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Gradient critical phenomena in the Ising quantum chain

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Abstract

We consider the behaviour of a critical system in the presence of a gradient perturbation of the couplings. In the direction of the gradient an interface region separates the ordered phase from the disordered one. We develop a scaling theory for the density profiles induced by the gradient perturbation which involves a characteristic length given by the width of the interface region. The scaling predictions are tested in the framework of the mean-field Ginzburg–Landau theory. Then we consider the Ising quantum chain in a linearly varying transverse field which corresponds to the extreme anisotropic limit of a classical two-dimensional Ising model. The quantum Hamiltonian can be diagonalized exactly in the scaling limit where the eigenvalue problem is the same as for the quantum harmonic oscillator. The energy density, the magnetization profile and the two-point correlation function are studied either analytically or by exact numerical calculations. Their scaling behaviour is in agreement with the predictions of the scaling theory.

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1. Introduction

Inhomogeneities may have a strong influence on the properties of a system in the vicinity of a second-order phase transition. Actually this influence will depend on the relevance of the perturbation introduced by the inhomogeneity (see [1] for a review). A relevant inhomogeneity may change the universality class of the system or even suppress the critical point as, for instance, in a finite-size system [2]. The critical behaviour may be altered by the presence of quenched disorder [3] or aperiodic modulation of the couplings [4, 5]. It will be modified locally (i.e., within a correlation length) at a flat free surface, at a corner [6–12] or at the tip of a parabolic-shape system [1, 13]. Line defects may have also some influence on the local critical behaviour [1, 14–16]. One may mention the case of films where the presence

of boundaries, by breaking translation invariance, leads to the formation of specific profiles [17–24].

Other types of inhomogeneities are linked to the application of external fields like magnetic, gravitational or thermal fields. These fields influence the behaviour of physical quantities like the magnetization, the particle or the energy density in the vicinity of the homogeneous system critical point. One should first mention an early work on the xy-quantum chain in a linearly varying z-field [25] for which exact results were obtained in different scaling limits. Phase coexistence induced by antiparallel magnetic fields at the surfaces of a film was studied in [26–30]. The effect of gravity was considered in [28–30] where it was found that it restores two-phase coexistence up to the bulk critical point, above the wetting temperature. The effect of a temperature gradient on an interface at equilibrium was considered in [31] for a symmetric binary system below its critical point. Phase separation induced by temperature gradients was studied in [32–34]. The effect of temperature gradients on interfacial premelting was considered in [35].

The influence of inhomogeneities on the critical behaviour was also considered in a series of works on gradient percolation [36–40] where the perturbation was introduced as a tool allowing for high-precision estimates of the percolation threshold and the percolation exponents.

In this work we begin with a presentation of the scaling theory for the density profiles in the presence of gradient field inhomogeneities. Specifically, we consider a system with a deviation from the critical coupling which varies linearly in one space direction. The coupling is at its critical value in the middle of the system where an interface region separates the ordered phase on the left from the disordered phase on the right. We test the validity of the scaling arguments, first at the mean-field level, within Ginzburg–Landau theory. Then we present a study of the Ising quantum chain in a linearly varying transverse field, $h_l = 1 + gl$, which corresponds to the extreme anisotropic limit of the two-dimensional classical Ising model with a linear variation of the couplings. We work in the scaling limit where the size L of the system goes to infinity while the gradient g goes to zero with the product gL held fixed. The excitation spectrum of the inhomogeneous Ising quantum chain is obtained exactly in terms of the solution of an harmonic oscillator eigenvalue problem. The knowledge of the eigenvectors allows us to obtain the energy density profile, the magnetization profile and the behaviour of the spin–spin correlation function. Their scaling forms are in complete agreement with the results of the scaling theory.

The paper is organized as follows: in section 2 we present a scaling analysis for the density profiles which is confirmed in section 3 in the framework of a mean-field approximation. Section 4 deals with the study of the Ising quantum in a linearly varying transverse field. First, the form of the quantum Hamiltonian is deduced from the classical Ising problem. Then the Hamiltonian is diagonalized exactly in the scaling limit. In the following subsections, analytical and numerical results for the energy density, the magnetization profile and the correlation function are confronted to the results of the scaling theory. We summarize our results in the last section.

2. Scaling arguments

Let us consider a critical system perturbed by a constant gradient g along the z-direction, such that the deviation from the critical coupling is given by

$$K(z) - K_c = -\Delta(z) = -gz, \qquad g > 0. \tag{2.1}$$

Thus around the origin there is an interface between the ordered phase on the left-hand side where $\Delta < 0$ and the disordered phase on the right side where $\Delta > 0$. Let ℓ denote the width of this interface. If the system is infinite ℓ is expected to depend on g only and to diverge when g vanishes.

Under a change of the length scale by a factor b, the thermal perturbation $\Delta(z)$ with scaling dimension $y_t = 1/\nu$, where ν is the correlation length exponent, transforms as

$$g'z' = b^{1/\nu} gz = g' \frac{z}{b}, \tag{2.2}$$

so that

$$g' = b^{1+1/\nu} g. \tag{2.3}$$

The interface width transforms as

$$\ell' = \ell(g') = \frac{\ell}{b} = \ell(b^{1+1/\nu} g), \tag{2.4}$$

with $b = g^{-\nu/(1+\nu)}$, one finally obtains

$$\ell \propto g^{-\nu/(1+\nu)}, \tag{2.5}$$

for the typical length introduced by the thermal gradient g.

The same result can be obtained self-consistently [36] by noting that with the width ℓ is associated a typical deviation from the critical coupling $\Delta(\ell) = g\ell$ from which a characteristic length $[\Delta(\ell)]^{-\nu}$ can be constructed. Since the only length in the problem is the interface width, ℓ, it satisfies

$$\ell \propto (g\ell)^{-\nu}. \tag{2.6}$$

Solving for ℓ, one immediately recovers (2.5).

Let us now study the influence of the thermal gradient on the scaling behaviour of the density φ with scaling dimension x_φ. This density can be the magnetization density m or the singular part of the energy density e. In the perturbed critical system it is a function $\varphi(z, \ell)$ or, alternatively, according to (2.5), a function $\varphi(z, g)$ transforming as

$$\varphi' = \varphi(z', g') = b^{x_\varphi} \varphi(z, g) \tag{2.7}$$

under a change of scale, so that

$$\varphi(z, g) = b^{-x_\varphi} \varphi\left(\frac{z}{b}, b^{1+1/\nu} g\right). \tag{2.8}$$

With $b = g^{-\nu/(1+\nu)} \propto \ell$ one obtains the scaling form

$$\varphi(z, g) = g^{\nu x_\varphi/(1+\nu)} \Phi[g^{\nu/(1+\nu)} z]. \tag{2.9}$$

One may note that, according to (2.5), the prefactor in (2.9) exhibits the finite-size behaviour $\varphi \propto \ell^{-x_\varphi}$ expected for a critical system with a transverse size ℓ.

For a magnetic system the magnetization density, $m(z, g)$, with scaling dimension $x_\mathrm{m} = \beta/\nu$, is non-vanishing in the ordered region $z < 0$, and one expects the same local critical behaviour as for the homogeneous system at the same value of the coupling, i.e.,

$$m(z, g) \propto |\Delta(z)|^\beta \propto |gz|^{\nu x_\mathrm{m}}, \qquad z < 0. \tag{2.10}$$

for not too large values of $|\Delta(z)|$. Here and in the following, we suppose that $m(z, g) \geqslant 0$. Comparing (2.10) to (2.9) with $\varphi = m$, one obtains the form of the scaling function in this region:

$$\Phi_\mathrm{m}(u) \sim |u|^{\nu x_\mathrm{m}}, \qquad u < 0. \tag{2.11}$$

Just at the interface one expects $\Phi_{\rm m}(0) = \text{const} \neq 0$, so that the local magnetization is non-vanishing and behaves as the prefactor in (2.9), displaying the finite-size behaviour $m(0, g) \propto \ell^{-x_{\rm m}}$. Since $m(z, g) > m(0, g)$ when $z < 0$, the scaling behaviour given in equations (2.10) and (2.11) is valid only when $|gz|^{\nu x_{\rm m}} > \ell^{-x_{\rm m}}$. Using (2.5), this translates into $z < -\ell$.

On the right-hand side of the interface, in the weak-coupling region, the magnetization density is expected to display the same exponential decay as the two-point correlation function $\Gamma(z) = \langle m(0)m(z)\rangle$. For a homogeneous system in its disordered phase, with a constant deviation Δ from the critical coupling, one has

$$\Gamma(z) \sim \exp\left(-\text{const}\,\frac{z}{\xi}\right) \sim \exp\left(-\text{const}\,\frac{z}{\Delta^{-\nu}}\right), \qquad z \gg \xi, \tag{2.12}$$

where ξ is the correlation length. Assuming the same behaviour for the inhomogeneous system, with the correlation length taking a value governed by the local deviation from the critical point, $\xi \propto [\Delta(z)]^{-\nu}$, one obtains [13]

$$m(z, g) \sim \exp(-\text{const}\, g^{\nu} z^{1+\nu}). \tag{2.13}$$

Equations (2.9) and (2.13) give the form of the scaling function for the order parameter when $z \gg 0$:

$$m(z, g) = g^{\nu x_{\rm m}/(1+\nu)} \Phi_{\rm m}[g^{\nu/(1+\nu)} z], \qquad \Phi_{\rm m}(u) \sim \exp(-\text{const}\, u^{1+\nu}). \tag{2.14}$$

The same type of arguments leads to the scaling behaviour of the singular part of the energy density:

$$e(z, g) = g^{\nu x_{\rm e}/(1+\nu)} \Phi_{\rm e}[g^{\nu/(1+\nu)} z], \qquad \Phi_{\rm e}(u) \sim \exp(-\text{const}\,|u|^{1+\nu}), \tag{2.15}$$

for both sides of the interface. Here $x_{\rm e} = d - 1/\nu$ is the scaling dimension of the energy density.

The two-point correlation function, with scaling dimension $2x_{\rm m}$, can also be written under the scaling form

$$\Gamma(z, g) = g^{2\nu x_{\rm m}/(1+\nu)} \Phi_{\Gamma}[g^{\nu/(1+\nu)} z], \tag{2.16}$$

with the exponential decay, $\Phi_{\Gamma}(u) \sim \exp(-\text{const}\, u^{1+\nu})$, for the connected part, $\Gamma_{\rm c}(z, g) = \Gamma(z, g) - \langle m(0)\rangle\langle m(z)\rangle$.

3. Mean-field theory

In order to check our scaling assumptions, let us now study the gradient perturbation problem in mean-field theory. With a scalar order parameter m and up–down symmetry, the Ginzburg–Landau free energy functional of the critical system perturbed by the gradient term reads

$$G[m] = G[0] + \int_V \left[\frac{C}{2}(\nabla m)^2 + \frac{\Delta(z)}{2} m^2 + \frac{B}{4} m^4 - Hm\right] \mathrm{d}V, \tag{3.1}$$

where B and C are positive constants. The first term is the energy contribution coming from inhomogeneities. The quadratic term is the thermal gradient perturbation with, as before, $\Delta(z) = gz$ and $g > 0$. The quartic term ensures the stability of the system in the ordered region for $z < 0$. The last term gives the interaction with the external field H.

In the mean-field approximation the equilibrium value of the order parameter minimizes $G[m]$. Thus the variation of the free energy, δG, vanishes to first order in δm. This leads to the Ginzburg–Landau equation

$$-C\frac{\mathrm{d}^2 m}{\mathrm{d}z^2} + gzm(z) + Bm^3(z) = 0, \tag{3.2}$$

where it was assumed that $H = 0$ and that translation invariance is broken only in the z-direction.

Introducing the dimensionless variable, $\zeta = z/\ell$, the Ginzburg–Landau equation can be rewritten as

$$-\frac{C}{\ell^2}\frac{\mathrm{d}^2 m}{\mathrm{d}\zeta^2} + g\ell\zeta m(\zeta) + Bm^3(\zeta) = 0. \tag{3.3}$$

The coefficients of $\mathrm{d}^2 m/\mathrm{d}\zeta^2$ and $m(\zeta)$ have to scale in the same way. Thus $C/\ell^2 \propto g\ell$ and the interface width has the following scaling behaviour:

$$\ell \simeq \left(\frac{C}{g}\right)^{1/3} \propto g^{-\nu/(1+\nu)}, \tag{3.4}$$

since $\nu = 1/2$ in mean-field theory.

In the ordered region, for $z \ll -\ell$ or $\zeta \ll -1$ in (3.3), one can neglect the second derivative which is much smaller than the next term in the Ginzburg–Landau equation (3.2) so that we obtain

$$m(z, g) \simeq \left(\frac{-gz}{B}\right)^{1/2}, \tag{3.5}$$

which confirms the scaling prediction (2.10) since here $\beta = \nu x_{\mathrm{m}} = 1/2$.

The order parameter is very small for $z \gg 0$, and the cubic term in (3.2) can be neglected. With the change of variable $u = z(g/C)^{1/3}$ one obtains the Airy equation

$$\frac{\mathrm{d}^2 m}{\mathrm{d}u^2} - um(u) = 0. \tag{3.6}$$

The order parameter is then given by $m(z, g) \propto \mathrm{Ai}(u)$ with the leading asymptotic behaviour

$$m(z, g) \sim \exp(-\mathrm{const}\, u^{3/2}) \sim \exp(-\mathrm{const}\, g^{1/2} z^{3/2}), \tag{3.7}$$

when $z \gg 0$ in agreement with equation (2.14) with $\nu = 1/2$.

4. Ising quantum chain in a linearly varying transverse field

4.1. Quantum Hamiltonian

Let us consider the two-dimensional classical nearest-neighbour Ising model on a square lattice with vertical couplings $K_1(l)$ varying in the horizontal direction ($-L/2 < l < L/2$) and constant horizontal couplings K_2. The partition function can be written as

$$Z \propto \mathrm{Tr}\, \mathcal{T}^M, \tag{4.1}$$

where M is the number of horizontal rows and $\mathcal{T}$ is the row-to-row transfer matrix given by [41, 42]

$$\mathcal{T} = \exp\left[\sum_l K_1^*(l)\sigma_l^z\right] \exp\left[\sum_l K_2 \sigma_l^x \sigma_{l+1}^x\right]. \tag{4.2}$$

$\sigma^{x,z}$ are Pauli spin operators, $K_1^*(l) = -1/2 \ln \tanh[K_1(l)]$ is the dual of the vertical coupling and it is assumed to vary as

$$K_1^*(l) = K_1^*(1 + gl), \qquad g \geqslant 0. \tag{4.3}$$

In the extreme anisotropic limit [43–45] $K_1 \to \infty$ (so that $K_1^* \to 0$) and $K_2 \to 0$ while keeping the ratio $h = K_1^*/K_2$ constant, the transfer matrix $\mathcal{T}$ can be rewritten as

$$\mathcal{T} = 1 - 2K_2\mathcal{H}. \tag{4.4}$$

$\mathcal{H}$ is the Hamiltonian of the Ising quantum chain in a transverse field [46] and takes the following form:

$$\mathcal{H} = -\frac{1}{2}\sum_{l=-L/2}^{L/2-1}\sigma_l^x\sigma_{l+1}^x - \frac{1}{2}\sum_{l=-L/2}^{L/2} h_l\sigma_l^z, \qquad h_l = h(1+gl), \tag{4.5}$$

where $g = \theta/L$ with $\theta \geqslant 0$.

In the homogeneous case, $g = 0$, the system is self-dual and critical at $h = 1$ in the thermodynamic limit $L \to \infty$. For $h < 1$, the system is ordered with $\langle\sigma^x\rangle \neq 0$ whereas $\langle\sigma^x\rangle = 0$, when $h > 1$.

The perturbed system is assumed to be critical when $\theta = 0$ so that $h = 1$ in (4.5) and $h_l = 1 + \theta l/L = 1 + gl$. In order to keep $h_l \geqslant 0$, one has to take $\theta \leqslant 2$. The transverse field is smaller (greater) than its critical value on the left-hand side (right) of the origin. Thus, in the thermodynamic limit, the quantum chain is ordered for $l < 0$, and the value of the order parameter decreases to zero when $l \to +\infty$.

4.2. Diagonalization

After a Jordan–Wigner transformation [47], the Hamiltonian (4.5) becomes a quadratic form in fermion creation and annihilation operators which is diagonalized through a canonical transformation [46, 48] leading to

$$\mathcal{H} = \sum_{q=0}^{L}\varepsilon_q\left(\eta_q^\dagger\eta_q - \frac{1}{2}\right). \tag{4.6}$$

$\eta_q^\dagger$ (η_q) are diagonal fermion creation (annihilation) operators and ε_q are the energies of the fermionic excitations. They satisfy the following set of equations:

$$\mathsf{A}\psi_q = \varepsilon_q\phi_q, \qquad \mathsf{A}^\dagger\phi_q = \varepsilon_q\psi_q, \tag{4.7}$$

where

$$\mathsf{A} = \begin{pmatrix} -h_{-L/2} & 0 & 0 & 0 & 0 \\ 1 & -h_{-L/2+1} & 0 & 0 & 0 \\ & \ddots & \ddots & & \\ 0 & 0 & 1 & -h_{L/2-1} & 0 \\ 0 & 0 & 0 & 1 & -h_{L/2} \end{pmatrix} \tag{4.8}$$

and $\mathsf{A}^\dagger$ is the transposed matrix. According to (4.7), the normalized eigenvectors, ϕ_q and ψ_q, are solutions of the following eigenvalue equations:

$$\mathsf{A}\mathsf{A}^\dagger\phi_q = \varepsilon_q^2\phi_q, \qquad \mathsf{A}^\dagger\mathsf{A}\psi_q = \varepsilon_q^2\psi_q. \tag{4.9}$$

In the bulk of the system these eigenvalue equations can be written as

$$\begin{aligned} &h_{l-1}\phi_q(l-1) + \left[\varepsilon_q^2 - 1 - h_l^2\right]\phi_q(l) + h_l\phi_q(l+1) = 0, \\ &h_l\psi_q(l-1) + \left[\varepsilon_q^2 - 1 - h_l^2\right]\psi_q(l) + h_{l+1}\psi_q(l+1) = 0. \end{aligned} \tag{4.10}$$

Introducing the scaling variable $u = g^{1/2}l$, the difference equations in (4.10) can be expanded in the scaling limit where $L \to \infty$ and $g \to 0$ in such a way that the product, $gL = \theta$, is held fixed. Up to terms of the first order in g the expansions lead to the following harmonic oscillator eigenvalue equations:

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}u^2} + \left[\left(\frac{\varepsilon}{g^{1/2}}\right)^2 - 1 - u^2\right]\phi(u) = 0, \qquad \frac{\mathrm{d}^2\psi}{\mathrm{d}u^2} + \left[\left(\frac{\varepsilon}{g^{1/2}}\right)^2 + 1 - u^2\right]\psi(u) = 0. \tag{4.11}$$

With the boundary conditions $\phi(\pm\infty) = \psi(\pm\infty) = 0$, one obtains

$$\psi_n(u) = C_n\, \mathrm{e}^{-u^2/2} H_n(u), \quad \phi_{n+1}(u) = \psi_n(u), \quad \varepsilon_n = \sqrt{2ng}, \quad n = 0, 1, 2, \ldots, \tag{4.12}$$

where $H_n(u)$ is the Hermite polynomial of order n and $C_n = (g/\pi)^{1/4}(2^n n!)^{-1/2}$ is a normalization factor.

One may note that in the bulk, according to (4.8), the operators A and $\mathsf{A}^\dagger$ satisfy the commutation relation

$$[\mathsf{A}, \mathsf{A}^\dagger] = g\mathsf{C}, \qquad \mathsf{C}_{l,m} = \delta_{l-1,m} + \delta_{l+1,m}. \tag{4.13}$$

Introducing the normalized operators, $\mathsf{a} = \mathsf{A}/\sqrt{2g}$ and $\mathsf{a}^\dagger = \mathsf{A}^\dagger/\sqrt{2g}$, in (4.13) and applying the commutator to a test function, in the scaling limit one obtains the canonical bosonic commutation relation:

$$[\mathsf{a}, \mathsf{a}^\dagger] = 1 + \mathrm{O}(g). \tag{4.14}$$

Thus, once normalized in the same way, the equations in (4.7) correspond to the lowering and raising operations on the eigenstates ψ_n and ϕ_n of the harmonic oscillator.

The eigenstate $\phi_0(u)$, associated with the excitation ε_0 which is vanishing in the scaling limit, cannot be obtained from the harmonic oscillator equation since it is incompatible with the boundary condition at $-\infty$. It corresponds to a mode which is localized in the vicinity of the left boundary (we consider open boundary conditions) and which is related to the presence of a non-vanishing magnetization m_s at the left boundary of the system [50, 51]. In order to obtain the form of this localized mode and the actual value of the corresponding excitation, one has to come back to the original finite-size system with open boundary conditions. It can be shown that, when it vanishes faster than $1/L$, the lowest excitation is given by [52–54]

$$\varepsilon_0 \simeq m_\mathrm{s} m_\mathrm{s}^*, \tag{4.15}$$

where m_s^* is the magnetization of the dual chain at the left boundary. m_s and m_s^* are equal to the component $\phi_0(-L/2)$ of the normalized eigenvector and can be deduced from the second equation in (4.7) with $\varepsilon_0 = 0$. These boundary magnetizations take the following forms [50]:

$$m_\mathrm{s} = \left[1 + \sum_{k=-L/2}^{L/2} \prod_{l=-L/2}^{k} h_l^2\right]^{-1/2}, \qquad m_\mathrm{s}^* = \left[1 + \sum_{k=-L/2}^{L/2} \prod_{l=-L/2}^{k} h_l^{-2}\right]^{-1/2}. \tag{4.16}$$

With $h_l = 1 + gl$ it is straightforward to show that m_s is O(1) whereas the dual magnetization is exponentially small:

$$m_\mathrm{s}^* \simeq \left(\frac{g}{\pi}\right)^{1/4} \exp\left(-\frac{gL^2}{8}\right). \tag{4.17}$$

As a consequence, the smallest excitation vanishes exponentially with the size of the system as

$$\varepsilon_0 \sim \mathrm{e}^{-gL^2/8}. \tag{4.18}$$

Using the second equation in (4.7) with $\varepsilon_0 \sim 0$, one obtains

$$\phi_0(-L/2 + l) \simeq \phi_0(-L/2)\, \mathrm{e}^{-l/l_0}, \qquad l_0^{-1} = |\ln(1 - gL/2)|. \tag{4.19}$$

The localization length l_0 diverges as $(\theta/2)^{-1}$ when the local deviation from the critical transverse field, $\theta/2 = 1 - h_{-L/2}$, vanishes. It behaves as the local correlation length since $\nu = 1$ for the Ising quantum chain. In the scaling limit $g \to 0$ and $L \to \infty$ while $\theta = gL$ remains constant; thus the localization length l_0 also remains constant and the localized mode, $\phi_0(u)$, has a vanishing amplitude in the bulk.

This completes the diagonalization of the model in the continuum limit.

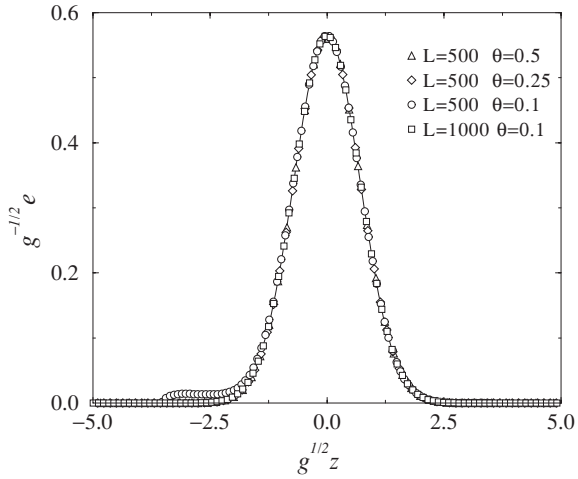

Figure 1. Rescaled energy density profiles for different chain sizes L and θ values. The corresponding values of the gradient are $g = 1 \times 10^{-3}, 5 \times 10^{-4}, 2 \times 10^{-4}, 1 \times 10^{-4}$ from top to bottom in the legend. The solid line is the analytic result in (4.24).

4.3. Energy density profile

Let us consider the connected autocorrelation function in imaginary time

$$G_{\mathrm{e}}(l,\tau) = \left\langle \sigma_l^z(\tau)\sigma_l^z \right\rangle - \left\langle \sigma_l^z \right\rangle^2, \tag{4.20}$$

where $\sigma_l^z(\tau) = \mathrm{e}^{\tau\mathcal{H}}\sigma_l^z\,\mathrm{e}^{-\tau\mathcal{H}}$. It can be rewritten as the eigenstate expansion

$$G_{\mathrm{e}}(l,\tau) = \sum_{i>0} \left|\langle \mathrm{i}|\sigma_l^z|0\rangle\right|^2 \mathrm{e}^{-\tau(E_i-E_0)}, \tag{4.21}$$

where $|0\rangle$ is the ground state of $\mathcal{H}$ with eigenvalue E_0 and $|\mathrm{i}\rangle$ an excited state with eigenvalue E_i. Since the operator σ_l^z is a two-fermion operator, the only non-vanishing matrix elements in the expansion are the two-fermion states $|\mathrm{i}\rangle = \eta_q^\dagger\eta_p^\dagger|0\rangle$. When $\tau \to \infty$, the amplitude of the dominant term defines the off-diagonal energy density

$$e(l) = \left|\langle \epsilon|\sigma_l^z|0\rangle\right|, \tag{4.22}$$

where $|\epsilon\rangle = \eta_1^\dagger\eta_0^\dagger|0\rangle$ is the first even excited state. The expansion of σ_l^z in terms of diagonal fermions leads to [56]

$$e(l) = |\psi_1(l)\phi_0(l) - \psi_0(l)\phi_1(l)|. \tag{4.23}$$

Inserting (4.12) into (4.23), one finally obtains the Gaussian profile:

$$e(l) = |\psi_0(l)|^2 = \sqrt{\frac{g}{\pi}}\exp(-gl^2), \tag{4.24}$$

which is in agreement with the form (2.15) deduced from scaling considerations since $\nu = x_{\mathrm{e}} = 1$ in the Ising model.

In order to reduce the boundary effects due to the localized mode, one has to consider sizes $L \gg l_0 \sim \theta^{-1}$ for small θ. Typically, for $\theta = 0.1, l_0 \simeq 20$ and taking $L > 10 \times l_0$ is sufficient to suppress the localized mode effect. The behaviour of the off-diagonal energy density, deduced from (4.23) through numerically exact diagonalization for chains of size up to $L = 1000$, is shown in figure 1. An excellent agreement with the analytic result in (4.24) is obtained.

4.4. Magnetization profile

Due to the Z_2 symmetry of the Hamiltonian, the ground state expectation value of σ_l^x identically vanishes. In order to obtain the magnetization profile one has to break this symmetry. Since the ground state $|0\rangle$ is asymptotically degenerate with the lowest one-fermion state $|\sigma\rangle = \eta_0^+|0\rangle$ such that $E_\sigma - E_0 = \varepsilon_0 \simeq 0$, one can construct the state

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |\sigma\rangle) \tag{4.25}$$

and take the expectation value of σ_l^x in that state which leads to[1]

$$m(l) = \langle +|\sigma_l^x|+\rangle = \langle \sigma|\sigma_l^x|0\rangle. \tag{4.26}$$

One may also note that the imaginary time autocorrelation function has the following asymptotic behaviour:

$$\lim_{\tau\to\infty} G_m(l,\tau) = m^2(l) = \langle \sigma|\sigma_l^x|0\rangle^2, \tag{4.27}$$

which is another way to justify the use of the off-diagonal matrix element for the magnetization profile.

Rewriting σ_l^x in terms of diagonal fermions and using Wick's theorem, the local magnetization can be expressed as a determinant [55]:

$$m(l) = \begin{vmatrix} H_{-L/2} & G_{-L/2,-L/2} & G_{-L/2,-L/2+1} & \dots & G_{-L/2,l-1} \\ H_{-L/2+1} & G_{-L/2+1,-L/2} & G_{-L/2+1,-L/2+1} & \dots & G_{-L/2+1,l-1} \\ \vdots & \vdots & \vdots & & \vdots \\ H_{l-1} & G_{l-1,-L/2} & G_{l-1,-L/2+1} & \dots & G_{l-1,l-1} \\ H_l & G_{l,-L/2} & G_{l,-L/2+1} & \dots & G_{l,l-1} \end{vmatrix}, \tag{4.28}$$

where

$$H_j = \phi_0(j), \qquad G_{j,k} = -\sum_{n=0}^{L} \phi_n(j)\psi_n(k). \tag{4.29}$$

Figure 2 shows the rescaled magnetization profile obtained for chain sizes up to $L = 1000$ and different values of θ. The numerical results are in excellent agreement with the scaling behaviour of equation (2.14) with $\nu = 1$ and $x_{\rm m} = 1/8$ for the Ising quantum chain in a transverse field.

In order to test the scaling assumption (2.10), $m^{1/(\nu x_{\rm m})} = m^8$ is plotted as a function of gz in figure 3. The spontaneous magnetization of the homogeneous Ising chain varies as $m = (1-h^2)^{1/8}$ as a function of the transverse field [46] for $h \leqslant 1$. Replacing h by its local value $h(z) = 1 + gz$ in the inhomogeneous system, one obtains $[m(z,g)]^8 = -2gz - g^2z^2$ for $z < 0$ in very good agreement with the numerical data. One may note that the second term in this expression does not fit with the scaling form which follows from (2.9), but this term becomes negligible in the scaling limit where $g \to 0$ as may be verified in figure 3.

Figure 4 shows the behaviour of the rescaled magnetization profile in the disordered region on a linear-logarithmic scale in order to check the exponential decay, $\exp(-\text{const}\, gz^2)$, expected from equation (2.14). The exact numerical results are once again in quite good agreement with the expected scaling behaviour.

[1] More generally, with the linear combination $|\alpha\rangle = \frac{|0\rangle+\alpha|\sigma\rangle}{\sqrt{1+\rho^2}}$, where $\alpha = \rho\, e^{i\theta}$, one obtains $\langle\alpha|\sigma_l^x|\alpha\rangle = \frac{2\rho\cos\theta}{1+\rho^2}\langle\sigma|\sigma_l^x|0\rangle$ which is maximum for $\alpha = 1$ when $\langle\alpha|\sigma_l^x|\alpha\rangle = \langle\sigma|\sigma_l^x|0\rangle$.

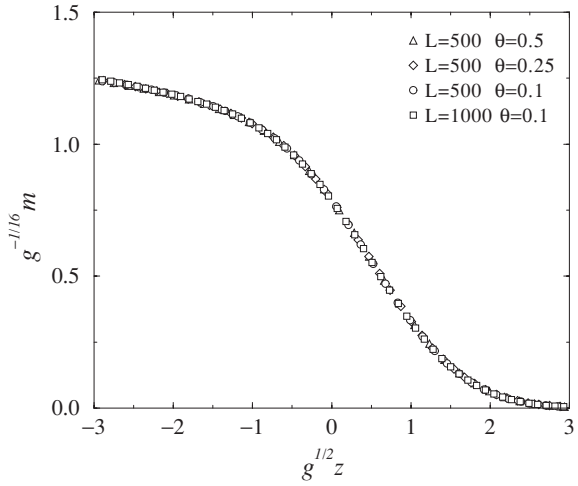

Figure 2. Rescaled magnetization profiles for different chain sizes L and θ values. The values of the gradient are the same as in figure 1.

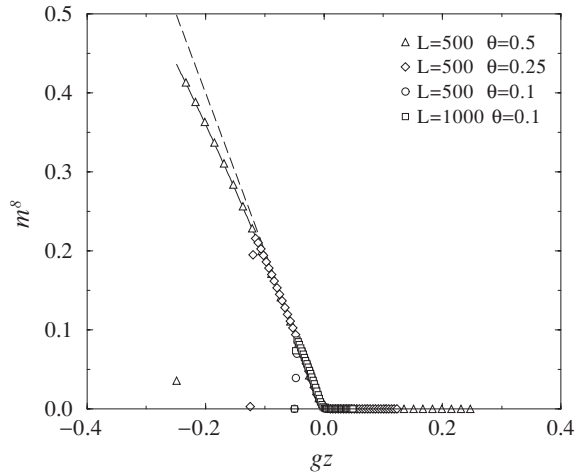

Figure 3. Behaviour of the magnetization profile for $z < 0$. The dashed line gives $m^8 = -2gz$, the behaviour expected from equation (2.10), valid in the scaling limit where $g \to 0$. The solid line corresponds to $m^8 = -2gz - g^2z^2$ (see text). The values of the gradient are the same as in figure 1.

4.5. Correlation functions

The correlation between a spin at l and the central spin is measured by the correlation function,

$$\Gamma(l) = \langle 0|\sigma_0^x \sigma_l^x|0\rangle, \tag{4.30}$$

given by the determinant [46]

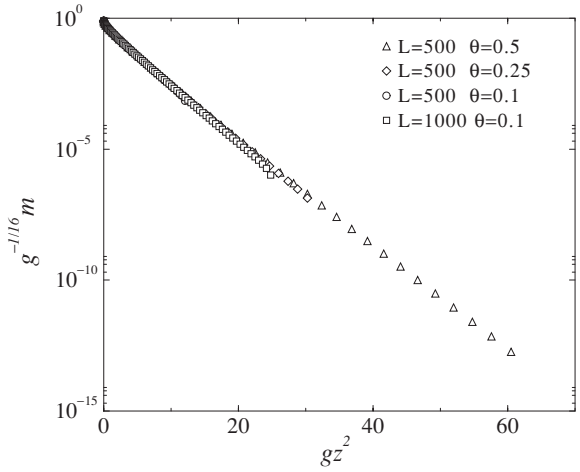

Figure 4. Semi-logarithmic plot of the rescaled magnetization profile in the disordered region, $z > 0$. A linear behaviour is expected from equation (2.14). The values of the gradient are the same as in figure 1.

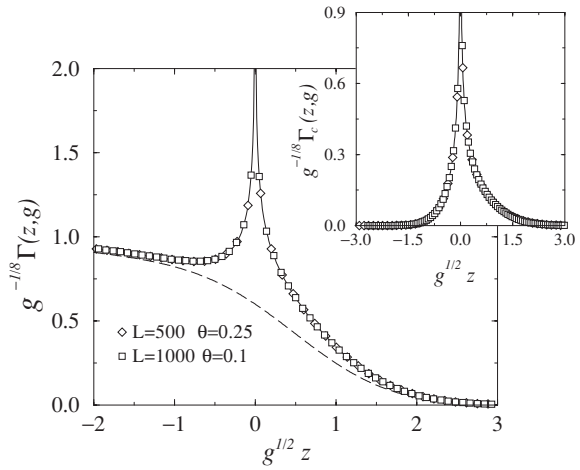

Figure 5. Scaling behaviour of the spin–spin correlation function $\Gamma(z, g)$ for $g = 5 \times 10^{-4}$ (diamond), 1×10^{-4} (square). The dashed line corresponds to the product $\langle m(0)\rangle\langle m(z)\rangle$ and the inset gives the behaviour of the connected part.

$$\Gamma(l) = \begin{vmatrix} G_{1,0} & G_{1,1} & \dots & G_{1,l-1} \\ G_{2,0} & G_{2,1} & \dots & G_{2,l-1} \\ \vdots & \vdots & & \vdots \\ G_{l,0} & G_{l,1} & \dots & G_{l,l-1} \end{vmatrix} \tag{4.31}$$

which involves the contractions already defined in (4.29).

The numerical results, shown in figure 5, confirm the scaling form given in (2.16). The behaviour of the connected part is shown in the inset. A closer analysis of the decay of $\Gamma_c(z, g)$

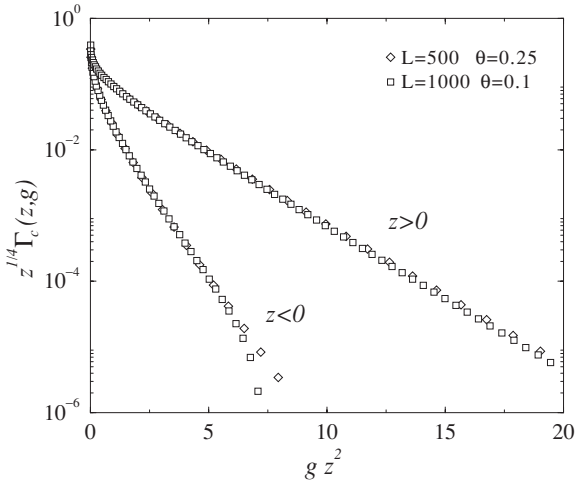

Figure 6. Semi-logarithmic plot of the rescaled connected part of the spin–spin correlation function as a function of gz^2. The linear behaviour is in agreement with (4.32).

points to the following Gaussian behaviour:

$$\Gamma_c \sim z^{-1/4} \exp(-\text{const}\, gz^2) \tag{4.32}$$

in agreement with the scaling prediction (2.16). The constant takes a different value on the two sides of the system (see figure 6).

5. Summary and conclusion

We have presented a scaling theory for the behaviour of the magnetization profile, the energy density profile and the two-point correlation function in a critical system in the presence of a linearly varying deviation from the critical coupling, $\Delta(z) = gz$. The gradient g introduces a new length scale in the problem, $\ell \sim g^{-\nu/(1+\nu)}$, which depends on the correlation length exponent ν in the case of a thermal perturbation considered here. The form of the scaling functions has been obtained by assuming that the different physical quantities have locally the same functional form as in the homogeneous system with the deviation from the critical point, Δ, replaced by its local value, $\Delta(z)$, in the inhomogeneous system.

The results of the scaling theory have been confirmed, first in mean-field theory and then in a study of the Ising quantum chain in a linearly varying transverse field. In this latter case, the excitation spectrum of the quantum Hamiltonian has been obtained exactly in the scaling limit where the size of the system $L \to \infty$, the gradient $g \to 0$ while the product Lg is held fixed. In this continuum limit one recovers the eigenvalue equation of the harmonic oscillator problem. Knowledge of the eigenvectors allows us to calculate exactly the energy density profile and to obtain numerically exact results for the magnetization density and the two-point correlation function. The very good agreement with the scaling results strongly supports the locality assumption used to deduce the form of the scaling functions.

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