(1 + u_\sigma/u_\rho)} \quad (4.4)$$

As stated above, Ω_W is in fact independent of r . This is a special feature of the Luttinger/Fermi liquid that does not generalize. The Wilson ratio has most often been considered in the past in the context of Luttinger/Fermi liquids, and this is perhaps the reason why its universal, non-trivial, dependence on the ratio H/T at generic quantum-critical points has not heretofore been pointed out.

B. Dilute Fermi Gas

Consider a gas of fermions (with spin j) in d dimensions described by the following Hamiltonian

$$\mathcal{H} = \sum_k \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c_k^\dagger c_k + \mathcal{H}_{\text{int}} \quad (4.5)$$

where c_k annihilates fermions with momentum k , and \mathcal{H}_{int} contains only repulsive interactions. This model has a $T = 0$ quantum phase transition as a function of μ at $\mu = 0$. The density of fermions vanishes for $\mu < 0$, and increases as $\sim \mu^{d/2}$ for $\mu > 0$. The scaling properties of this quantum transition are very similar to those of the corresponding transition for bosons which has been studied elsewhere [22]. From this analysis [22] we may conclude that the exponent $z = 2$. Also, it can be shown that the interactions in \mathcal{H}_{int} are irrelevant at

this transition for $d > 2$ (they are in fact also irrelevant below $d = 2$ for spinless electrons). Thus, for $d > 2$, we may compute the scaling properties of the free energy in the free fermion model.

The conserved charge we focus on here is the density of the fermions. The field conjugate to this density is μ and therefore plays the role here of the ‘magnetic’ field. Thus consistent with (3.3) the free fermion free energy density obeys

$$\begin{aligned} \mathcal{F}(\mu, T) &= -(2j + 1)(k_B T)^{1+d/2} \left(\frac{2m}{\hbar^2}\right)^{d/2} \Omega\left(\frac{\mu}{k_B T}\right) \\ \Omega(r) &= \int \frac{d^d y}{(2\pi)^d} \log\left(1 + e^{-y^2+r}\right) \end{aligned} \quad (4.6)$$

Unlike Section IV A, note that $\Omega(r)$ is quite a non-trivial function of r , and leads to correspondingly non-trivial r -dependences in the scaling results for the density (which plays the role of ‘magnetization’), specific heat, and Wilson ratio.

C. Bhatt-Lee model.

This is a simple phenomenological model of the spin-fluid phase (*i.e.* no spin-glass order) of spin-1/2 random antiferromagnetic spin systems [20]. It has been quite successful in describing experiments in lightly doped semiconductors [23]. We now show that this model in fact satisfies all of the constraints discussed above on quantum-critical spin fluctuations. Thus the entire spin-fluid *phase* may in fact be critical in random systems, and not just its transition to a magnetically ordered state. Additional evidence for such a scenario has appeared in recent solutions of random Heisenberg antiferromagnets with infinite-range interactions [24].

The Bhatt-Lee model [20] describes the random antiferromagnet as independent pairs of spins which have an antiferromagnetic exchange interaction J with probability $P(J) \sim J^{-\alpha}$. The exponent α is estimated from numerical work to be approximately 0.6 in $d = 3$. The free energy of this model in an external field H , is obtained by summing the contributions of each pair of spins and is therefore

$$\mathcal{F} = \mathcal{F}_0 - k_B T \int dJ P(J) \log\left[1 + e^{-J/k_B T} (1 + 2 \cosh(gH/k_B T))\right] \quad (4.7)$$

This can easily be collapsed into the scaling form (3.3) with $p = 2 - \alpha$ and the universal scaling function $\Omega(r)$:

$$\Omega(r) = \int_0^\infty dy y^{-\alpha} \log\left[1 + e^{-y} (1 + 2 \cosh r)\right] \quad (4.8)$$

The value of $\Omega(r = 0)$ has been chosen for convenience; apart from this single scale, the function $\Omega(r)$ is otherwise universal. If we assume hyperscaling then we get the dynamic exponent

$$z = \frac{d}{1 - \alpha} \quad (4.9)$$

The integral in (4.8) cannot be evaluated exactly, but we quote some useful asymptotic limits:

$$\Omega(r) = \begin{cases} -\Gamma(1-\alpha) [\text{Li}_{2-\alpha}(-3) + r^2 \text{Li}_{1-\alpha}(-3)/3] & r \rightarrow 0 \\ r^{2-\alpha} / ((2-\alpha)(1-\alpha)) + \pi^2 r^{-\alpha} / 6 & r \rightarrow \infty \end{cases} \quad (4.10)$$

where $\text{Li}_p(z)$ is the polylogarithm function, defined by analytic continuation of the series:

$$\text{Li}_p(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^p} \quad (4.11)$$

The scaling functions for the magnetization (Ω_M), specific heat (Ω_C), and the Wilson ratio (Ω_W) can now be easily obtained by taking suitable derivatives of $\Omega(r)$: The results are plotted in Figs 1 and 2 for the value $\alpha = 0.6$ (a function closely related to Ω_M was evaluated and compared with experiments in Ref. [23]). As we noted earlier, the results for Ω_W are totally independent of any choice of an overall scale - we state below the asymptotic limits of Ω_W :

$$\Omega_W(r) = \begin{cases} \frac{2\text{Li}_{1-\alpha}(-3)}{3(1-\alpha)(2-\alpha)\text{Li}_{2-\alpha}(-3)} & r \rightarrow 0 \\ \frac{1}{\pi^2(1-\alpha)} & r \rightarrow \infty \end{cases} \quad (4.12)$$

Note also in Fig 2 the non-monotonic behavior of Ω_W between these two limits.

Our identification of the exponent z also allows us to make a new prediction on the temperature dependence of the spin diffusion constant D . The scaling dimension of D is $z - 2$, leading to the low temperature dependence

$$D \sim T^{1-2/z} = T^{(d-2+2\alpha)/d}. \quad (4.13)$$

D. $O(N)$ sigma model in 2+1 dimensions

We first generalize the $O(3)$ sigma model of Section II 2 to the $O(N)$ model by allowing n_a to have N components, $a = 1 \dots N$. The external field H must now generate one of the rotations of the $O(N)$ group. These rotations can be built out of combinations of rotations in the $N(N-1)/2$ different hyperplanes in N dimensions. For general N , unlike $N = 3$, not all such rotations are equivalent, and cannot be transformed into each other by a change of co-ordinates: this is related to the presence of more than a single Casimir invariant in the $O(N)$ group. We will therefore choose a specific orientation of the magnetic field to facilitate a simple large N limit: other orientations of the magnetic field will have physically different properties (for $N > 3$). We choose a magnetic field to generate a simultaneous rotation by the same angle in the $(1, 2), (3, 4), \dots, ((2p-1)N, 2pN)$ hyperplanes, with no rotation in the remaining $N(1-2p)$ hyperplanes; the fraction p is chosen such that pN is an integer, and $p \leq 1/2$. The large N limit will be taken with p fixed. Clearly, the model relevant to collinear quantum antiferromagnets is $N = 3$, $p = 1/3$. These considerations lead to the following action for the $O(N)$ sigma model in a magnetic field:

$$S = \frac{N}{2t} \int d\tau \int d^2x \left[\sum_{a=1}^N (\nabla_x n_a)^2 + \frac{1}{c^2} \sum_{a=1}^{pN} [(\partial_\tau n_{2a-1} - igHn_{2a})^2 + (\partial_\tau n_{2a} + igHn_{2a-1})^2] + \frac{1}{c^2} \sum_{a=2pN+1}^N (\partial_\tau n_a)^2 \right], \quad (4.14)$$

where the coupling constant t determines the strength of the quantum fluctuations and c is the spin-wave velocity.

The $T = 0$ phase diagram of S can be deduced by a straightforward extension of the methods of Ref. [13] and the $d = 1$ analysis of Affleck [25]; the results are summarized in Fig 3. In zero external field, there are quantum disordered and Néel ordered phases separated by a critical point at $t = t_c$. This critical point has $z = 1$. The quantum disordered phase has a gap Δ which vanishes near t_c as $\Delta \sim (t - t_c)^\nu$. For finite H the Néel ordered phase transforms into a second ordered phase in which the spin-condensate is preferentially oriented in the pN planes in which the field generates rotation. For the physical case $pN = 1$ this phase has XY order and is so identified in Fig 3. The transition between the finite H ordered phase and the quantum disordered phase occurs exactly at the field $H = H_c$ where the zero-field gap Δ equals gH . This quantum transition has $z = 2$ and is studied in some detail in a separate paper [26].

The $T \neq 0$, $H \neq 0$ properties of S are quite different for the cases $pN = 1$ and $pN > 1$. We discuss first the case $pN = 1$, which is summarized in Figs 4-6. The $T = 0$ XY order survives at finite temperature as quasi-long-range order. There is a Kosterlitz-Thouless transition from this state at a temperature T_{KT} to a fully disordered state. The dependence of T_{KT} on H depends crucially on the value of t . We found (See Figs 4-6)

$$k_B T_{KT} = \begin{cases} 2\pi\rho_s / \log(\rho_s/H) & t < t_c \\ \mathcal{K}gH & t = t_c \\ \frac{g(H - H_c)}{4} \frac{\log(\Lambda/(H - H_c))}{\log \log(\Lambda/(H - H_c))} & t > t_c \end{cases} \quad (4.15)$$

The result for $t < t_c$ can be deduced from the results of Nelson and Pelcovits [27] on a closely related model; here ρ_s is the fully renormalized spin stiffness of the ordered state of the $T = 0$, $H = 0$, sigma model. The situation for $t > t_c$ follows from the work of Popov [28], and is discussed in more detail elsewhere [26]. Our main focus here is on the $t = t_c$ case: the finite T , finite H properties can then be deduced by applying the scaling methods of this paper to the $z = 1$ critical point at $t = t_c$. The free-energy of the model continues to satisfy (3.3). The existence of a finite T Kosterlitz-Thouless transition implies that the function $\Omega(r)$ must be non-analytic at, say, $r = \mathcal{K}$: this leads to the result above for T_{KT} at $t = t_c$. Moreover as there are no non-universal factors in the scale of r , the number \mathcal{K} is *universal*.

The finite T properties for $pN > 1$ are simpler - there is no phase transition at any finite T . The windows of quantum-critical behavior with $z = 1$ (as in Fig 5) and $z = 2$ (as in Fig 6) are however still defined.

We will now present the $N = \infty$ computation of the universal function $\Omega(r)$ in the vicinity of the $T = 0$, $H = 0$ critical point at $t = t_c$. As the large N limit is taken with p fixed, we necessarily have $pN > 1$ and there is no finite temperature Kosterlitz Thouless

transition as in Fig 5. Nevertheless, from the insight gained in Ref. [13], we expect that our results for $\Omega(r)$ are reasonable accurate for the physical case $N = 3$, $p = 1$ provided $r \gg 1$ or $gH \gg k_B T$.

The technical steps in obtaining the $N = \infty$ free energy of S are quite similar to those in Ref. [13] - we will therefore be quite brief. We impose the length constraint on the n_a field by a Lagrange multiplier; at $N = \infty$ this Lagrange multiplier is frozen at its saddle-point value and gives a ‘mass’ m to the n_a field. The value of m is determined by solving the saddle point equation, which at $t = t_c$ is (using units in which $\hbar = k_B = c = 1$)

$$T \sum_{\omega_n} \int \frac{d^2 k}{4\pi^2} \left(\frac{1 - 2p}{k^2 + \omega_n^2 + m^2} + \frac{2p}{k^2 + (\omega_n - igH)^2 + m^2} \right) = \int \frac{d^3 q}{8\pi^3} \frac{1}{q^2} \quad (4.16)$$

It is easy to check that $m = 0$ is a solution at $T = H = 0$, confirming that the system is indeed at $t = t_c$. As in Ref. [13] it can be shown that the leading term in the solution for m is independent of the nature of the ultra-violet cutoff. Evaluating the frequency summations, and a subsequent momentum integration we find that (4.16) reduces to

$$(1 - 2p) \log(1 - e^{-\Theta}) + p \log(1 - e^{-\Theta-r}) + p \log(1 - e^{-\Theta+r}) = -\frac{\Theta}{2} \quad (4.17)$$

where

$$r = \frac{gH}{k_B T} \quad \Theta = \frac{m}{T} \quad (4.18)$$

The Eqn. (4.17) implicitly determines Θ as a function only of r .

The $N = \infty$ result for the free energy is

$$\frac{\mathcal{F}}{N} = \frac{T}{2} \sum_{\omega_n} \int \frac{d^2 k}{4\pi^2} \left((1 - 2p) \log(k^2 + \omega_n^2 + m^2) + 2p \log(k^2 + (\omega_n - igH)^2 + m^2) \right) - \frac{m^2}{2g} \quad (4.19)$$

We evaluate (4.19) using the methods of Ref. [13] and find (after reinserting factors of k_B , \hbar , c)

$$\mathcal{F}(H, T) = \mathcal{F}(0, 0) - N \frac{(k_B T)^3}{(\hbar c)^2} \Omega \left(\frac{gH}{k_B T} \right) \quad (4.20)$$

with

$$\Omega(r) = \frac{\Theta^3}{12\pi} - \frac{1}{2\pi} \int_{\Theta}^{\infty} y dy \left[(1 - 2p) \log(1 - e^{-y}) + p \log(1 - e^{-y-r}) + p \log(1 - e^{-y+r}) \right] \quad (4.21)$$

where Θ is also a function of r specified by (4.17). Exact evaluation of the integrals in $\Omega(r)$ is not possible, but we have obtained the following asymptotic results

$$\Omega(r) = \begin{cases} \frac{2\zeta(3)}{5\pi} + \frac{\sqrt{5}p}{2\pi} \log\left(\frac{\sqrt{5}+1}{2}\right) r^2 & r \rightarrow 0 \\ \frac{1}{12\pi} r^3 + \frac{p\pi}{12} r + \frac{p\zeta(3)}{2\pi} & r \rightarrow \infty \end{cases} \quad (4.22)$$

where ζ denotes the Reimann zeta function. In obtaining the above result we have used the non-trivial polylogarithm identities discussed in Ref. [29].

Results for the scaling functions for the specific heat and magnetization now follow as before and are plotted in Fig 7. The Wilson ratio (Eqn (3.8)) can be obtained by taking the appropriate ratio, and the results are shown in Fig 8. The scaling function has the asymptotic limits

$$\Omega_W(r) = \begin{cases} \frac{5\sqrt{5}p}{12\zeta(3)} \log\left(\frac{\sqrt{5}+1}{2}\right) & r \rightarrow 0 \\ \frac{3}{2p\pi^2} & r \rightarrow \infty \end{cases} \quad (4.23)$$

V. PHASE TRANSITIONS IN QUANTUM FERROMAGNETS

We now consider the application of the ideas of this paper to one of the very first models of quantum phase transitions that was considered by Hertz [1]: the zero temperature transition from ferromagnet to a paramagnet in an itinerant Fermi gas. The order parameter for this transition is clearly the local magnetization density, $m_a(x, \tau)$ ($a = 1, 2, 3$). This transition is special in that m_a has a dual role - it is also the conserved charge density associated with global spin rotation invariance.

The order parameter susceptibility

$$\chi(x, \tau) = \langle m_a(x, \tau) \cdot m_a(0, 0) \rangle \quad (5.1)$$

is expected to satisfy the following homogeneity relationship at the quantum fixed point

$$\chi'(x', \tau') = s^{d+z-2+\eta} \chi(x, \tau) \quad (5.2)$$

This relationship defines the value of the critical exponent η . The scaling dimension of m_a is then immediately fixed at $(d+z-2+\eta)/2$. However, m_a is a conserved charge density, and below the upper critical dimension its scaling dimension must be precisely d . Equating the two scaling dimensions we get one of our main results

$$z = d + 2 - \eta \quad (5.3)$$

Thus the three independent exponents z, η, ν have been reduced for the paramagnet-ferromagnet transition to just two - the values of z and η are no longer independent.

It is not difficult to see that Hertz's simple paramagnon model in fact violates the exponent equality (5.3) below its upper critical dimension. In his model

$$z = 3 + \mathcal{O}(\epsilon^2) \quad \eta = 0 + \mathcal{O}(\epsilon^2) \quad (5.4)$$

where $\epsilon = 1 - d$ is the deviation from the upper critical dimension. It is clear that these relationships are inconsistent with (5.3) at order ϵ .

We believe that this discrepancy can be traced to a more basic difficulty with Hertz's effective action: the incomplete treatment of the Ward identity (2.22) associated with total spin conservation. In the vector-formulation (equivalent to our m_a) of the effective action there clearly must be cubic terms present if (2.22) is satisfied; such terms are absent in Hertz's treatment. Hertz also has a scalar-field formulation in which no such cubic terms will arise; however the full symmetry of the effective action is then hidden, and one cannot expect a proper treatment of the critical phenomena.

A complete analysis of this problem clearly requires a more detailed consideration of the effective action of paramagnons, including the effect of cubic paramagnon vertex Γ . A preliminary analysis along these lines suggests that the identification of the upper critical dimension of $d = 1$ is incorrect.

VI. CONCLUSIONS

This paper has discussed the theory of the non-linear response to an external field, H , of a bulk quantum system in the finite temperature *quantum-critical* [11,5,12,13] region of a zero temperature, second-order phase transition. In particular, we have considered the case where H couples to a conserved charge. For such a field, we obtained the general result that the scaling dimension of H is equal to that of $k_B T$, even in the absence of hyperscaling. This result is encapsulated in the scaling form (3.3). We also introduced a generalized Wilson ratio (3.8) associated with the non-linear response, and argued that it was a fully universal function of $H/k_B T$. These principles were illustrated by calculations on some model systems.

Tsvetik and collaborators [7,8] have also recently studied the non-linear field dependence of the thermodynamics of heavy-fermion alloys. However they did not consider the special consequences of having a total conserved spin. The experimental data appear to indicate that the scaling dimension of H is unequal to that of $k_B T$ [7]. Using our results we may then conclude that any theory with a conserved total spin (some of the speculative proposals in Ref. [8] have a conserved spin) cannot explain the data. Spin-orbit scattering from the impurity sites must be included in an essential way in the final theory.

ACKNOWLEDGMENTS

I am grateful to B. Delamott and A. Georges for hospitality at the University of Paris and Ecole Normale while this work was carried out. This work grew out of an earlier collaboration with A. Chubukov [12], and I benefited from helpful discussions with him. I thank T. Senthil for many useful discussions and for assistance with some of the technical computations in Section IV D, and N. Read and R. Shankar for helpful comments on the manuscript. This work has been supported by NSF Grant DMR-9224290.

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FIGURES

FIG. 1. The universal scaling function Ω_M and Ω_C for the magnetization and specific heat (Eqn (3.7)) for the Bhatt-Lee model with $\alpha = 0.6$. The functions are obtained by taking appropriate derivatives of (4.8). The coordinate $r = gH/(k_B T)$.

FIG. 2. The universal scaling function Ω_W for the Wilson ratio (Eqn (3.8)) for the Bhatt-Lee model with $\alpha = 0.6$.

FIG. 3. Ground states of the $2 + 1$ dimensional $O(N)$ sigma model in a magnetic field H described by the action (4.14). We have specialized to $N = 3$, $p = 1/3$. The coupling t measures the strength of the quantum fluctuations. The $H = 0$ critical point at $t = t_c$ has the dynamic critical exponent $z = 1$. The line separating the quantum-disordered and XY ordered phases represents second-order transitions with $z = 2$. This phase boundary approaches $H = 0$ as $H \sim (t - t_c)^\nu$ where ν is correlation length exponent of the classical Heisenberg ferromagnet in three dimensions.

FIG. 4. Finite temperature properties of the model of Fig 3 for $t < t_c$. There is a Kosterlitz-Thouless transition at T_{KT} separating a phase with algebraic XY order from complete disorder. The dependence of T_{KT} on H at small H can be deduced from the results of Ref. [27]; here ρ_s is the fully renormalized spin stiffness of the Heisenberg order at $T = 0$, $H = 0$.

FIG. 5. Finite temperature properties of the model of Fig 3 for $t = t_c$. The number \mathcal{K} is universal. The small T, H properties are described by the $z = 1$ critical point at $T = 0$, $H = 0$, $t = t_c$ and obey the scaling form (3.3). The scaling function $\Omega(r)$ has a singularity at $r = \mathcal{K}$.

FIG. 6. Finite temperature properties of the model of Fig 3 for $t > t_c$. The physics of this phase diagram is discussed in some detail in Ref. [26]. The dashed line represents a crossover, while the full line is a Kosterlitz-Thouless transition. The functional form of T_{KT} is deduced from Ref. [28].

FIG. 7. The universal scaling function Ω_M and Ω_C for the magnetization and specific heat (Eqn (3.7)) for the $O(N)$ model in a field (4.14) at $t = t_c$. The results are obtained in the large N limit and plotted for $N = 3$, $p = 1/3$. The scaling functions are obtained by taking appropriate derivatives of (4.17,4.21). The coordinate $r = gH/(k_B T)$. The actual scaling function for $pN = 1$ will have a weak singularity at $r = \mathcal{K}$ (corresponding to the Kosterlitz-Thouless transition of Fig 5) which does not appear in the large N calculation.

FIG. 8. As in Fig 7, but with the results for the scaling function Ω_W for the fully universal Wilson ratio (Eqn (3.8)). The asymptotic limits of Ω_W are given in Eqn (4.23).















