Generalized Ginzburg-Landau theory of pseudo-one-dimensional systems

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A generalized Ginzburg-Landau theory is suggested to describe the phase transition of an array of weakly coupled pseudo-one-dimensional chains. Using a mean-field approximation, the coupled-chain problem is reduced to that of a single chain in an effective field. The finite-range correlations which develop along the chain are treated using exact one-dimensional solutions. The results obtained are then used to construct a generalized Ginzburg-Landau theory. We argue that this approach provides a means of treating the remaining slowly varying long-range fluctuations. Results are given for a variety of arrays consisting of Ising, classical Heisenberg, real and complex ψ^4 chains.

I. INTRODUCTION

There exist a number of materials which may be viewed as arrays of quasi-one-dimensional systems. These substances are generally characterized by molecular arrangements which lead to strong coupling along linear chains and weak coupling between the chains. Some examples of such systems are tetramethyl manganese chloride (TMMC),[1] an $S = \frac{5}{2}$ Heisenberg antiferromagnet; *α-bis*-(N-methylsalicylaldiminato)-Cu *α*-(Cu-N-Sal),[2] an $S = \frac{1}{2}$ Heisenberg antiferromagnet; most of the salts based on the organic acceptor tetracyanoquinodimethane (TCNQ),[3] which have been described as exhibiting a wide variety of pseudo-one-dimensional electronic behavior ranging from localized spin magnetism to band behavior to strong electron-lattice coupling; mixed-valency Pt salts[4] such as $K_2Pt(CN)_4Br_{0.3} \cdot 3H_2O$, which appears to undergo a one-dimensional Peierls distortion and then at lower temperatures to develop (short-range) three-dimensional order.

As is well known,[5] a strictly one-dimensional system with short-range interactions does not develop long-range order at a finite temperature. Nevertheless, once kT decreases below the energy characteristic of the intrachain interaction, significant short-range correlations develop along the chain. These correlations may often be well described by one-dimensional models over a wide temperature range. However, at some sufficiently low temperature, the interchain coupling becomes important, and the array of chains may undergo a phase transition to a state which has long-range order.

Here we develop a generalized Ginzburg-Landau theory[6,7] to describe the phase transition of an array of weakly coupled chains. The work proceeds in three stages: (a) A mean-field theory is developed in which the interchain coupling is approximated by a mean field and the resulting one-dimensional-chain problem is solved exactly. (b) The mean field is replaced by a slowly varying order parameter whose configuration energy is given by a Ginzburg-Landau[8] functional. (c) Using this energy functional the statistical mechanics of the order-parameter field is expressed in terms of functional integrals over all order-parameter configurations.

Basically, the procedure is similar in spirit to all Ginzburg-Landau theories—the short-range correlations are integrated out, leaving only the slowly varying configurations to be averaged over. In the present case the "short-range" correlations are very anisotropic and may, in fact, extend along the chain for many fundamental chain lengths. The exact solutions, usually available for one-dimensional problems, allow one to accurately treat these "short-range" correlations. Once this is done, the problem can be rescaled such that distances along the chain are measured in terms of the one-dimensional correlation length. The resulting generalized Ginzburg-Landau theory is then isotropic and, although it usually cannot be exactly solved, a great deal is known both theoretically and experimentally about it.

To illustrate this procedure, we treat a one-dimensional array of weakly coupled Ising chains in Sec. II. Replacing the interchain interaction by a mean field,[9] the wave-vector-dependent magnetic susceptibility $\chi(q)$ and the free energy per spin f are obtained. The susceptibility exhibits the usual Ornstein-Zernike form and gives an approximate expression for the transition temperature of the array. An order parameter is introduced to describe slow spatial variations of the mean field. Then the results for $\chi(q)$ and f are used to construct a Ginzburg-Landau func-

tional which gives the energy of the slowly varying mean-field configuration. Using this functional, a generalized Ginzburg-Landau formulation of the low-temperature phase transition of the array is obtained.

In Sec. III we apply these same ideas to the case of a two-dimensional array of weakly coupled ψ^4 chains. Here the statistical mechanics of an isolated chain is assumed to be described by a real-ψ^4 Ginzburg-Landau theory. The salient features of the theory are summarized in Sec. IV, and it is applied to two other examples: (i) a two-dimensional array of classical Heisenberg spin chains, and (ii) a two-dimensional array of ψ^4 chains with ψ a complex order parameter. It is straightforward to apply our formalism to any array for which the one-dimensional problem can be solved.[10]

II. WEAKLY COUPLED ISING CHAINS

The Hamiltonian describing a weakly coupled one-dimensional (planar) array of Ising chains in an external magnetic field is

$$H=-\sum_{nm}(J_{\parallel}\sigma_{n+1,m}\sigma_{nm}+J_{\perp}\sigma_{n,m+1}\sigma_{nm}+h_{nm}\sigma_{nm}). \tag{1}$$

Here the (n,m) spin can be up or down corresponding to $\sigma_{nm}=\pm 1$. $J_{\parallel}$ is the exchange coupling along a chain, $J_{\perp}$ is the interchain coupling, and h_{nm} is the Zeeman energy at the (n,m) site. In this work we take both $J_{\parallel}$ and $J_{\perp}>0$. We are interested in the situation where $J_{\parallel}\gg J_{\perp}$, so that the system develops important short-range correlations along the chains before the two-dimensional phase transition occurs. The generalization of this to a three-dimensional lattice consisting of a two-dimensional array of chains is straightforward.

For a given q dependence the Zeeman energy has the form

$$h_{nm}=h(\vec{q})e^{i(q_{\parallel}d_{\parallel}n+q_{\perp}d_{\perp}m)}+\text{c.c.} \tag{2}$$

Here $\vec{q}=(q_{\parallel},q_{\perp})$ and $(d_{\parallel},d_{\perp})$ are the distances between the spins parallel and perpendicular to the chains, respectively. The expectation value of the spin on site (n,m) is given in linear response by

$$\langle\sigma_{nm}\rangle=e^{i(q_{\parallel}d_{\parallel}n+q_{\perp}d_{\perp}m)}\langle\sigma(\vec{q})\rangle+\text{c.c.}, \tag{3}$$

with

$$\langle\sigma(\vec{q})\rangle=\chi(\vec{q})h(\vec{q}). \tag{4}$$

Here $\chi(\vec{q})$ is the $\vec{q}$-dependent susceptibility.

If the spins $\sigma_{n,m\pm1}$ on the two chains adjacent to the mth chain are replaced by their self-consistent mean-field values using Eq. (3), the problem becomes that of a one-dimensional chain in an effective field. Dropping the m index, the Hamiltonian for this one-dimensional problem is

$$H=-\sum_{n}J_{\parallel}\sigma_{n+1}\sigma_{n}-h_{\text{eff}}(q)\sum_{n}e^{iq_{\parallel}d_{\parallel}n}\sigma_{n}, \tag{5}$$

with

$$h_{\text{eff}}(q)=h(q)+2J_{\perp}(q_{\perp})\langle\sigma(q)\rangle. \tag{6}$$

$J_{\perp}(q_{\perp})$ is the $q_{\perp}$ Fourier transform of the interchain interaction

$$J_{\perp}(q_{\perp})=\frac{J_{\perp}}{2}\sum_{m=\pm1}e^{iq_{\perp}d_{\perp}m}=J_{\perp}\cos q_{\perp}d_{\perp}. \tag{7}$$

Above the transition temperature, the self-consistent expectation value $\langle\sigma(q)\rangle$ is given by the usual linear-response form

$$\langle\sigma(\vec{q})\rangle=\chi_{1D}(q_{\parallel})h_{\text{eff}}(q_{\parallel},q_{\perp}). \tag{8}$$

Here $\chi_{1D}(q_{\parallel})$ is the $q_{\parallel}$ susceptibility per spin for a one-dimensional Ising chain. Substituting Eq. (6) into Eq. (8) we have

$$\langle\sigma(q_{\parallel},q_{\perp})\rangle=\frac{\chi_{1D}(q_{\parallel})}{1-2J_{\perp}(q_{\perp})\chi_{1D}(q_{\parallel})}h(q_{\parallel},q_{\perp}). \tag{9}$$

Therefore, in this approximation the q-dependent susceptibility for the array of chains is simply related to $J_{\perp}(q_{\perp})$ and $\chi_{1D}(q_{\parallel})$:

$$\chi(q_{\parallel},q_{\perp})=\frac{\chi_{1D}(q_{\parallel})}{1-2J_{\perp}(q_{\perp})\chi_{1D}(q_{\parallel})}. \tag{10}$$

The transfer-matrix solution[11,12] of the one-dimensional Ising model gives the result

$$\chi_{1D}(q_{\parallel})=\frac{1}{kT}\sum_{l}(\tanh\beta J_{\parallel})^{|l|}e^{iq_{\parallel}d_{\parallel}l}. \tag{11}$$

When $J_{\perp}\ll J_{\parallel}$, the temperature region in which the intrachain coupling becomes important is such that $\beta J_{\parallel}\gg 1$. In this limit Eq. (11) sums to the simple form

$$\chi_{1D}(q_{\parallel})=\frac{\chi_{1D}(0)}{1+(\xi_1 q_{\parallel})^2}, \tag{12}$$

where $\chi_{1D}(0)=2\xi_1/kTd_{\parallel}$ and $\xi_1(T)$ is the one-dimensional correlation length which for $\beta J_{\parallel}\gg 1$ is given by

$$\xi_1(T)=\tfrac{1}{2}d_{\parallel}e^{2\beta J_{\parallel}}. \tag{13}$$

The $\vec{q}=0$ limit of Eq. (10) is

$$\chi(0)=\frac{\chi_{1D}(0)}{1-2J_{\perp}\chi_{1D}(0)}. \tag{14}$$

At temperatures where $2J_{\perp}\chi_{1D}(0)\ll 1$ this reduces to the one-dimensional result. However, as the temperature is reduced and $\chi_{1D}(0)$ increases, the interchain coupling enhances $\chi(0)$, and the system becomes two dimensional when $t\lesssim kT_c/J_{\parallel}$. It turns out that this region is also the two-dimensional

Ginzburg[13] critical region.

Within our present mean-field treatment of the interchain coupling, $\chi(0)$ diverges at a temperature determined by the condition

$$1 - 2J_\perp \chi_{1D}(0) = 0. \tag{15}$$

For the case in which $J_\parallel \gg J_\perp$, an explicit expression for the transition temperature T_c can be obtained:

$$kT_c \cong 2J_\parallel / \ln(J_\parallel / J_\perp). \tag{16}$$

This has the same form as the exact result[11] obtained by expanding $1 = \sinh(2J_\parallel / kT_c)\sinh(2J_\perp / kT_c)$ for the case $J_\parallel \gg J_\perp$:

$$kT_c \cong 2J_\parallel / \ln(2J_\parallel / J_\perp). \tag{17}$$

The approximate expression given by Eq. (16) overestimates the transition temperature by a factor of order $[1 + \ln 2 / \ln(2J_\parallel / J_\perp)]$. This difference between the exact result, Eq. (17), and our equation (16) reflects the slight suppression of T_c due to the two-dimensional fluctuations which are neglected by our present mean-field approximation.

For temperatures near T_c, in the two-dimensional regime, where

$$|t| = |(T - T_c)/T_c| < kT_c / 2J_\parallel, \tag{18}$$

our mean-field $q = 0$ susceptibility has the "Curie-Weiss" form

$$\chi(0) \cong (kT_c / 4J_\parallel J_\perp)\, 1/t\,. \tag{19}$$

In this same temperature region the small-$\vec{q}$ ($q_\parallel \xi_1 \ll 1$, $q_\perp d_\perp \ll 1$) expansion of $\chi(q)$ has the usual Ornstein-Zernike structure:

$$\chi(q) \simeq \frac{1}{2J_\perp} \frac{1}{(2J_\parallel / kT_c)t + \xi_1^2 q_\parallel^2 + (d_\perp^2 q_\perp^2 / 2)}\,. \tag{20}$$

This gives the characteristic lengths

$$\xi_\parallel = \left(\frac{kT_c}{2J_\parallel}\right)^{1/2} \frac{\xi_1(T_c)}{t^{1/2}}\,, \quad \xi_\perp = \left(\frac{kT_c}{4J_\parallel}\right)^{1/2} \frac{d_\perp}{t^{1/2}}\,, \tag{21}$$

which describe the spin correlations in the parallel and perpendicular directions, respectively. These lengths diverge in the usual mean field way as $(T_c)^{1/2}/(T - T_c)^{1/2}$ when $T \to T_c$.

In calculating $\chi(q_\parallel, q_\perp)$ [Eq. (10)] outside the temperature region set by Eq. (18), the temperature variation of ξ_1 and χ_{1D} must be taken into account. In this case, one has the more general result

$$\chi(q_\parallel, q_\perp) = \frac{\chi_{1D}(0)}{a(t) + [(\xi_1 q_\parallel)^2 + (d_\perp q_\perp)^2/2]\, 2J_\perp \chi_{1D}(0)}\,, \tag{22}$$

with

$$a(t) = 1 - 2J_\perp \chi_{1D}(0). \tag{23}$$

Here we continue to assume that $\xi_1 q_\parallel$ and $d_\perp q_\perp$ are small compared to 1.

Continuing with the mean-field treatment of the perpendicular coupling, we turn to the free energy. The free energy f per spin can be expanded in terms of the uniform ($q = 0$) mean field $\langle\sigma\rangle$. In the absence of an external magnetic field, the solution of this one-dimensional problem with $J_\parallel \gg J_\perp$ gives

$$f = -J_\parallel + J_\perp [a\langle\sigma\rangle^2 + b\langle\sigma\rangle^4 + O(\langle\sigma\rangle^6)]. \tag{24}$$

Here a is the same coefficient that appeared in $\chi(q)$ [see Eqs. (22) and (23)] and

$$b = \tfrac{1}{4}(2J_\perp)^3 \chi_{1D}^3(0) \cong \tfrac{1}{4}, \tag{25}$$

where the last approximate equality holds in the temperature region given by Eq. (18). Minimizing f with respect to $\langle\sigma\rangle$ gives the usual mean-field result for the behavior of $\langle\sigma\rangle$:

$$\begin{aligned} \langle\sigma\rangle^2 &= 0, \quad T > T_c \\ &= -a/2b, \quad T < T_c. \end{aligned} \tag{26}$$

Close to T_c, when the condition given by Eq. (18) holds, b can be approximated by $\frac{1}{4}$ and a by $(2J_\parallel / kT_c)t$. In this case, for $T < T_c$,

$$\langle\sigma\rangle^2 \cong (4J_\parallel / kT_c)|t|\,. \tag{27}$$

Thus the buildup of the order parameter below the ordering temperature is enhanced by the large factor $4J_\parallel / kT_c \cong 2\ln(J_\parallel / J_\perp)$.

In order to go beyond these mean-field results it is necessary to develop a scheme to take into account the remaining fluctuations. These fluctuations are most important when $|t| < kT_c / 2J_\parallel$. In this region the interchain correlation length becomes larger than $d_\perp$, which means that two-dimensional correlations become important. This region is the same as the one estimated from the Ginzburg criterion for critical fluctuations. Physically, the spin correlations vary slowly on a scale set by $\xi_1(T_c)$ along a chain and $d_\perp$ perpendicular to the chains. Thus one would expect a generalized Ginzburg-Landau theory based on the mean-field results for $\chi(q)$ and f with the correlation lengths $\xi_\parallel \gg \xi_1$, $\xi_\perp \gg d_\perp$ to be a valid approximation. Using $\chi(q)$ and f it follows that the energy of a slowly varying mean-field configuration described by an order parameter $\Psi(x)$ can be expressed as

$$F[\Psi(x)] = \frac{J_\perp}{d_\parallel d_\perp} \int d^2x \left[a\Psi^2(x) + b\Psi^4(x) + \xi_1^2 \left(\frac{d\Psi}{dx_\parallel}\right)^2 + \frac{d_\perp^2}{2} \left(\frac{d\Psi}{dx_\perp}\right)^2 \right]. \tag{28}$$

Here the order parameter $\Psi(x)$ can be understood

as the average of the spin over a chain length $\xi_1(T_c)$ centered at position $x \equiv (x_\parallel, x_\perp)$:

$$\Psi(x) = \frac{d_\parallel}{\xi_1(T_c)} \sum_{n'}{}' \langle \sigma_{n'm} \rangle, \tag{29}$$

with $x_\parallel = nd_\parallel$, $x_\perp = md_\perp$, and the sum over n' such that $|n' - n| d_\parallel < \frac{1}{2}\xi_1$. It is convenient to scale the dimensions so that $x_\parallel = \xi_1 y_\parallel$ and $x_\perp = (d_\perp/\sqrt{2}) y_\perp$. Then the functional $F[\psi(y)]$ has the isotropic form

$$F[\Psi] = \frac{J_\perp}{\sqrt{2}} \frac{\xi_1}{d_\parallel} \int d^2y \, [a\Psi^2(y) + b\Psi^4(y) + |\nabla_y \Psi|^2], \tag{30}$$

where ∇_y is the two-dimensional gradient. The energy functional F in Eqs. (28) and (30) does not include the configuration-independent contributions of $-J_\parallel$ per spin which arise from the first term of Eq. (24).

In arriving at the Ginzburg-Landau functions, Eq. (30), we have integrated out the short-range one-dimensional correlations. The $J_\parallel$ coupling now simply serves to set the parameters ξ_1 and $\chi_{1D}(0)$. In order to treat fluctuations, we now propose that $F[\Psi]$, Eq. (30), be used as the energy functional for a generalized Ginzburg-Landau theory.[7] Here the partition function is given by the functional integration

$$Z = \int \delta\Psi \, e^{-\beta F[\Psi]}, \tag{31}$$

and the correlation function by

$$\langle \Psi(x)\Psi(x') \rangle = \int \delta\Psi (e^{-\beta F[\Psi]}/z) \Psi(x)\Psi(x'). \tag{32}$$

While these functional integrals cannot be carried out exactly, this formulation reduces the problem of an array of weakly coupled chains to the standard form for an isotropic phase transition.

III. ARRAYS OF REAL-ψ^4 GINZBURG-LANDAU CHAINS

This same type of approach can be applied to arrays of chains described by a continuous real-field order parameter.[14] Here we consider a two-dimensional array of weakly coupled chains oriented along the x axis. The ith chain is described by a real order parameter $\psi_i(x)$, and the energy of a given configuration is given by

$$F = \sum_i \int_0^L dx \left[\bar{a}\psi_i^2 + \bar{b}\psi_i^4 + \bar{c}_\parallel \left(\frac{d\psi_i}{dx} \right)^2 \right] - 2 \sum_{i \neq j} \bar{c}_\perp \int_0^L \psi_i \psi_j \, dx, \tag{33}$$

where $\bar{a} = (T - T_c^\circ)\bar{a}'$ and $\bar{a}'$, $\bar{b}$, $\bar{c}_\parallel$, and $\bar{c}_\perp$ are positive constants. The $i \neq j$ sum is over near neighbors. The temperature T_c° is the mean-field transition temperature of an isolated chain. As is well known, for the case of a single chain, fluctuations prevent the system from ordering and give rise to a broad continuous transition region of characteristic width ΔT given by[13]

$$\Delta T = 2T_c^\circ (\bar{b} k T_c^\circ)^{2/3} / \bar{a}'. \tag{34}$$

If the array interacts with an external field h which couples linearly to ψ, there is the additional interaction energy

$$-\sum_i \int_0^L h_i(x)\psi_i(x)\, dx. \tag{35}$$

Proceeding as in Sec. II, a mean-field approximation of the interchain coupling is made, and the problem is reduced to that of a single one-dimensional chain in an effective field. The q-dependent susceptibility of the array in this approximation has the same structure as Eq. (10),

$$\chi(q_\parallel, q_\perp) = \frac{\chi_{1D}(q_\parallel)}{1 - 2z_\perp \bar{c}_\perp(\vec{q}_\perp)\chi_{1D}(q_\parallel)}, \tag{36}$$

with $\chi_{1D}(q_\parallel)$ the susceptibility of a single chain and

$$\bar{c}_\perp(\vec{q}_\perp) = \frac{\bar{c}_\perp}{z_\perp} \sum e^{i\vec{q}_\perp \cdot \vec{R}_{ij}}. \tag{37}$$

Here $\vec{R}_{ij}$ are the perpendicular near-neighbor distances between chains and $z_\perp$ is the number of near-neighbor chains of a given chain. For $\bar{c}_\perp$ positive, the susceptibility diverges first for $\vec{q} = 0$, and the mean-field prediction for the transition temperature T_c of the array is given by

$$1 - 2z_\perp \bar{c}_\perp \chi_{1D}(0) = 0. \tag{38}$$

The single-chain problem can be solved by well-known transfer-matrix techniques which reduce it to finding the eigenstates $|n\rangle$ and eigenenergies ϵ_n of the effective Hamiltonian,[15]

$$H = -\frac{1}{4\beta\bar{c}_\parallel} \frac{\partial^2}{\partial\psi^2} + \bar{a}\psi^2 + \bar{b}\psi^4. \tag{39}$$

In Eq. (39) ψ is simply a variable and not the field $\psi(x)$. It can be shown that the one-dimensional susceptibility of a single chain is given by

$$\chi_{1D}(q_\parallel) = \frac{1}{kT} \int dx \, e^{iq_\parallel x} \langle \psi(x)\psi(0) \rangle \cong \frac{|\langle 1|\psi|0\rangle|^2}{kT} \frac{2\xi_1}{1 + (q_\parallel \xi_1)^2}, \tag{40}$$

with $\langle 1|\psi|0\rangle$ the matrix element of the variable ψ between the ground state $|0\rangle$ and first excited state $|1\rangle$ of Eq. (39), and

$$\xi_1^{-1} = \beta(\epsilon_\perp - \epsilon_0). \tag{41}$$

From Eq. (40), we have $\chi_{1D}(0) \cong |\langle 1|\psi|0\rangle|^2 2\xi_1/kT$, so that the condition specifying T_c, Eq. (38), becomes

$$1 = 4z_\perp c_\perp \xi_1 |\langle 1|\psi|0\rangle|^2/kT. \tag{42}$$

We will say that the chains are weakly coupled if T_c for the array is less than $T_c^\circ - \Delta T$, where ΔT is given by Eq. (34). In this case, setting $T = T_c$, one finds from the solutions of the effective Hamiltonian, Eq. (39), that

$$|\langle 1|\psi|0\rangle|^2 \cong \langle 0|\psi^2|0\rangle \cong (\bar{a}'/2\bar{b})(T_c^\circ - T_c) \tag{43}$$

and

$$\xi_1 \cong (T_c^\circ/\Delta T)^{1/2} \xi_0 \exp[(T_c^\circ - T)/\Delta T], \tag{44}$$

with $\xi_0 = \bar{c}_\parallel^{1/2}/\bar{a}^1 k T_c^\circ$. Substituting these expressions into Eq. (42) we find that

$$T_c \cong \frac{T_c^\circ}{\ln(\bar{c}_\parallel/z_\perp \bar{c}_\perp \xi_0^2)} . \tag{45}$$

Thus weak coupling means that the ratio of the transverse coupling to the longitudinal coupling $z_\perp \bar{c}_\perp \xi_0^2/\bar{c}_\parallel$ is small compared with unity. This ratio plays the same role as $J_\perp/J_\parallel$ for the Ising model discussed in Sec. II. In the continuous model, described by the energy functional $F[\psi_i(x)]$ of Eq. (33), $\bar{c}_\perp$ has dimensions of energy per unit length, so that $z_\perp \bar{c}_\perp \xi_0$ represents the effective transverse coupling energy, and $\bar{c}_\parallel$ has dimensions of energy times length, so that $\bar{c}_\parallel/\xi_0$ represents the effective longitudinal coupling energy.

Assuming that $q_\parallel \xi_1$ and $\vec{q}_\perp \cdot \vec{d}_\perp$ are both small compared to unity, the q-dependent susceptibility becomes

$$\chi(q) = \frac{\chi_{1D}(0)}{a(T) + 2z_\perp \bar{c}_\perp \chi_{1D}(0)[(\xi_1 q_\parallel)^2 + (\vec{d}_\perp \cdot \vec{q}_\perp)^2/2]}, \tag{46}$$

with $a(T) = 1 - 2z_\perp \bar{c}_\perp \chi_{1D}(0)$. The parallel and perpendicular coherence lengths are therefore given by

$$\xi_\parallel = \left(\frac{2z_\perp \bar{c}_\perp \chi_{1D}}{a(T)}\right)^{1/2} \xi_1, \quad \xi_\perp = \frac{d_\perp}{[2a(T)]^{1/2}} . \tag{47}$$

For temperatures near the ordering temperature T_c of the array, the expression for $\chi(q)$ reduces to

$$\chi(q) \cong \frac{1}{2z_\perp \bar{c}_\perp} \frac{1}{(T - T_c/\Delta T) + \xi_1^2 q_\parallel^2 + (\vec{d}_\perp \vec{q})^2/2} . \tag{48}$$

The calculation of the free-energy density (free energy per chain per unit length) is straightforward within our present approximation in which the interchain coupling is replaced by a mean field. The Hamiltonian, Eq. (40), becomes

$$H = -\frac{1}{4\beta \bar{c}_\parallel} \frac{\partial^2}{\partial \psi^2} + \bar{a}\psi^2 + \bar{b}\psi^4 - 2z_\perp \bar{c}_\perp \langle\psi\rangle \psi. \tag{49}$$

At temperatures near T_c, which for weakly coupled chains are well below T_c°, only the ground and first excited state of H are important. Diagonalizing the Hamiltonian, Eq. (49), in this basis and expanding the ground-state energy in powers of $\langle\psi\rangle$ through order $\langle\psi\rangle^4$ one obtains

$$\epsilon_0 - \frac{(2z_\perp \bar{c}_\perp)^2}{\epsilon_1 - \epsilon_0} |\langle 1|\psi|0\rangle|^2 \langle\psi\rangle^2 + \frac{(2z_\perp \bar{c}_\perp)^4}{(\epsilon_1 - \epsilon_0)^3} |\langle 1|\psi|0\rangle^4 \langle\psi\rangle^4. \tag{50}$$

According to the transfer-matrix theory, this is just the Gibbs free-energy density. Adding the self-consistent field interaction energy $\frac{1}{2}\bar{c}_\perp z_\perp \langle\psi\rangle^2$ to this gives the free-energy density we seek:

$$f = \epsilon_0 + z_\perp \bar{c}_\perp (a\langle\psi\rangle^2 + b|\langle 0|\psi^2|0\rangle|\langle\psi\rangle^4), \tag{51}$$

with

$$a = 1 - 2z_\perp \bar{c}_\perp \chi_{1D}(0) \cong (T - T_c)/\Delta T \tag{52}$$

and

$$b = \tfrac{1}{4}[2z_\perp \bar{c}_\perp \chi_{1D}(0)]^3 \cong \tfrac{1}{4}. \tag{53}$$

Here we have replaced $2|\langle 1|\psi|0\rangle|^2/(\epsilon_1 - \epsilon_0)$ by $\chi_{1D}(0)$, set $|\langle 1|\psi|0\rangle|^2 \cong \langle 0|\psi^2|0\rangle$, and in the last form of Eq. (53) taken $2z_\perp \bar{c}_\perp \chi_{1D} = 1$, its value at T_c.

Now, just as before, we introduce a new order parameter $\Psi(x)$ which is a ratio of $\psi(x)$ averaged over a length $\xi_1(T_c)$ along the chain to $(\langle 0|\psi^2|0\rangle)^{1/2}$. It follows from the expressions for χ and f that a slowly varying $\Psi(x)$ configuration has energy

$$F[\Psi(x)] = \frac{z_\perp \bar{c}_\perp \langle 0|\psi^2|0\rangle}{d_\perp^2} \int d^3x \left[a\Psi^2(x) + b\Psi^4(x) + \xi_1^2 \left(\frac{d\Psi}{dx}\right)^2 + \tfrac{1}{2}(\vec{d}_\perp \cdot \vec{\nabla}_\perp \Psi)^2 \right]. \tag{54}$$

Here we have not included the configuration-independent contribution $NL\epsilon_0(T)$ which represents the free energy of N noninteracting chains of length L. Scaling $\vec{x}$ such that $x_\parallel = \xi_1 y_\parallel$ and $\vec{x}_\perp = (\vec{d}_\perp/\sqrt{2})\vec{y}$ gives the isotropic form

$$F[\Psi(y)] = \tfrac{1}{2}(z_\perp \bar{c}_\perp \xi_1 \langle 0|\psi^2|0\rangle) \times \int d^3y [a\Psi^2(y) + b\Psi^4(y) + |\nabla\Psi(y)|^2]. \tag{55}$$

This functional has the same form as Eq. (30) of Sec. II for the Ising problem. There is again a substantial amount of order along the chains, and the configuration energy is set by the interchain or transverse energy $\frac{1}{2}z_\perp c_\perp \xi_1 \langle 0|\psi^2|0\rangle$. Using Eq. (55) the generalized Ginzburg-Landau theory is constructed as discussed at the end of Sec. II.

IV. SUMMARY AND CONCLUSION

The problem of a weakly coupled array of chains is characterized by two scales of energy. The longitudinal intrachain coupling energy is large compared to the transverse interchain coupling energy. This difference of energy scales can be removed and the problem homogenized by using the single-chain (one-dimensional) solution to integrate out the "short-range" one-dimensional correlations. The procedure for carrying this out has been discussed in Secs. II and III for two specific examples.

Treating the interchain coupling within mean field, expressions for the q-dependent susceptibility $\chi(q_\parallel, \tilde{q}_\perp)$ [Eqs. (20) and (46)] and the free-energy density f [Eqs. (24) and (51)] were obtained. These expressions provide an adequate approximation outside the critical ordering region and give an approximate expression for T_c. In the critical region, interchain fluctuations are treated by a generalized Ginzburg-Landau formalism using a free-energy functional F [Eqs. (28) and (54)] with parameters obtained from χ and f. All of these functions are constructed from the solution of the one-dimensional problem. Specifically, the one-dimensional linear response $\chi_{1D}(q)$ and the lowest-order nonlinear response must be evaluated.

We conclude with two additional examples. First consider a two-dimensional array of classical Heisenberg spin chains. The jth chain has a Hamiltonian

$$H_j = -\sum_i 2J_\parallel \vec{S}_{i+1,j} \cdot \vec{S}_{i,j}, \tag{56}$$

and the chains are coupled by a near-neighbor exchange $J_\perp$:

$$-\sum_{ij} 2J_\perp \vec{S}_{ij+1} \cdot \vec{S}_{ij}. \tag{57}$$

Here $\vec{S}$ is a classical unit vector and $J_{\parallel,\perp} = S(S+1)\mathcal{J}_{\parallel,\perp}$, where $\mathcal{J}$ is the Heisenberg exchange. We will treat the case in which the coupling along a chain is antiferromagnetic ($J_\parallel < 0$), while the coupling between the chains is ferromagnetic ($J_\perp > 0$).

Fisher[16] has calculated the correlation functions leading to the staggered susceptibility for the one-dimensional chain. In the $q_\parallel = 0$ limit

$$\chi_{1D}(0) = (1/3k_BT)[(1-u)/(1+u)], \tag{58}$$

with $u = (\coth K - 1/K)$ and $K = 2J_\parallel/kT$. Just as before [Eqs. (15) and (38)], this leads to an estimate of the ordering temperature of the array given by $1 = 2z_\perp J_\perp \chi_{1D}(0)$. For $J_\parallel \gg kT_c$ we find that

$$kT_c \cong J_\parallel (\tfrac{8}{3} z_\perp J_\perp / J_\parallel)^{1/2}. \tag{59}$$

The change in the dependence of T_c on $z_\perp J_\perp / J_\parallel$ from logarithmic for the Ising model to square root for the mean-field estimate of the classical vector model reflects the change in symmetry of the order parameter. More generally, one may expect that $kT_c/J_\parallel$ varies as $(z_\perp J_\perp/J_\parallel)^{\alpha'}$, where the index α' depends on the number of components of the order parameter and the dimensions of the array.

For kT small compared to $J_\parallel$, spin correlations develop along the chains and

$$\chi_{1D}(q_\parallel) \cong \chi_{1D}(0)/[1 + (q_\parallel \xi_1)^2], \tag{60}$$

with a correlation length $\xi_1 = 2J_\parallel d_\parallel/kT$. The q-dependent susceptibility of the array is given by Eq. (10). Finally, it is straightforward to calculate the nonlinear (H^2) susceptibility for T near T_c.[17] From this one finds that

$$F[\vec{\Psi}] = 2J_\perp z_\perp \int \frac{d^3x}{d_\parallel^2 d_\parallel} \left(a|\vec{\Psi}|^2 + b|\vec{\Psi}|^4 + \xi_1^2 \left| \frac{d\vec{\Psi}}{dx} \right|^2 + \frac{d_\perp^2}{2} |\nabla_\perp \vec{\Psi}|^2 \right), \tag{61}$$

with $a = 1 - 2z_\perp J_\perp \chi_{1D}(0)$ and $b = \frac{11}{20}$. The order parameter $\vec{\Psi}$ is equal to the average value of $\vec{S}_i$ over a length ξ_1 along a chain [see Eq. (29)]. In this case the crossover region between 1D and 3D behavior as well as the 3D critical region occur for $|t| \lesssim 1$.

As a final example, we conclude by giving some results for a complex Ψ field. The notation is that of Sec. III. The susceptibility of a single chain is approximately given by

$$\chi_{1D}(q_\parallel) = \frac{\langle O||\Psi|^2|O\rangle}{kT} \frac{\xi_1}{1 + (q_\parallel \xi_1)^2}. \tag{62}$$

Numerical results for ξ_1^{-1} are plotted in Ref. 15.

For $T < T_c^\circ$, one has $\xi_1^{-1} \cong \bar{b} kT/2\bar{c}|\bar{a}|$. The transition temperature of the array can be expressed in the weak-coupling limit as

$$T_c \simeq T_c^\circ \left(\frac{2z_\perp \bar{c}_\perp \xi_0^2}{\bar{c}_\parallel} \right)^{1/2}, \tag{63}$$

with $\xi_0^2 = \bar{c}_\parallel/\bar{a}' kT_c^\circ$. Just as for the real field, the weak-coupling limit is set by the requirement that $z_\perp \bar{c}_\perp \xi_0^2/\bar{c}_\parallel$ be small compared to unity. The square-root dependence on this relative coupling strength which appears in Eq. (63) is similar to that obtained for the classical spin case. The change in dependences on this ratio of coupling strengths from logarithmic for the real field to square root for the complex field reflects the change from exponential to power-law growth of the correlation length ξ_1. As previously noted, the square root in Eq. (63) is a mean-field result, and in an exact theory it would be replaced by a different

index. Near $T_{c'}$ a new complex order parameter $\Psi(x)$ is obtained by averaging $\psi(x)$ over a length $\xi_1(T_c)$ and normalizing it to $(\langle O||\psi|^2|O\rangle)^{1/2}$. The free-energy functional is

$$F[\Psi] = \frac{z_\perp \bar{c}_\perp \langle O||\psi|^2|O\rangle}{d_\perp^2} \int d^3x \left(a|\Psi|^2 + b|\Psi|^4 + \xi_1 \left|\frac{d\Psi}{dx_\parallel}\right|^2 + \frac{d_\perp^2}{2} |\nabla_\perp \Psi|^2 \right), \quad (64)$$

with $a = 1 - z_\perp \bar{c}_\perp \chi_{1D}(q_\parallel = 0)$ and $b \cong 1$.

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