

## Quantum phases of the Shraiman-Siggia model

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We examine phases of the Shraiman-Siggia model of lightly doped, square lattice quantum antiferromagnets in a self-consistent, two-loop, interacting magnon analysis. We find magnetically ordered and quantum-disordered phases both with and without incommensurate spin correlations. The quantum-disordered phases have a pseudogap in the spin excitation spectrum. The quantum transition between the magnetically ordered and commensurate quantum-disordered phases is argued to have the dynamic critical exponent  $z = 1$  and the same leading critical behavior as the disordering transition in the pure  $O(3)$   $\sigma$  model. The relationship to experiments on the doped cuprates is discussed.

### I. INTRODUCTION

The last few years have seen numerous experiments examining the magnetic properties of the doped copper oxide compounds in some detail. Neutron scattering experiments on  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  have shown that the commensurate long-range-ordered Néel state at  $x = 0$  evolves into a phase with short-range incommensurate spin correlations above  $x = 0.075$ .<sup>1</sup> However, our theoretical understanding has not kept in step, partly due to the numerous competing effects and ensuing complexity of these materials: At low temperatures the effects of disorder are paramagnetic, and at larger doping there is the onset of superconductivity.

On the theoretical side, a popular model for investigating the interplay of doping and antiferromagnetic spin correlations has been the  $t$ - $J$  model. Numerical and high-temperature series studies of this model have been especially valuable as a testing ground for various theoretical ideas. In an important advance, Shraiman and Siggia<sup>2</sup> (SS) proposed a phenomenological description of the long-wavelength interplay between spin and charge transport in this model. There are numerous theoretical reasons for believing that their long-wavelength model is a correct description of the  $t$ - $J$  model at low temperatures and small doping. In this latter regime, it is expected that the SS model is quite robust, and will describe a whole class of doped antiferromagnets, not just the  $t$ - $J$  model. However, at some finite doping, an approach based upon long-wavelength distortions of the background antiferromagnetic order must eventually become invalid; the mechanism of this breakdown of the SS model is not understood and remains an important open problem. This paper shall examine the SS model in an approach which is designed to explicate the nature of the quantum-disordered phases i.e., the phases with no long-range magnetic order. These phases appear at a reasonably small doping concentration. We conjecture, although we certainly cannot rule out the contrary, that these phases are also present in the  $t$ - $J$  model, and are

not artifacts of using the SS model. We will also discuss the relationship of our results to other theoretical work and some experiments in Sec. IV.

We begin by writing down a simplified version of the action  $S$  of the Shraiman-Siggia model:

$$S = \int_0^{\beta\hbar} d\tau \int d^2r [S_n + S_f + S_c], \quad (1.1)$$

with  $\tau$  the Matsubara time,  $r = (x, y)$  the spatial coordinates,  $\beta = 1/(k_B T)$ , and  $T$  the absolute temperature. The first part,  $S_n$ , describes fluctuations of the antiferromagnetic order parameter  $n_\ell$ . Here  $n_\ell$  is a three-component vector and is taken to have unit length

$$\sum_{\ell=1}^3 n_\ell^2 = 1. \quad (1.2)$$

We then have

$$S_n = \frac{\rho_s^0}{2\hbar} \left[ (\partial_x n_\ell)^2 + (\partial_y n_\ell)^2 + \frac{1}{c_0^2} \left( \frac{\partial n_\ell}{\partial \tau} \right)^2 \right], \quad (1.3)$$

with  $\rho_s^0$  the bare spin stiffness and  $c_0$  the bare spin-wave velocity. The momentum of the  $n_\ell$  field is restricted to be smaller than an ultraviolet cutoff  $\Lambda$ , which is also the scale at which the coupling constants are defined.

The action of the fermionic dopant holes is given by  $S_f$ . The holes are described by fermionic spinor fields  $\Phi_{v\alpha}$  where  $\alpha = \uparrow, \downarrow$  is the spin index, and  $v$  is "valley" index. The valleys are regions in the Brillouin zone around the minima of the fermion dispersion spectrum. For the square-lattice  $t$ - $J$  model there is a great deal of evidence that there are two valleys centered at the points  $(\pi/2, \pm\pi/2)$  in the reduced Brillouin zone.<sup>3,4</sup> We will rotate our coordinate system from the conventional one, so that our  $x$  axis is at an angle of  $45^\circ$  to the axes of the square lattice, and the principal axes of the valleys are along the new  $x$  and  $y$  axes; the index  $v$  will therefore take the values  $v = x, y$ . Further, we will measure momenta

from the center of the valleys. With these conventions, the fermionic action  $S_f$  is

$$S_f = \Phi_{x\alpha}^\dagger \left( \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2m_l} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_h} \frac{\partial^2}{\partial y^2} \right) \Phi_{x\alpha} + \Phi_{y\alpha}^\dagger \left( \frac{\partial}{\partial \tau} - \frac{\hbar^2}{2m_h} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_l} \frac{\partial^2}{\partial y^2} \right) \Phi_{y\alpha}, \quad (1.4)$$

where  $m_l$ ,  $m_h$  are the light and heavy masses of the hole.

It is important to realize that there is no simple relationship between the bare fermionic field  $c_{i\alpha}^\dagger$  of the  $t$ - $J$  model ( $i$  is the site index) and the continuum fields  $(n_\ell, \Phi_{v\alpha})$  of the hydrodynamic SS model. Crudely speaking, one may consider this field transmutation as a form of spin-charge separation in which the spin-1/2, charge- $e$   $c_{i\alpha}^\dagger$  fermionic field has separated into the spin-1, charge-0, bosonic  $n_\ell$  quanta and the spin-1/2, charge- $e$ ,  $\Phi_{v\alpha}$  fermions.

Finally, we will consider only the leading term in the coupling,  $S_c$ , between the holes and the  $n_\ell$  field, which is responsible for inducing local incommensurate spin correlations. It is expected that the remaining terms in the SS model are innocuous and do not change the results of this paper qualitatively. We have

$$S_c = \kappa (\Phi_{v\alpha}^\dagger \sigma_{\alpha\beta}^\ell \Phi_{v\beta}) (\epsilon_{lmnp} n_m \partial_v n_p), \quad (1.5)$$

where  $\sigma^\ell$  are three Pauli matrices, and  $\kappa$  is a coupling constant. A crucial feature of the SS model is that there is no three-body coupling like  $n_\ell \Phi_{v\alpha}^\dagger \sigma_{\alpha\beta}^\ell \Phi_{v\beta}$  between the fermions and  $n_\ell$  quanta.<sup>5</sup> Such a term is forbidden by a sublattice interchange symmetry of the SS model<sup>2</sup> under which  $n_\ell$  change sign while the  $\Phi_{v\alpha}$  remain invariant. Other models of nearly antiferromagnetic Fermi liquids<sup>6,7</sup> possess such a term and, as a result, have quantum disordered phases with rather different properties.

We wish to clarify a crucial point about our particular form of  $S$  at the outset. SS have shown that there is a mapping, in principle exact, to an alternative form of  $S$  in which the degrees of freedom are a spin-1/2, charge-0, complex scalar  $z_\alpha$  with  $\alpha = \uparrow, \downarrow$  and *spinless*, charge- $e$  fermions  $\Psi_{v\alpha}$  where  $\alpha = A, B$  is a sublattice index. The  $(n_\ell, \Phi_{v\alpha})$  fields are related to the  $(z_\alpha, \Psi_{v\alpha})$  fields by

$$n_\ell = z_\alpha^* \sigma_{\alpha\beta}^\ell z_\beta, \quad \begin{pmatrix} \Phi_{v\uparrow} \\ \Phi_{v\downarrow} \end{pmatrix} = \begin{pmatrix} z_\uparrow & -z_\downarrow^* \\ z_\downarrow & z_\uparrow^* \end{pmatrix} \begin{pmatrix} \Psi_{vA} \\ \Psi_{vB} \end{pmatrix}. \quad (1.6)$$

Note that there is a U(1) gauge transformation on the  $(z_\alpha, \Psi_{v\alpha})$  fields which leaves the  $(n_\ell, \Phi_{v\alpha})$  fields invariant:

$$z_\alpha \rightarrow z_\alpha e^{i\phi}, \quad \Psi_{vA} \rightarrow \Psi_{vA} e^{-i\phi}, \quad \Psi_{vB} e^{i\phi}, \quad (1.7)$$

where  $\phi$  has an arbitrary dependence on spacetime. The action in terms of the  $(z_\alpha, \Psi_{v\alpha})$  will therefore also have to be invariant under the gauge transformation; there is no such restriction on the action in the  $(n_\ell, \Phi_{v\alpha})$  variables. This latter absence of gauge restrictions and associated long-range gauge forces will be quite useful to us in our analysis.

SS go on to state that equivalent results are obtained in computations using either choice of fields. In principle, this statement is correct. In practice, however, one is usually restricted in the analysis to perturbation theory, in which the quantum numbers of the low-lying excitations are essentially identical to those of the degrees of freedom in the action. Equivalent results in both theories have been obtained in the vicinity of magnetically ordered states, where one is performing a small fluctuation, spin-wave analysis. On the other hand, the choice of fields is expected to have dramatic consequences in a quantum-disordered state. Kane *et al.* and others<sup>8</sup> made a choice of fields equivalent to the  $(z_\alpha, \Psi_{v\alpha})$  formulation of the SS model. Thus, not surprisingly, their Schwinger-boson mean-field theory yielded a quantum-disordered phase with deconfined, spin-1/2, charge-0, bosonic spinons (the  $z_\alpha$ ) and spinless, charge- $e$  fermions ( $\Psi_{v\alpha}$ ).

In this paper, we use another approach and shall examine the phases of the SS model which are obtained naturally in the  $(n_\ell, \Phi_{v\alpha})$  formulation. Some of the results of our calculations were noted some time ago.<sup>9</sup> While, in the end, we have no formal justification for claiming that the  $(n_\ell, \Phi_{v\alpha})$  formulation is more accurate than the  $(z_\alpha, \Psi_{v\alpha})$  approach, we can offer the following motivations. The  $n_\ell$  field formulation has been quite successful in describing the undoped, frustrated antiferromagnet. The long-wavelength action of the undoped antiferromagnet<sup>10</sup> is simply the  $O(3)$   $\sigma$  model,  $S_n$ , and it is expected to display a quantum-disordered phase in which massive  $n$  quanta form the lowest excitations and carry spin 1.<sup>11</sup> Consistent with this, recent investigations of the quantum-critical behavior in these systems have argued for the superiority of the  $n$ -field-based approach, and have successfully explained a number of experimental and numerical computations on the square lattice antiferromagnet.<sup>9,12</sup> Further, careful analysis of fluctuations<sup>13</sup> in the  $z_\alpha$ -based theories of the undoped antiferromagnet has yielded quantum-disordered phases in which the quantum numbers of the low-lying excitations are identical to those of the  $n$  field, which means that fluctuations in fact confine bosonic spinons into  $S = 1$  particles. It is then natural to explore the consequences of doping in a model in which the correct physics in the limit of zero doping is captured most directly, i.e., in the  $(n_\ell, \Phi_{v\alpha})$  approach. We shall argue later in this paper that the results of such an investigation are consistent with the available numerical and experimental data on doped antiferromagnets.

## A. Summary of results

We now discuss the main results of our calculations. We will distinguish the quantum phases by the properties of the equal-time  $n_\ell$  correlator

$$\tilde{S}(q) = \langle |n_\ell(q)|^2 \rangle \quad (1.8)$$

as  $T \rightarrow 0$ , as a function of the momentum  $q$ . [We emphasize that  $\tilde{S}(q)$  is *not* the full structure factor  $S(q)$  measured in neutron scattering experiments;  $S(q)$  will con-

tain additional terms involving the contribution of the spin-1/2  $\Phi_{v\alpha}$  fields. Determining these terms requires knowledge of the connection between the  $\Phi_{v\alpha}$  fields and the bare  $c_{i\alpha}$  electrons, which we do not have.] Phases with magnetic long-range order have a  $\delta$ -function term in  $\tilde{S}(q)$  at  $T = 0$ ; this  $\delta$ -function is at  $q = 0$  in the commensurate long-range-ordered phase (hereafter referred to as CLRO) and at  $q \neq 0$  for the case of incommensurate long-range order (ILRO) [ $q$  is measured from  $(\pi, \pi)$ ]. The quantum-disordered phases have no  $\delta$ -function terms at  $T = 0$ , but only a peak of finite, though possibly small, width. This peak is at  $q = 0$  in the commensurate quantum-disordered phase (CQD) and at  $q \neq 0$  in the incommensurate case (IQD). In agreement with the SS analysis<sup>2</sup> and experimental results,<sup>1</sup> the peak in the ILRO and IQD phases was found to occur along the conventional (1, 0) and (0, 1) axes of the square lattice [these are the (1, 1) and (1, -1) axes in our rotated coordinate system].

We will have little to add here to existing studies<sup>2,14-16</sup> of the properties of the magnetically ordered phases (CLRO and ILRO): Their low-lying excitations are spin waves involving long-wavelength deformations of the ordered state. Our focus will mainly be upon the new quantum-disordered phases (CQD and IQD) and their unusual properties. The  $n_\ell$  quanta in both phases were found to be fully gapped. The low-lying excitations in the  $n_\ell$  sector consist of a triply degenerate spin-1 particle with a finite energy. However, the spin 1/2  $\Phi_{v\alpha}$  particles continue to form a Fermi sea which possesses gapless fermionic excitations with charge  $e$  and spin 1/2. Despite the presence of these gapless excitations, the  $n_\ell$  gap is robust as there is no term in the SS model which permits the decay of a  $n_\ell$  quantum to a fermion particle-hole pair. The importance of the absence of the three-body term noted above is now evident. Taken as a whole, the model thus only has a pseudogap to spin excitations in the CQD and IQD phases. One of the consequences of the presence of the gapless spin-1/2 fermions is that the uniform spin susceptibility of the CQD and IQD phases will be finite at  $T = 0$  due to the Pauli contribution.<sup>5</sup> We also note that our calculation has completely neglected the effect of Berry phases; in the context of undoped antiferromagnets it has been argued<sup>13</sup> that Berry phases should induce spin-Peierls long-range order in the CQD phases. It is possible that such spin-Peierls order will also exist in the CQD phase of the doped antiferromagnet.

We have numerically solved the equations of a self-consistent, two-loop, interacting magnon approximation to  $S$  and thus obtained a partial survey of its phase diagram as a function of  $\rho_s^0$ ,  $\kappa$ , and the hole density. Parameters were always chosen so that the zero doping state was CLRO. This CLRO state was always found to be stable over a small, but finite, doping concentration. Over some of the regime examined, the sequence of phases with increasing doping was CLRO-CQD-IQD. We studied the  $T = 0$  quantum transition between the CLRO and CQD phases and will present evidence indicating that it has dynamic critical exponent  $z = 1$  and the same leading critical behavior as the transition in the pure  $O(3)$   $\sigma$  model; however, the corrections to scaling

in the two models were found to be quite different. The boundary between the CQD and IQD phases is an example of a disorder line.<sup>17</sup> Our calculation only found a nonanalyticity in the dependence of the structure factor on the bare coupling constants at the disorder line, but no strong long-wavelength fluctuations.

In a region of the phase diagram with  $\kappa$  large, we found the sequence CLRO-ILRO with increasing doping. In principle, there should eventually be a ILRO to IQD transition, but for the parameters examined, we did not find one before a doping level where the incommensuration wave vector was almost as large as the momentum upper cutoff.

We will argue from the above numerical results, and from theoretical considerations, that there is a Lifshitz point in the  $\rho_s^0, \kappa$  plane where all the four phases, CLRO, ILRO, CQD, IQD, meet. Some properties of this multicritical point will be discussed.

We also have extensive results on the temperature dependence of equal-time correlation functions in the various phases. In particular, the temperature dependences in the spin correlation length and the structure factor are quite instructive, and will be described later.

## II. CALCULATIONS

For the case of the undoped antiferromagnet, the  $1/N$  expansion on the  $O(N)$  nonlinear  $\sigma$  model offers a convenient and accurate method for exploring properties in the vicinity of  $T = 0$  quantum transitions.<sup>12</sup> The extension of the  $1/N$  expansion to the doped antiferromagnet is however not straightforward because of the presence of the third-rank  $\epsilon_{lmp}$  tensor in  $S_c$  [Eq. (1.5)], which is special to the case  $N = 3$ . Even with this complication, it is still possible to justify perturbative  $1/N$  calculations, although in a rather inelegant way: After the fermions have been integrated out, the coupling  $\kappa$  in the effective action of the  $n$  field has to be scaled by  $1/N^\mu$  where  $0 < \mu < 1/2$ . Not much is learned from this extension to general  $N$ , and we will therefore spare the reader the details. We will be satisfied, instead, in restricting our discussion to the special case of  $N = 3$ , and viewing our  $1/N$  calculation as a physically motivated, self-consistent, interacting magnon approximation. The magnon-magnon interactions are computed in a manner which is directly inspired by the  $1/N$  expansion of the undoped antiferromagnet.<sup>12</sup>

An important property of our approach is that spin-rotation invariance is explicitly preserved at all stages of the calculation. This is crucial for a proper study of the quantum-disordered phases of the model, especially when the  $n$  quanta acquire a gap. We thus expect our approximations to work best in the quantum-disordered phase, at the  $T = 0$  quantum transition, and in the intermediate-temperature quantum-critical region.<sup>10,12</sup> At the same time, the low-temperature properties in a region with magnetic long-range order (the renormalized classical region<sup>10</sup>) in the ground state may not be well described. Even in the undoped antiferromagnet, the  $1/N$  expansion is singular in the renormalized-

classical region, and a careful interpretation of the results is required.<sup>12</sup> We therefore will focus below mainly on the quantum-disordered phases.

We begin by expressing the action in suitable dimensionless parameters. We rescale lengths such that the upper cutoff in momentum space for the  $n$  field is 1; thus

$$r \rightarrow \frac{r}{\Lambda}. \quad (2.1)$$

Similarly, the times  $\tau$  are rescaled so that the bare spin-wave velocity of the  $n$  field is unity:

$$\tau \rightarrow \frac{\tau}{c_0 \Lambda}. \quad (2.2)$$

After rescaling the temperature

$$T \rightarrow T \frac{\hbar c_0 \Lambda}{k_B}, \quad (2.3)$$

we then have the following modified form of  $S_n$ :

$$S_n = \frac{1}{2g} [(\partial_x n_\ell)^2 + (\partial_y n_\ell)^2 + (\partial_\tau n_\ell)^2], \quad (2.4)$$

where the dimensionless coupling constant  $g$  is given by

$$g = \frac{\hbar c_0 \Lambda}{\rho_s^0}. \quad (2.5)$$

The fermionic action will retain its form after rescaling the field  $\Phi \rightarrow \Lambda \Phi$  and rescaling to the dimensionless effective masses

$$m_{h,l} \rightarrow m_{h,l} \frac{\Lambda \hbar}{c_0}. \quad (2.6)$$

Finally in  $S_c$  we replace  $\kappa \rightarrow \kappa c_0$ .

We will impose the constraint (1.2) by a Lagrange multiplier field  $\lambda$ . Thus we need to evaluate the functional integral

$$Z = \int \mathcal{D}n_\ell \mathcal{D}\Phi_{v\alpha} \mathcal{D}\lambda \exp\left(-S - i \int_0^{1/T} d\tau \int d^2x \frac{\lambda}{2g} (n_\ell^2 - 1)\right). \quad (2.7)$$

It is now possible to set up a rotationally invariant, diagrammatic expansion of all observables associated with  $Z$ . We will work at finite  $T$ , and so no breaking of spin-rotation invariance can occur; the properties of the ground state will be elucidated by taking the  $T \rightarrow 0$  limit. We treat the  $\lambda$  field in much the same way as in the undoped system.<sup>11</sup> We assume that fluctuations of  $i\lambda$  occur about a saddle point value  $\bar{\lambda}$ ; we therefore write

$$i\lambda = \bar{\lambda} + i\tilde{\lambda}, \quad (2.8)$$

where  $\tilde{\lambda}$  is the fluctuating part of  $\lambda$ . The value of  $\bar{\lambda}$  is to be determined at the end of the calculation to satisfy the constraint (1.2). The diagrammatic expansion now has three bare propagators: the conventional Green's function of the fermions  $\Phi_{v\alpha}$ , the propagator  $G^0$  of the  $n_\ell$  field,

$$G^0(q, i\omega_n) = \frac{1}{q^2 + \omega_n^2 + \bar{\lambda}} \quad (2.9)$$

( $q$  is the wave vector and  $\omega_n$  is a Matsubara frequency), and the propagator  $1/\Pi$  of  $\tilde{\lambda}$ , with<sup>11</sup>

$$\Pi(q, i\omega_n) = T \sum_{\epsilon_n} \int \frac{d^2k}{4\pi^2} G^0(k+q, i\epsilon_n + i\omega_n) G^0(k, i\epsilon_n). \quad (2.10)$$

There are two interaction vertices: the four-body ( $n$ - $n$ - $\Phi$ - $\Phi$ ) coupling in  $S_c$  and a three-body ( $\tilde{\lambda}$ - $n$ - $n$ ) vertex with the value  $i/(2g)$ . Finally, there is a rule to prevent overcounting: No  $\tilde{\lambda}$  propagator can be followed by a bubble consisting just of two  $G^0$  propagators.

We may now write the fully renormalized correlator of the  $n$  field in the form

$$G(q, i\omega_n) = \frac{1}{q^2 + \omega_n^2 + m^2 + \Sigma(q, i\omega_n) - \Sigma(0, 0)}, \quad (2.11)$$

where  $\Sigma$  is the self-energy and the "mass"  $m$  is given by

$$m^2 = \bar{\lambda} + \Sigma(0, 0). \quad (2.12)$$

The lowest-order contributions to  $\Sigma$  from magnon-magnon ( $\Sigma_n$ ) and magnon-fermion ( $\Sigma_f$ ) interactions are shown in Fig. 1, and their values are

$$\begin{aligned} \Sigma &= \Sigma_n + \Sigma_f, \\ \Sigma_n(q, i\omega_n) &= \frac{2}{3} T \sum_{\epsilon_n} \int \frac{d^2k}{4\pi^2} \frac{G^0(k+q, i\epsilon_n + i\omega_n)}{\Pi(k, i\epsilon_n)}, \\ \Sigma_f(q, i\omega_n) &= -4g^2 \kappa^2 T \sum_{\epsilon_n} \int \frac{d^2k}{4\pi^2} (2q_v + k_v)^2 \chi_v(k, i\epsilon_n) \\ &\quad \times G^0(k+q, i\epsilon_n + i\omega_n), \end{aligned} \quad (2.13)$$

where  $\chi_v$  is polarization of the fermion in valley  $v$ . We will assume that the fermions continue to form a conventional Fermi liquid even in the presence of  $n_\ell$  field fluctuations. We therefore used the following expression for  $\chi_v$ , appropriate for an elliptical Fermi surface:

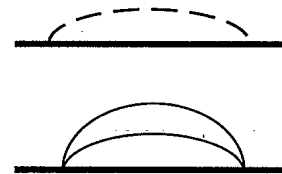


FIG. 1. Feynman diagrams for the  $n$  self-energy. The thick, solid line is the  $n$  propagator, the thin, solid lines are the hole fermions, and the dashed line is the  $\lambda$  propagator.

$$\chi_x(q, i\epsilon_n) = \chi_0(T) \left( 1 - \frac{|\epsilon_n|}{[\epsilon_n^2 + v_F^2 \{q_x^2 (m_h/m_l)^{1/2} + q_y^2 (m_l/m_h)^{1/2}\}]^{1/2}} \right) \quad (2.14)$$

and similarly for  $\chi_y$ . The Fermi velocity  $v_F$ , the Fermi wave vector  $k_F$ , and the doping concentration  $\delta$  are related by the equations

$$v_F = \frac{k_F}{\sqrt{m_l m_h}}, \quad \delta = \frac{k_F^2}{\pi}, \quad (2.15)$$

and the polarization is taken to vanish unless

$$[q_x^2 (m_h/m_l)^{1/2} + q_y^2 (m_l/m_h)^{1/2}]^{1/2} < 2k_F. \quad (2.16)$$

The prefactor  $\chi_0$  we chose as the compressibility of a free Fermi gas at a temperature  $T$ :

$$\chi_0(T) = \frac{\sqrt{m_l m_h}}{2\pi} \left( 1 - e^{-k_F v_F / (2T)} \right). \quad (2.17)$$

The restriction (2.16) will have a crucial effect on the structure of  $\Sigma_f$  in the small doping limit. In particular, it is easy to see that both  $\Sigma_f(0,0)$  and  $\partial\Sigma_f/\partial q^2(0,0)$  vanish as  $k_F \rightarrow 0$ . The fermions therefore only have a weak effect on the undoped state in this limit, and the insulating CLRO state is always stable towards infinitesimal doping. In this respect our results differ from those of SS, who did not consider the consequences of spin fluctuations. What we have found here is that because the dynamic range of the spin fluctuations is much larger at small doping than that of the fermions, the fermions only have a weak effect on the  $n$  quanta.

Our approach consisted of using the above approximation for  $\Sigma$  and then solving the constraint equation (1.2), or

$$3gT \sum_{\omega_n} \int \frac{d^2q}{4\pi^2} G(q, i\omega_n) = 1 \quad (2.18)$$

for the value of  $m^2$  (or equivalently  $\bar{\lambda}$ ). The dependence of  $\Sigma$  on  $G^0$  was made partially self-consistent by replacing  $\bar{\lambda}$  by  $m^2$  in (2.9), thus using  $G^0(q, i\omega_n) = 1/(q^2 + \omega_n^2 + m^2)$  in (2.10) and (2.13). A fully self-consistent approach would require we replace  $G^0$  by  $G$  in these equations; this is computationally much more difficult and was not numerically implemented. Our approximation thus amounts to replacing  $G^0$  by  $G$ , but then ignoring the momentum and frequency dependence of the self-energy in  $G$ . For the most part, this omission is not expected to be serious, as corrections can be organized order by order in  $\kappa$ . However, we cannot rule out the possibility, especially in the quantum-disordered phases, that there is some entirely different, possibly gapless, solution of the fully self-consistent equations; such a solution will clearly be nonperturbative in  $\kappa$ . We also note here that in our analytical considerations below of the boundaries between the phases we will include the full  $G$  in (2.13).

The numerical determination  $m^2$  as a function of  $T, \delta$  was carried out on a HP-RISC workstation. A meaningful solution always existed at all finite  $T$ , with no phase transitions as a function of  $T$  or  $\delta$ . Phase transitions are however present at  $T = 0$ , and were examined by studying the  $T \rightarrow 0$  limit of our solutions. The computations required about 3 weeks of computer time.

### III. RESULTS

We now describe the results of our numerical calculations. The nature of the ground state can be determined from the values and  $T$  dependences of  $q_c$  and  $\bar{m}$  where  $q = q_c$  is the location of the maximum of  $G(q, i\omega_n = 0)$ , and

$$\bar{m}^2 = m^2 + \Sigma(q_c, i\omega_n = 0) - \Sigma(0,0). \quad (3.1)$$

It is easy to see from (2.11) that  $\bar{m}$  is roughly the inverse correlation length ("roughly" because this neglects  $\partial\Sigma/\partial q^2$ ; including this term yields corrections of the order of unity which are not strongly  $T$  dependent). The various phases can be identified by studying the  $T$  dependence of  $\bar{m}$  as  $T \rightarrow 0$ , as will be described below. The values of  $q_c$  were approximately  $T$  independent and distinguish between commensurate and incommensurate phases.

Two samples of our results are contained in Figs. 2 and 4 which plot the  $T$  and doping dependence of  $\bar{m}$  for two sets of coupling constants. For completeness we also

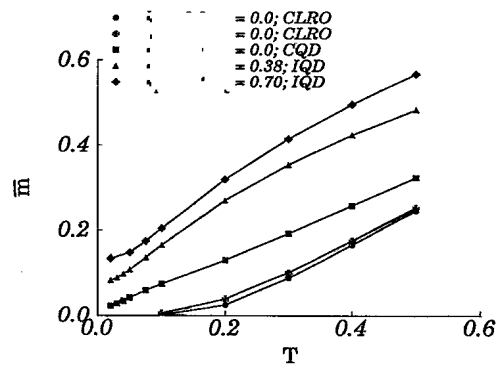


FIG. 2. Values of  $\bar{m}$  [defined in Eq. (3.1); it is roughly the inverse correlation length] as a function of  $T$  for various doping levels specified by  $k_F$ . The coupling constants were  $g = 3$ ,  $\kappa = 1.5$ ,  $(m_l m_h)^{1/2} = 0.6$ ,  $m_l/m_h = 0.1296$ . The maxima in the structure factor are at  $q = q_c(\pm 1, \pm 1)/\sqrt{2}$  in our rotated coordinate system; this places them at  $(\pi \pm q_c, \pi)$  and  $(\pi, \pi \pm q_c)$  in the conventional Brillouin zone of the square lattice. All parameters are measured in the dimensionless units described in Sec. II. The small- $T$  behavior of  $\bar{m}$ , and the value of  $q_c$  identifies the nature of the ground state (CLRO, ILRO, CQD, IQD) which is also noted.

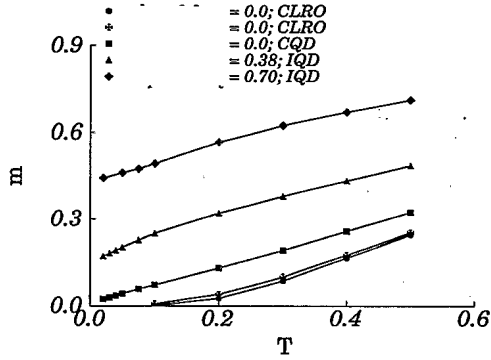


FIG. 3. The values of  $m$  associated with the results for  $\bar{m}$  in Fig. 2 for the commensurate states  $m = \bar{m}$ .

show in Figs. 3 and 5 the values of  $m$  for the same samples. We will now describe the properties of the phases in these figures and follow that up with some general discussion on the nature of the quantum transitions between them.

#### A. Long-range-ordered states

The states with magnetic order are expected to have  $\bar{m} \rightarrow 0$  as  $T \rightarrow 0$ . In particular, the low- $T$  dependence should be<sup>18</sup>

$$\bar{m} \sim \exp\left(-\frac{2\pi\rho_s}{k_B T}\right), \quad (3.2)$$

where  $\rho_s$  is the fully renormalized spin stiffness. Numerical solutions at very lower  $T$  took longer times to converge, and so it was difficult to see this exponential behavior in some of the doped samples. We simply identified the samples in which  $\bar{m}$  vanished with an upward curvature as  $T \rightarrow 0$ , as possessing magnetic long-range order. Further states with  $q_c = 0$  ( $q_c \neq 0$ ) were identified as CLRO (ILRO).

#### B. Quantum-disordered states

These states have  $\bar{m}$  saturating at a finite value as  $T \rightarrow 0$ , which is roughly the gap,  $\Delta \sim \bar{m}(T \rightarrow 0)$ , in the

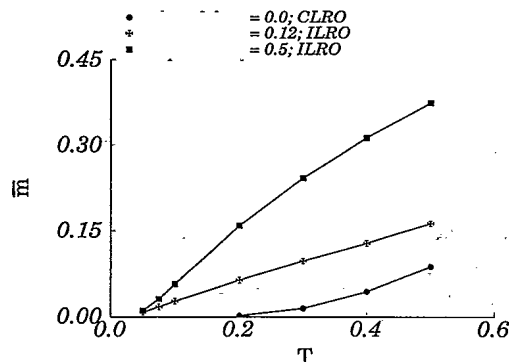


FIG. 4. As in Fig. 2 but for  $g = 6$ ,  $\kappa = 2$ ,  $(m_\ell m_h)^{1/2} = 0.6$ ,  $m_\ell/m_h = 0.1296$ .

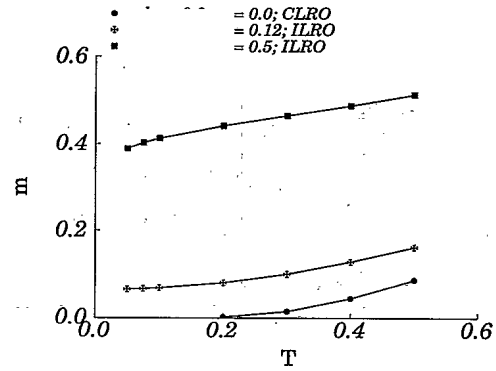


FIG. 5. The values of  $m$  associated with the results for  $\bar{m}$  in Fig. 4.

$n$  sector. Again, the value of  $q_c$  distinguishes between the CQD and IQD states.

We examine the nature of the spin correlations at a point in the IQD phase by plotting the  $n$  field contribution to the structure factor  $\tilde{S}(q)$ ,

$$\tilde{S}(q) = gT \sum_{\omega_n} G(q, \omega_n), \quad (3.3)$$

in Fig. 6. Notice that there is strong overlap between the peaks at high temperature. Upon lowering the temperature, the peaks first sharpen considerably, but then their width saturates.

Let us discuss the form of the  $n$  spectrum at  $T = 0$  in the CQD phase. We will focus on real frequencies,  $\omega$  just above the gap  $\Delta$ , and small momenta  $q$ . The magnon contribution to the self-energy  $\Sigma_n$  in (2.13) does not acquire an imaginary part until  $\omega = 3\Delta$  and can therefore be completely ignored. The damping from the fermion particle-hole continuum  $\Sigma_f$  is however not so innocuous. We find<sup>19</sup>

$$\text{Im}\Sigma_f(q, \omega) \sim \begin{cases} 0, & 0 < \omega < \Delta, \\ |q|(\omega - \Delta)^2, & 0 < \omega - \Delta \ll \frac{q^2}{2\Delta}, \\ \Delta^{1/2}(\omega - \Delta)^{5/2}, & \omega - \Delta \gg \frac{q^2}{2\Delta}, \end{cases} \quad (3.4)$$

and  $\text{Im}\Sigma_f(q, -\omega) = -\text{Im}\Sigma_f(q, \omega)$ . The  $n$  spectral weight is then given by

$$G(q, \omega) \sim \frac{1}{\Delta^2 + q^2 - \omega^2 + \Sigma_f(q, \omega)}. \quad (3.5)$$

From the above results it follows that at  $q = 0$  we have

$$\text{Im}G(q = 0, \omega \geq \Delta) = \frac{a_1}{\Delta} \delta(\omega - \Delta) + \frac{a_2}{\Delta^{3/2}} (\omega - \Delta)^{1/2} \quad (3.6)$$

for some constants  $a_1, a_2$ . Thus there is a sharp spin-1 quasiparticle peak, and a second background term which is a direct consequence of the coupling of the  $n$  quanta to the particle-hole continuum. At small, but finite  $q$ , the

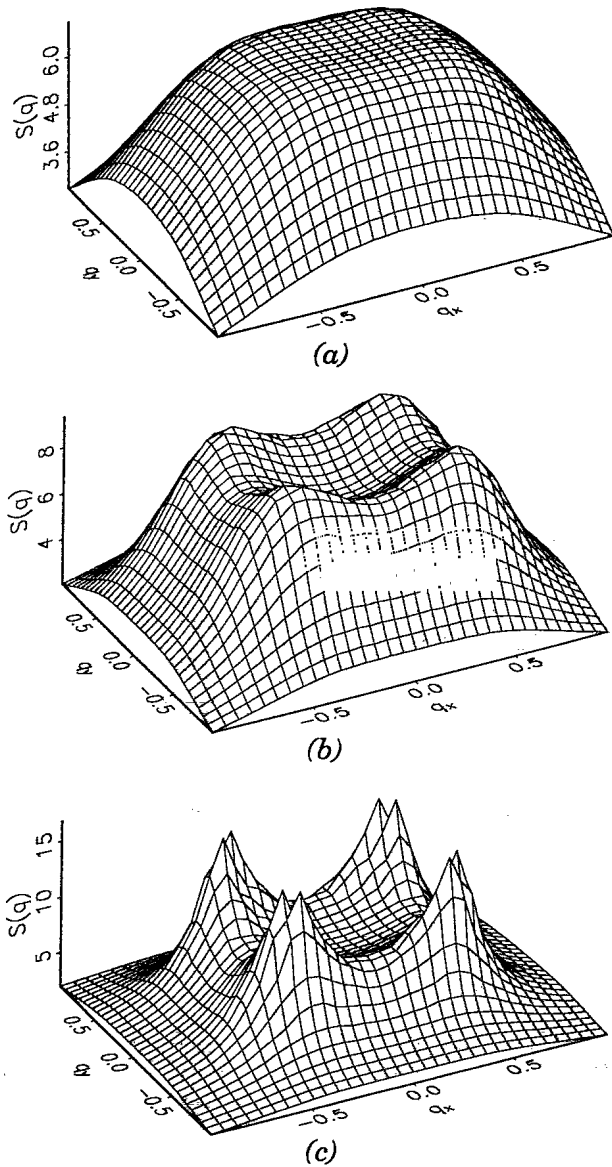


FIG. 6. Contribution of the  $n$  field to the structure factor,  $\tilde{S}(q)$ , in the IQD phase. We use the coupling constants of Fig. 2 at  $k_F = 0.3$ . The temperatures are (a)  $T = 0.5$ , (b)  $T = 0.2$ , and (c)  $T = 0.02$ . The jagged double peaks in (c) are an artifact of the plotting routine.

sharp peak moves to  $\omega \sim \Delta + q^2/(2\Delta)$  and acquires a finite width; there is absorption at all frequencies greater than  $\Delta$ .

The spectral properties of the IQD phase are essentially identical except that the role of the point  $q = 0$  is replaced by  $q = q_c$ ; in obtaining this result it is, of course, necessary to replace  $G^0$  by  $G$  in (2.13).

### C. Quantum transitions

Our results in Figs. 2 and 4 show two sequences of quantum transitions with increasing doping: CLRO-CQD-IQD and CLRO-ILRO. In the second case there should eventually be a ILRO to IQD transition, but for

the parameters examined, we did not find one before a doping level where the incommensuration wave vector was almost as large as the momentum upper cutoff. We now present a theoretical analysis of some issues raised by the existence of these quantum transitions.

#### 1. CLRO to CQD quantum transition

An important ingredient in determining the universality class of this transition is the analytic structure of the  $n$  field self-energy  $\Sigma_f$  as  $T \rightarrow 0$  in the Néel phase and the quantum-critical point. We consider (2.13) in the limit  $m \rightarrow 0$ , and  $T \rightarrow 0$  when the frequencies become continuous variables, and the Matsubara summations can be converted to integrations. It is evident that  $\Sigma_f(q, i\omega)$  is an even function of  $\omega$ . Moreover, it is not difficult to show that there are no infrared divergences in either  $\partial\Sigma_f/\partial q^2|_{q=\omega=0}$  or  $\partial\Sigma_f/\partial\omega^2|_{q=0, \omega \searrow 0}$ . This implies that for  $q, \omega$  small we have

$$\Sigma_f(q, i\omega) = \Sigma_f(0, 0) + b_1 q^2 + b_2 \omega^2 + \dots \quad (3.7)$$

Thus the gapless fermion particle-hole sea has not induced any nonanalyticities in  $\Sigma_f$  to this order. There are indeed nonanalytic terms present at higher order in  $\Sigma_f$  which are signaled by infrared divergences in higher derivatives of  $\Sigma_f$ ; we will discuss the form of such terms below. For our purposes, it is sufficient to note here that all such higher gradient terms are expected to be irrelevant at the CLRO to CQD transition. Thus the gapless fermion particle-hole excitations have had a relatively innocuous effect: They have mainly lead to renormalizations of the spin-wave velocity and spin stiffness. The universality class of the CLRO-CQD transition is thus expected to be the same as that in the undoped  $\sigma$  model. This is a transition with dynamic critical exponent  $z = 1$  and its leading universal properties have been discussed in some detail by Chubukov *et al.*<sup>12</sup> All of the scaling functions of Chubukov *et al.*<sup>12</sup> should therefore also apply to the present doped antiferromagnet. The main effect of the fermions has been to change the value of the effective coupling constant and renormalize the spin-wave velocity. Consistent with this identification, observe the linear dependence of  $\bar{m}$  with  $T$  in Fig. 2 at  $k_F = 0.2$  over a wide temperature region. This value of  $k_F$  places the system quite close to the quantum-critical point as the value of  $\Delta$  is very small. At the quantum-critical point of the  $\sigma$  model, it is predicted that  $\xi^{-1} = C_Q k_B T / \hbar c$  with  $C_Q \approx 1$  a universal number. The slope of  $m$  versus  $T$  at  $k_F = 0.2$  in Fig. 2 is about 0.65—this matches with the expected result if there is renormalization of spin-wave velocity  $c/c_0 \approx 1/0.65$ . A renormalization of the spin-wave velocity of order unity is to be expected, as the fermionic polarization  $\chi$  in (2.17) is not suppressed by a factor that vanishes as  $\delta \rightarrow 0$ .

Differences between the quantum transition in the doped and undoped antiferromagnet do however show up at the correction to scaling level. The higher-order nonanalytic terms in  $\Sigma_f$  will have a form which is quite specific to the doped model. One such term can be ob-

tained by analytically continuing to real frequencies and computing  $\text{Im}\Sigma_f$  at the critical point. We find

$$\text{Im}\Sigma_f(q, \omega) \sim q\omega^2 \quad \text{at the quantum-critical point.} \quad (3.8)$$

### 2. Lifshitz point

The existence of a direct CLRO to ILRO transition in Fig. 4 has a strong consequence for the phase diagram of the SS model. As both phases can be transformed into their quantum-disordered partners simply by increasing the value of  $g$ , we conclude that there must be a point in the phase diagram where all the four phases CLRO, CQD, IRLO, and IQD meet. Such a point is called a Lifshitz point.<sup>20</sup> Lifshitz points have so far been studied primarily in the context of thermal transitions in classical spin systems.<sup>21</sup> An important result is that such points can exist only above a lower critical dimension determined as follows:<sup>22</sup> A system in  $D$  dimensions, with incommensurate instabilities in  $m$  of those dimensions, has lower critical dimension  $2 + m/2$ . This result appears to be in conflict with our results here for the doped antiferromagnet. For we have incommensuration in  $m = 2$  spatial dimensions, giving a lower critical dimensionality equal to the spacetime dimension  $D = 3$ . So how can a Lifshitz point exist?

The answer to this apparent inconsistency lies in the form of  $\Sigma_f$ . At the Lifshitz point we clearly have  $\partial G^{-1}/\partial q^2|_{q=0, \omega=0} = 0$ . Thus the leading  $q$  dependence of  $G^{-1}$  at small  $q$  will come from higher-order terms in  $\Sigma_f$ . Let us assume that  $G^{-1} \sim \omega^2 + q^p$  at the Lifshitz point. Inserting this fully renormalized  $G$  in the result (2.13) for  $\Sigma_f$  we find by power counting

$$\Sigma_f(q, 0) = \Sigma_f(0, 0) + b_1 q^2 + b_3 q^{4-p/2} + \dots \quad (3.9)$$

Consistency now demands that  $p = 4 - p/2$  which yields  $p = 8/3$ . This differs from the value  $p = 4$  use in classical spin systems.<sup>21</sup> With this modified form of  $G$  we may repeat the calculation of Grest and Sak<sup>22</sup> and verify that spacetime dimension  $D = 3$  is above the lower critical dimension which is  $D = 7/3$ . Thus it is possible to have a Lifshitz point in  $D = 3$ .

Finally we note that a point where CLRO, ILRO, CQD, and IQD phases meet was also found in the large- $N$ ,  $\text{Sp}(N)$  theory of frustrated, two-dimensional quantum Heisenberg antiferromagnets.<sup>23</sup> The nature of this point appears to be quite different from the Lifshitz point in the present theory. In particular, the IQD phase of the  $\text{Sp}(N)$  frustrated antiferromagnets<sup>23</sup> contains deconfined, bosonic, spin-1/2 spinons, while here we have found massive, triply degenerate  $n$  quanta. Perhaps related to this difference is the fact that the large- $N$ ,  $\text{Sp}(N)$  theory<sup>23</sup> finds no softening in the spinon spectrum at the CQD-IQD boundary. Instead, at the boundary the parabolic spinon spectrum splits into two parabola with minima at incommensurate points; the curvature at the minima of the parabola always remains finite. Contrast this with the behavior of the  $n$  spectrum found here: The curvature at the minimum of the  $n$  spectrum

vanishes at the CQD-IQD boundary leading to double minima at incommensurate points in the IQD phase.

## IV. CONCLUSIONS

The most notable features of our results on the Shraiman-Siggia<sup>2</sup> model lightly doped antiferromagnets are the quantum disordered phases with a spin pseudogap. These phases possess fully gapped, triply degenerate, spin-1 magnons, and gapless, spin-1/2, charge- $e$  fermions. Several other investigators<sup>24-28</sup> have also recently explored models of the normal state of the lightly doped cuprates which have spin gaps and/or pseudogaps. This interest in pseudogaps is of course motivated by numerous experiments on the underdoped cuprates showing gaplike features in the normal state.<sup>29-31</sup> There are also interesting trends in the doping and temperature dependence of uniform spin susceptibility of the cuprates.<sup>32</sup>

For completeness we review some of the previous theoretical results, and point out the differences to our results. A number of the models<sup>24</sup> are related to resonating valence-bond-type mean-field theories;<sup>25</sup> there is a BCS-like pairing of spin-1/2, neutral spinons in the normal state at low doping, leading to a gaplike feature in the spectrum at finite temperature. However, unlike our results, this state extrapolates to a true gap at  $T = 0$ . An extension of these models to a three-band,  $\text{CuO}_2$  layer model<sup>26</sup> did possess gapless, spin-1/2, charge- $e$  fermionic excitations on the oxygen sites. However the above-gap spectrum in all of these models<sup>24,26</sup> consists of unbound spin-1/2, neutral fermions; in contrast, the spin spectral weight above the gap of our model is dominated by a spin-1, bosonic magnon. Millis and Monien have attributed the gaps to interlayer couplings in the yttrium-based cuprates.<sup>28</sup> The recent work of Sokol and collaborators<sup>27</sup> is perhaps closest in spirit to ours, although their scenario for the mixing between the  $n$  quanta and the fermions appears to be somewhat different.

Also relevant to our result is the recent high-temperature series analysis of the CLRO to CQD transition in the  $t$ - $J$  model.<sup>33</sup> This work provides some evidence in support of our result that  $z = 1$  at this transition.

Finally, if our model is to provide a complete picture of the cuprates, it should also explain the nature of the photoemission spectrum.<sup>34</sup> For this one needs to understand better the connection between the bare electron ejected in the photoemission and the  $(n_\ell, \Phi_{va})$  fields. This problem is currently under investigation.

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