Spin Dynamics in the Square-Lattice Antiferromagnet

Assa Auerbach
Physics Department, Brookhaven National Laboratory, Upton, New York 11973

and

Daniel P. Arovas
James Franck Institute, University of Chicago, Chicago, Illinois 60637
(Received 16 May 1988)

We apply the Schwinger boson mean-field theory to the square-lattice Heisenberg antiferromagnet at low temperatures. For spin $\frac{1}{2}$ we confirm the renormalized classical behavior of the correlation length $\kappa^{-1}(T)$ without appealing to spin-wave theory. We also present a detailed calculation of the dynamical structure factor. A quasielastic peak is featured near $\mathbf{q}=(\pi,\pi)$, while for $|\mathbf{q}-(\pi,\pi)| \gg \kappa$, spin-wave ridges appear. The uniform susceptibility interpolates between spin-wave results at $T=0$ and the high-temperature series of Rushbrooke and Wood. Our theory is distinct from theories in which fermionic spinon excitations determine the low-temperature spin dynamics.

PACS numbers: 75.10.Jm, 67.40.Db, 75.10.+x

Interest in the two-dimensional quantum Heisenberg model has been greatly revived since the discovery[1] of quasi-two-dimensional antiferromagnetism in the undoped, insulating La_2CuO_4. This behavior may be fundamentally related to the fact that the material becomes a high-T_c superconductor under doping of Sr or Ba. A similar antiferromagnetic phase has been observed[2] in $YBa_2Cu_3O_{6+x}$ for $x<0.5$. As a first approximation, the copper spin dynamics can be modeled by the square lattice $S=\frac{1}{2}$ quantum antiferromagnet,

$$H=J\sum_{\langle i,j\rangle} \mathbf{S}_i\cdot\mathbf{S}_j;\quad \mathbf{S}^2=S(S+1), \tag{1}$$

where $J>0$ is the superexchange energy, and the sum is taken over all bonds in the lattice.

The continuum theory which corresponds to the d-dimensional quantum Heisenberg model is that of the $(d+1)$-dimensional nonlinear σ model[3] with coupling constant g; g is a decreasing function of the spin S. Since the three-dimensional σ model orders at $g \le g_c \ne 0$, this suggests that a critical spin S_c can be defined such that for $S>S_c$ and $d=2$ the ground state of the quantum antiferromagnet possesses long-range order. In this regime, the disordering effects of quantum fluctuations can be treated perturbatively [in $(2S)^{-1}$] by expansion around a broken-symmetry Néel state by use of spin-wave theory (SWT). In a recent Letter,[4] Chakravarty, Halperin, and Nelson (CHN) have evaluated the temperature-dependent correlation length κ^{-1} by studying the model in a slab of finite thickness. They applied Oguchi's SWT[5] to determine the appropriate value of the coupling at $S=\frac{1}{2}$, and found that $g<g_c$, and that the correlation length has renormalized classical behavior $\kappa^{-1}=\exp[-A/T]$, where A is weakly temperature dependent and finite at $T=0$. They also demonstrated the consistency of their $\kappa(T)$ with the experimentally determined correlations.[1]

In a different approach, we recently developed the "Schwinger boson mean-field theory"[6] (SBMFT) as a useful way of treating a large class of lattice quantum antiferromagnets in their rotationally invariant phases. For the square lattice model, we arrived at the same conclusion as CHN, *without* assuming that the ground state is ordered and the spin-wave expansion applicable. Conventional SWT which describes quantum fluctuations about a putative ordered ground state, breaks down at finite temperature in low dimensions because of the Mermin-Wagner theorem.[7] Our theory, which preserves rotational invariance, describes a finite-temperature magnetically disordered phase. It hinges on a steepest-descents approximation to a functional integral, and is exact in the large-N limit of a class of generalized SU(N) invariant models. Like SWT, our theory provides an appealingly simple *Bose-liquid* description of the excitations.

In recent literature, there have been several alternative descriptions of the quasiparticles of the (perhaps frustrated) quantum antiferromagnet. Some of the prominent proposals are, e.g., fermionic "spinons" of the resonating valence-bond theory,[8] neutral fermions of certain (2+1)-dimensional field theories,[9] and excitations analogous to those in the fractional-quantum-Hall theory.[10] These theories describe various "quantum spin-liquid" ground states, i.e., disordered phases, and excitations that are distinct from bosonic spin waves. Many of them have been linked to proposed mechanisms of high-T_c superconductivity in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$.

In order to allow experiments to distinguish between the models, we present a detailed calculation of the dynamical structure factor $S(\mathbf{q},\omega;T)$, as well as the uniform susceptibility and specific heat. We also make connection with $T=0$ SWT, and with high-temperature series.

The spin operators are represented by two Schwinger bosons ($m=1,2$), viz., $[a_{im},a^\dagger_{i'm'}]=\delta_{ii'}\delta_{mm'}$, with the constraint $\sum_{m=1}^2 a^\dagger_{im}a_{im}=2S$. The spin operators of Eq. (1) are given by $a_1^\dagger a_2 \equiv S^+ \, (-S^-)$ and $(a_1^\dagger a_1 - a_2^\dagger a_2)/2 \equiv S^z \, (-S^z)$ on sublattice A (B). The Hamiltonian (1) is written as

$$H=-\tfrac{1}{2}J\sum_{\langle i,j\rangle}A^\dagger_{i,j}A_{i,j}+2NJS^2, \qquad (2)$$

where N is the number of lattice sites, and $A^\dagger_{i,j} \equiv \sum_m a^\dagger_{im}a^\dagger_{jm}$. It is easy to check that Eq. (2) constitutes a faithful representation of Eq. (1). We use units of $\hbar=k_B=a=1$, where a is the lattice constant.

We first apply a Hubbard-Stratonovich transformation to the Langrangean in the path integral representation of the partition function using a complex variable $Q_{i,j}$ at each bond. The constraint, given above, is enforced by a "chemical potential" field λ_i at each site. The mean-field (MF) theory amounts to a steepest-descents approximation, where Q and λ acquire static uniform values, that are determined by our extremizing the free energy. The MF Hamiltonian is given by

$$H^{\rm MF}=\sum_{i,m}[\lambda a^\dagger_{i,m}a_{i,m}+g\mu \mathbf{h}(i,t)\mathbf{S}+\tfrac{1}{2}Q\sum_\delta(a^\dagger_{i,m}a^\dagger_{i+\delta,m}+a_{i,m}a_{i+\delta,m})]-N\lambda S+NQ^2/J+2NS^2. \qquad (3)$$

Here $\mathbf{h}(i,t)$ is the dynamical magnetic field. For $\mathbf{h}=0$, it can easily be verified that the Hamiltonian does not break rotational symmetry. $H^{\rm MF}$ is readily diagonalized by the quasiparticle operators: $\alpha_{\mathbf{k}m}=\cosh\theta_\mathbf{k} a_{\mathbf{k}m}+\sinh\theta_\mathbf{k} a^\dagger_{-\mathbf{k}m}$, where $a_{\mathbf{k}m}=\sum_j \exp(i\mathbf{k}\cdot \mathbf{j})a_{jm}$. Here, $\tanh(2\theta_\mathbf{k})=-4Q\gamma_\mathbf{k}/\lambda$ and $\gamma_\mathbf{k}=\frac{1}{2}(\cos k_x+\cos k_y)$. The dispersion of the quasiparticles $\{\alpha_\mathbf{k}\}$ is $\omega_\mathbf{k}=[\lambda^2-(4Q\gamma_\mathbf{k})^2]^{1/2}$.

The steepest-descents equations are derivatives of the MF free energy $f^{\rm MF}$ with respect to the MF parameters:

$$\tfrac{1}{2}\,df^{\rm MF}/d\lambda=\int[d^2\mathbf{k}/(2\pi)^2]\cosh(2\theta_\mathbf{k})(n_\mathbf{k}+\tfrac{1}{2})-(S+\tfrac{1}{2})=0, \qquad (4)$$

$$\tfrac{1}{2}\,df^{\rm MF}/dQ=-4\int[d^2\mathbf{k}/(2\pi)^2]\gamma_\mathbf{k}\sinh(2\theta_\mathbf{k})(n_\mathbf{k}+\tfrac{1}{2})+4Q/J=0. \qquad (5)$$

Here, $n_\mathbf{k}$ is the Bose occupation $[\exp(\omega_\mathbf{k}/T)-1]^{-1}$. The structure factor ${\rm Im}\langle S^z(\mathbf{q},\omega)S^z(-\mathbf{q},\omega)\rangle$ is

$$S^{\rm MF}=\tfrac{1}{4}\pi\sum_\mathbf{k}\{\cosh[2(\theta_\mathbf{k}+\theta_{\mathbf{k}+\tilde{\mathbf{q}}})]+1\}n_\mathbf{k}(n_{\mathbf{k}+\tilde{\mathbf{q}}}+1)\delta(\omega_{\mathbf{k}+\tilde{\mathbf{q}}}-\omega_\mathbf{k}-\omega)+\tfrac{1}{8}\pi\sum_\mathbf{k}\{\cosh[2(\theta_\mathbf{k}+\theta_{\mathbf{k}+\tilde{\mathbf{q}}})]-1\}$$
$$\times[n_\mathbf{k}+\Theta(\omega)][n_{\mathbf{k}+\tilde{\mathbf{q}}}+\Theta(\omega)]\delta(\omega_{\mathbf{k}+\tilde{\mathbf{q}}}+\omega_\mathbf{k}-|\omega|), \qquad (6)$$

where $\Theta(\omega)$ is the step function. The first term corresponds to "normal" scattering of spin waves, while the second is the "anomalous" contribution, representing creation and anhilation processes of two spin-wave excitations. Here it is convenient to measure the reduced momentum with respect to the antiferromagnetic vector, i.e., $\tilde{\mathbf{q}}\equiv\mathbf{q}-(\pi,\pi)$. In (6) we have exploited the decoupling of the two Schwinger bosons, in the Hamiltonian (3).

It is convenient to parametrize the dispersion $\omega_\mathbf{k}$ in terms of the spin-wave velocity $c=\sqrt{8}Q$, and an inverse correlation length $c\kappa=\{8[\lambda^2-(4Q)^2]\}^{1/2}$. The dispersion is then given by $\omega_\mathbf{k}=c[(\kappa/2)^2+2(1-\gamma_\mathbf{k}^2)]^{1/2}$. We note that $\kappa/2$ serves as a cutoff in the momenta integrations in Eqs. (4)-(6). Our spin waves are therefore "massive" when $\kappa\neq 0$. The antiferromagnetic spin correlations were previously shown[6] to decay as $R^{-1}\times\exp(-\kappa R)$, for large distances R. At low temperatures, the solutions of Eqs. (4) and (5) yield

$$c=Z_c\sqrt{8}JS; \quad \kappa=\exp[-Z_\kappa 2\pi S(S+1)J/T]. \qquad (7)$$

The quantum renormalization factors $Z_c(T,S)$ and $Z_\kappa(T,S)$ are obtained numerically for $T\to 0$ and small values of S in Table I. It was also previously shown[6] that Eq. (4) ensures that Z_κ has a finite $T=0$ limit for all $S>S_c\approx 0.2$, and is only weakly T dependent for $T<JS(S+1)$. For large S, $\lim_{S\to\infty}Z_\kappa=1$, and Eq. (7) agrees, to one-loop order, with the renormalization-group calculation of the classical Heisenberg model.[11] Since $Z_\kappa(S=\frac{1}{2})=0.246$, it is apparent that quantum fluctuations drastically reduce the correlation length at finite temperatures from its classical value. On the other hand, κ^{-1} still diverges at $T=0$, which implies that this system has a Néel ordered ground state, in agreement with perturbative analyses[12] and numerical results for finite-size systems.[13]

At this point we can compare our theory to SWT[4,5] at

TABLE I. Results of the SBMFT compared to SWT (Refs. 4 and 5), and to the σ model calculation (Ref. 4) (CHN). Z_c, Z_χ, and Z_κ are the $T\to 0$ limit of the renormalization constants of the spin-wave velocity, susceptibility, and correlation-length exponent, respectively.

Theory	Coefficient	$S=\frac{1}{2}$	$S=1$
SBMFT	Z_c	1.159	1.079
SWT	$Z_c=1+0.158/2S$	1.158	1.079
SBMFT	Z_χ	0.53 ± 0.01	0.73 ± 0.01
SWT	$Z_\chi=1-0.552/2S$	0.448	0.724
SBMFT	$JS(S+1)(dZ_\chi/d_T)$	0.22 ± 0.01	0.27 ± 0.01
SBMFT	Z_κ	0.246	0.442
CHN	$Z_\kappa=\hbar c Z_c Z_\chi/a\sqrt{8}(S+1)$	0.200	0.421
SBMFT	$\delta=C_v[T/S(S+1)J]^{-2}$	1.3 ± 0.05	1.2 ± 0.05

$T=0$, and we notice the following facts:

(1) The values of the spin-wave velocity renormalization Z_c, Eq. (7), agree well for $S=\frac{1}{2}$ and 1, as shown in Table I. Since κ vanishes at $T=0$, our quasiparticle dispersion matches the spin-wave result.

(2) The expression for f^{MF} is twice that of SWT. This is the same situation we have previously encountered when comparing our ferromagnetic Bose-liquid theory to Takahashi's[14] finite-temperature modified SWT, which has been quantitatively successful in reproducing the numerical Bethe *Ansatz* solution for the $S=\frac{1}{2}$ chain at low temperatures. In that system, we were able to explicitly show[6] that the Gaussian corrections reduce the overcounting of the leading term in f^{MF} by a multiplicative factor of $\frac{1}{2}$. For the square lattice antiferromagnet, however, we have not yet attempted to compute the Gaussian corrections.

(3) The spin-correlation function S^{MF} [Eq. (6)] is exactly $\frac{3}{2}$ times the *rotationally averaged* expression of SWT. It can be easily verified, by use of Eqs. (4) and (6), that the susceptibility sum rule yields $\sum_{\mathbf{q},q_n} S^{\mathrm{MF}}=S(S+1)/2$ which is exactly $\frac{3}{2}$ too large.

Therefore, in order to obey the condition that our theory should match SWT at $T=0$, for large S, and also obey the sum rule, we correct our free energy and correlation functions by $F=\frac{1}{2}f^{\mathrm{MF}}$, and $S(\mathbf{q},\omega)\equiv\frac{2}{3}S^{\mathrm{MF}}$. We suggest *without proof* that this normalization partly compensates for the fluctuation effects, missed by the static MF theory.

The calculation of Eq. (6) is greatly simplified by our expanding $\omega_{\mathbf{k}}$ to quadratic order in $\mathbf{k}$ and $\tilde{\mathbf{k}}$. This allows us to perform the angular integration analytically, and only the radial integration numerically. In Fig. 1, we plot Eq. (6) in the positive $\tilde{q},\omega$ quadrant, where $\tilde{q}\equiv|\mathbf{q}|$. For $(\omega,\tilde{q})<(T,T/c)$ there is a reflection symmetry on both energy and momentum axis. Two distinct regimes are observed: (a) $(\omega,\tilde{q})\leq(c\kappa,\kappa)$ and (b) $(\omega,\tilde{q})\gg(c\kappa,\kappa)$. Region (a) is a quasielastic peak, which increases, and narrows with decreasing κ. This peak turns into the magnetic Bragg peak at $T=0$, and its width reflects the overdamped nature of the spin waves with wavelength longer than the coherence length. In region (b), the κ integrations in Eq. (6) are dominated by $\mathbf{k}\approx 0$, and $\tilde{\mathbf{k}}\approx 0$. Using Eq. (4) and neglecting terms of order $c\tilde{q}/T$, we find

$$S^{\mathrm{MF}}\approx[\sqrt{2}c\pi(S-S_c)/3\omega][n_{\tilde{q}}+1]\delta(\omega-c\tilde{q}),$$

which is proportional to the naive SWT result. The spin-wave peaks, and the resulting $\tilde{q}^{-1}$ T-independent correlations, agree with those predicted by other approaches.[15] An important effect of finite temperatures is to "soften" the magnetization *group* velocity $\partial\omega_{\mathbf{q}}/\partial\tilde{q}$ in comparison to c at long wavelengths. We note that there is a gap between the normal $(\omega<c\tilde{q})$ and the anomalous $[\omega>c(\kappa^2+q^2)^{1/2}]$ contributions of Eq. (6). We suspect, however, that this structure is an artifact of the static MF approximation, and that it might be washed out by fluctuations in λ and Q. Nevertheless, it would be interesting to see whether any double-peak features could be experimentally resolved.

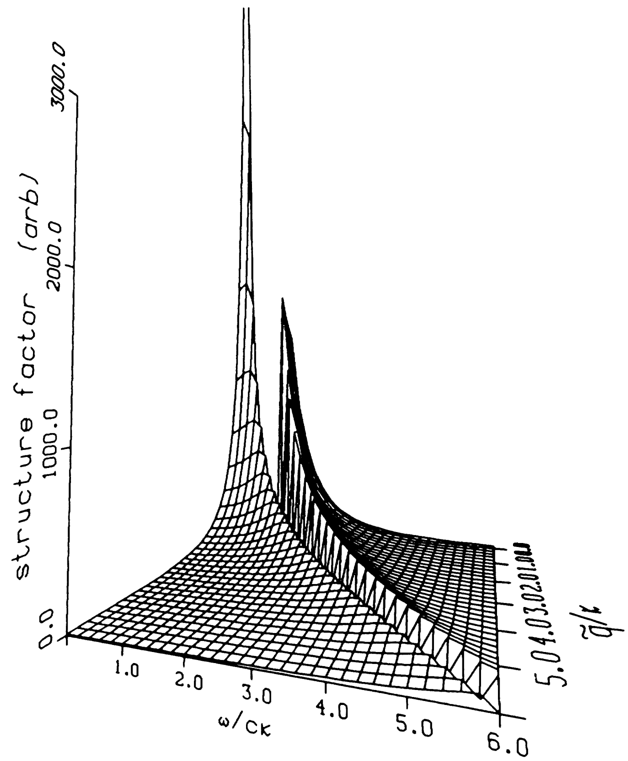

FIG. 1. The structure factor Eq. (6) at $T\ll JS(S+1)$. $\tilde{q}$ is the distance from the antiferromagnetic wave vector (π,π). κ is the inverse correlation length Eq. (8), and c is the spin-wave velocity. For low frequencies $\omega\ll T$, the structure factor is symmetric under reflection on both $\tilde{q}$ and ω axis.

The integrated ("equal time") correlation function is $\bar{S}(\mathbf{q})=\frac{2}{3}\int_{-\infty}^{\infty}d\omega\pi^{-1}S^{\mathrm{MF}}(\mathbf{q},\omega)$, where we included the correction factor of $\frac{2}{3}$ discussed above. In the regime of $c\tilde{q}\ll T\ll JS(S+1)$, $\bar{S}(\mathbf{q})$ is given by a sharply peaked function at small values of $\tilde{q}$, $\bar{S}(\mathbf{q})=\frac{16}{3}\pi^{-1}(ST/hc\kappa a)^2F(\tilde{q}/\kappa)$, where

$$F(x)=\int_0^{\infty}dk\,k((k^2+1)\{[(k+2x)^2+1][(k-2x)^2+1]\}^{1/2})^{-1}. \tag{8}$$

This limit represents the "classical" part of the fluctuations, which is distinct from the contributions of the spin-wave ridges. $\bar{S}$ at large $\tilde{q}/\kappa$ (but still $c\tilde{q}/T\ll 1$) goes as $T^2\ln\tilde{q}/\tilde{q}^2$. Equation (8) should be useful in the experimental fitting of the values of κ and c, in the region where most of the scattering is concentrated. In contrast to this result, the fer-

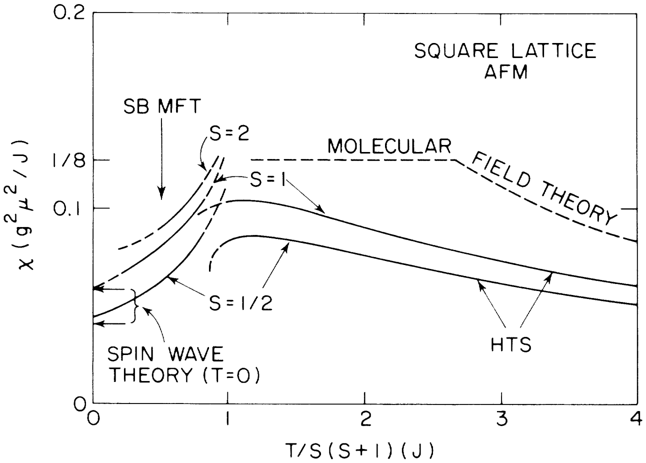

FIG. 2. The uniform magnetic susceptibility for different spin value S. High-temperature series (HTS) and the molecular-field theory are given in Refs. 16. The SWT (Refs. 4 and 5) susceptibility is rotationally averaged. The SBMFT interpolates between the two regimes.

mionic (MF) theory of Baskaran, Zou, and Anderson,[8] and also the flux phase of Affleck and Marston[8] yield $\bar{S}(\mathbf{q})$ which are spread throughout the Brillouin zone, with much weaker singularity[6] at $\tilde{q}=0$, even at $T=0$.

It is interesting to compute the uniform susceptibility, which is given by $\chi=(g^2\mu^2/T)\bar{S}(\mathbf{q}=0)\equiv g^2\mu^2 Z_\chi/8J$. In Fig. 2 we plot our $\chi(T)$ (for the applicable range of T) and show how it interpolates between the rotationally averaged SWT result[5] and the high-temperature series expansion of Rushbrooke and Wood.[16] It is also important to note slight discrepancies for the value of Z_χ between our result and that of Oguchi as seen in Table I. The disagreement, which affects CHN's determination of the correlation-length renormalization Z_κ, probably arises from either of the two reasons: (1) the smallness of $S=\frac{1}{2}$ or (2) the zero-temperature limit of the SWT in 2D is tricky since the $\mathbf{k}$ summations are logarithmically divergent. Numerical simulations might be able to determine which approximation is better in this limit. In any case, the agreement (as expected) improves with the size of S. We also present our result for the specific-heat T^2 coefficient δ in Table I.

Our formalism allows a natural extension to the three-dimensional problem with interplanar coupling ($J^{\text{ip}}\ll J$). The Schwinger boson dispersions would acquire a weak κ_z dependence, and therefore for $J(\kappa a)^2\gg J^{\text{ip}}$, disordered two-dimensional behavior is expected. At lower temperatures, the integrand in the summation of Eq. (4) is not sufficiently divergent, and a crossover to 3D behavior occurs, where κ vanishes at the Néel temperature $T=T_{\text{N}}$. The susceptibility would have a weak nonanalyticity at T_{N}, and would deviate from the 2D behavior for $T<T_{\text{N}}$. These conclusions agree with those arrived at by renormalization-group analysis.[4] We have also extended the theory to take into account the effects of frustrating antiferromagnetic next-nearest-neighbor interactions.

We thank S. Chakravarty and V. Emery for helpful conversations. One of us (A.A.) was supported by the Division of Material Sciences, U.S. Department of Energy, under Contract No. DE-AC02-76H00016. Another (D.P.A.) was supported in part by Grant No. DMR-MRL-85-19460.

[1]D. Vaknin *et al.*, Phys. Rev. Lett. **58**, 2802 (1987). Y. Endoh *et al.*, Phys. Rev. B **37**, 7443 (1988).

[2]J. M. Tranquada *et al.*, Phys. Rev. Lett. **60**, 156 (1988).

[3]F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983), and Phys. Lett. **93**, 464 (1983), and to be published.

[4]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988).

[5]T. Oguchi, Phys. Rev. **117**, 117 (1960).

[6]D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).

[7]N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[8]P. W. Anderson, Science **235**, 1196 (1987); G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987); I. Affleck and J. B. Marston, to be published.

[9]P. B. Weigmann, Phys. Rev. Lett. **60**, 821 (1988). In contrast to this field theory, absence of the Hopf invariant for the quantum-Heisenberg model was shown by T. Dombre and N. Read, to be published; F. D. M. Haldane, to be published.

[10]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[11]S. H. Shenker and J. Tobochnik, Phys. Rev. B **22**, 4462 (1980).

[12]Rajiv R. P. Singh, M. P. Gelfand, and D. A. Huse, to be published.

[13]J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978); J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).

[14]M. Takahashi, Phys. Rev. Lett. **58**, 168 (1987).

[15]J. Villain, J. Phys. (Paris) **35**, 27 (1974); G. Reiter, to be published.

[16]G. S. Rushbrooke and P. J. Wood, Mol. Phys. **1**, 257 (1958); M. E. Lines, Phys. Rev. **164**, 736 (1967); L. J. de Jongh and A. R. Miedema, Adv. Phys. **23**, 1 (1974).