Charge- and spin-density-wave ordering transitions in strongly correlated metals

Subir Sachdev
Department of Physics, P.O. Box 208120, Yale University, New Haven, Connecticut 06520-8120

Antoine Georges
Laboratoire de Physique Théorique de l'Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France
(Received 29 March 1995)

We study the quantum transition from a strongly correlated metal, with heavy fermionic quasiparticles, to a metal with commensurate charge- or spin-density-wave order. To this end, we introduce and numerically analyze a large dimensionality model of Ising spins, in a transverse field, coupled to two species of fermions; the analysis borrows heavily from recent progress in the solution of the Hubbard model in large dimensions. At low energies, the Ising order parameter fluctuations are characterized by the critical exponent $z\nu = 1$, while above an energy scale, Γ, there is a crossover to $z\nu = \frac{1}{2}$ criticality. We show that Γ is of the order of the width of the heavy quasiparticle band, and can be made arbitrarily small for a correlated metal close to a Mott-Hubbard insulator. Therefore, such a correlated metal has a significant intermediate energy range of $z\nu = \frac{1}{2}$ behavior, a single-particle spectrum with a narrow quasiparticle band, and well-formed analogs of the lower and upper Hubbard bands; we suggest that these features are intimately related in general.

I. INTRODUCTION

It has become increasingly clear that studies of magnetic ordering quantum transitions in metallic, fermionic systems will be of significant utility in understanding the properties of strongly correlated systems like the cuprates or the heavy-fermion compounds.[1–13] The reader is referred to a recent comprehensive study by Barzykin and Pines[14] comparing such ideas with experimental data on the cuprates.

We begin by discussing some background before introducing the question addressed in this paper. Consider a metal in the vicinity of a transition to a ground state with spin- or charge-density-wave order. We denote by $\Psi_\mu(x,\tau)$ the order parameter field as a function of space (x) and Matsubara time (τ)—the index $\mu = 1,\ldots,3$ for the case of vector spin-density-wave order and $\mu = 1$ for the case of scalar charge-density-wave order. The long-distance, long-time, zero-temperature (T) effective action for Ψ_μ obtained after integrating out all the fermionic degrees of freedom takes the form[1,5,9–11,13]

$$S = \int d^d q d\omega |\Psi_\mu(q,\omega)|^2 (r + q^2 + \gamma|\omega| + \omega^2/c_0^2) + \cdots . \tag{1.1}$$

We have Fourier transformed to wave vector q and Matsubara frequency ω, and introduced phenomenological constants r, γ, and c_0^2; the ellipsis represents higher order couplings between the Ψ_μ. We are considering here only the case originally considered by Hertz[1] in which[5] the ordering wave vector, $\vec{Q}$, is not a spanning wave vector of the Fermi surface, and it is possible to connect at least two points on the Fermi surface by $\vec{Q}$—for a spherical Fermi surface this last condition is $|\vec{Q}| < 2k_F$, where k_F is the Fermi wave vector. In the language of a recent paper by one of us, Chubukov, and Sokol,[13] we are considering only transitions of type B. Under these conditions, the density of particle-hole excitations with wave vector $\vec{Q}$ is linear in energy at small energies, and this is responsible for the dissipative $|\omega|$ term in S. The q^2 and ω^2 (Refs. 9–11, 13) terms are simply regular terms controlling spatial and dynamic fluctuations. Alternatively, the ω^2 term may be viewed as the simplest addition that makes the order parameter correlator have the correct $1/\omega^2$ decay at large frequencies.

In mean-field theory, S undergoes an ordering transition when the Landau-like parameter $r = 0$ —hence $r > 0$ measures the distance of the metal from the ordered state [we caution that an action like S is *not* appropriate for $r < 0$ (Ref. 13)]. For the usual reasons, the mean-field transition has a correlation length exponent $\nu = \frac{1}{2}$. At low energies, the $|\omega|$ is the most important term controlling the energy scale—comparing this with the q^2 term we get a mean-field value for the dynamic critical exponent of $z = 2$.[1] Later we will consider the solution of a model for such a transition in the limit of large dimensionality, where z and ν are not separately defined, but the energy scale exponent $z\nu$ is. Hence we prefer to quote the value of $z\nu$ which is $z\nu = 1$ for the present mean-field theory. It has been argued on theoretical and phenomenological grounds[15,6,9–11,13] that, under suitable conditions, the nearly ordered metallic state should exhibit a crossover at higher frequency or temperature scales to the region with the effective exponent $z = 1$, or in mean-field theory, $z\nu = \frac{1}{2}$ (at the $z = 1$ fixed point we still have $\nu = \frac{1}{2}$ in large d mean-field theory, but $\nu \approx 0.7$ in $d = 2$). It has also been suggested that this $z = 1$ behavior is observed in the cuprates not only at very low doping[4] but also at moderate dopings.[6,14] In a simple mean-field analysis of S, the energy/temperature scale above which $z\nu = \frac{1}{2}$ behavior appears is of order γc_0^2, as that is when the ω^2

term starts becoming more important than the $|\omega|$ term.

The question we address in this paper is the following: under what conditions does this crossover from $z\nu = 1$ to $z\nu = \frac{1}{2}$ actually occur? In other words, is there a reasonable scenario in which the crossover scale $\sim \gamma c_0^2$ is significantly smaller than all other higher energy cutoffs of the critical behavior, so that $z\nu = \frac{1}{2}$ behavior is clearly observable? At sufficiently high energies the behavior of the system must become dominated by lattice scale cutoffs, and hence nonuniversal, and it is therefore important to have the cutoff $\sim \gamma c_0^2$ be lower than such cutoffs.

We will answer this question here using the solution of a large dimensionality model of spinless fermions which has a charge-density-wave-like order parameter with a Z_2 symmetry (the solution uses recent progress in understanding the Hubbard model in large dimensions[16–20]). Our model exhibits a transition between metallic states with and without a mean value for the Z_2 order parameter. We will show that there is indeed a reasonable scenario in which the vicinity of this transition exhibits $z\nu = \frac{1}{2}$ behavior over a significant intermediate energy scale. Although we will explicitly display results only for a specific model, our arguments are quite generic; we expect that similar results apply to other models of ordering transitions in fermionic systems in infinite dimensions, including those with order parameters with a larger symmetry, e.g., the $O(3)$ symmetry in spin-density-wave transitions.

We now turn to a qualitative discussion of the region of parameter space where such behavior occurs. Rather than introducing the infinite-dimensional model at this point, let us discuss a more familiar example in two dimensions; this example has the virtue of having phases closely analogous to all of the phases of the infinite-dimensional model (and perhaps more). This will make the physical meaning of the phases transparent, allowing us, then, to jump directly to the phase diagram of the infinite-dimensional model.

Consider spin-$\frac{1}{2}$ electrons moving on a square lattice with first- (t_1) and second- (t_2) neighbor hopping matrix elements and short range repulsive interactions of scale U which prefer spin-density-wave ordering at the wave vector $\vec{Q} = (\pi, \pi)$ (see, e.g., Ref. 13). We need second-neighbor hopping to avoid effects from nested Fermi surfaces. On general grounds we anticipate four distinct ground states for this model at half-filling:

(A) Metal — this is a Fermi liquid whose Fermi surface crosses the boundary of the magnetic Brillouin zone. Such a Fermi surface is not nested and is also of the type in which spin fluctuations are described by an action like S.

(B) Metal with spin-density-wave order — the magnetic order causes gaps over portions of the Fermi surface, but the system remains metallic. Some details of the evolution of the Fermi surface and critical properties of the transition between phases (A) and (B) were discussed in Ref. 13. At very large values of U we can have two additional insulating phases.

(C) Insulator with Néel order — all charged excitations are now gapped. The appropriate model for spin excitations is the spin-$\frac{1}{2}$ Heisenberg spin model with first- and second-neighbor exchange—the so-called J_1-J_2 model.

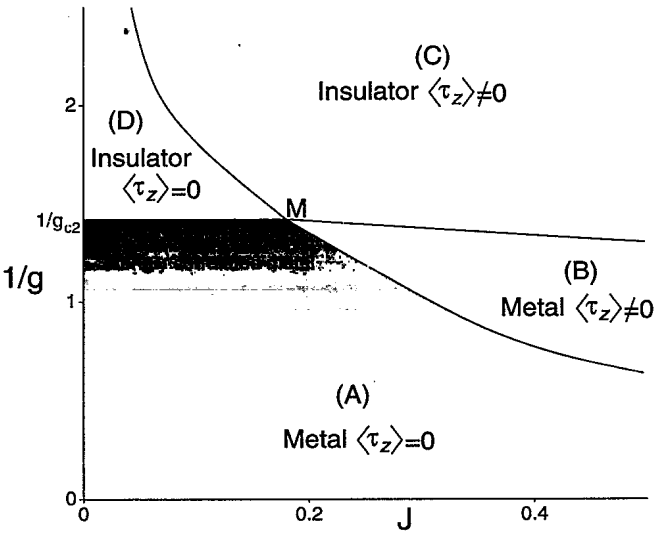

FIG. 1. Phase diagram of the Hamiltonian H (2.2) at half-filling in the $Z = \infty$ limit. We have chosen $t = 1$ and $\lambda = 2.5$. The metal-insulator transition between phases A and D is assumed to be a second-order transition at $g = g_{c2}$. However, phase D continues to be metastable for $g_{c1} < g < g_{c2}$ and the energy of this state crosses that of A at a point very close to $g = g_{c2}$. Thus this transition could be weakly first order, in which case g_{c2} and the multicritical point M will be in a metastable region. However, the critical theories at $g = g_{c2}$ and M could still be used to describe the shaded strongly correlated metal. The Ising order parameter is $\langle \tau_z \rangle$. We are interested mainly in the Ising transition between A and B from the shaded region of A: in this case the Ising fluctuations have $z\nu = 1$ at low energies and $z\nu = \frac{1}{2}$ at intermediate energies. The Ising transition between D and C has $z\nu = \frac{1}{2}$ at low and intermediate energies. The phase boundary between B and C is of no real interest to the discussion in this paper, and its position is based on an educated guess; positions of other phase boundaries were numerically determined.

(D) Insulating quantum paramagnet — or a Mott-Hubbard insulator. The J_1-J_2 model can have a ground state in which the magnetic order is short ranged.[21,22] This state can also have spin Peierls order,[22] but this is incidental to our considerations here.

Determining, in this two-dimensional model, the topology of the phase diagram with phases A, B, C, D, and possibly others, the nature of the phase transitions, and of the possible multicritical points, is a formidable problem which we shall not address here.

Turning then to the large dimensionality model to be introduced later in this paper, we show in Fig. 1 its phase diagram. The phases are closely analogous to phases A, B, C, and D above and are labeled as such in the figure. The model has a charge-density-wave-like Z_2 order parameter $\langle \tau_z \rangle$, but its role is analogous to the Néel order parameter above.

We are now ready to state the main result of this paper. We are interested in critical properties of the transition from phase A to phase B. Consider the region

of phase A which is close to the Mott-Hubbard insulator D. We identify this region as a "strongly correlated metal," and it has been shaded as such in Fig 1. In such a metal,[19,20,23,24] the fermionic quasiparticles are quite heavy and form a narrow band of width Γ around the chemical potential. A large part of the single-particle spectral weight is in the higher energy lower and upper Hubbard bands. Now consider the ordering transition from the strongly correlated metal to the metallic, ordered, phase B; in other words, the transition from A to B, not too far from the multicritical point M. We shall show that in the large dimensionality limit, the order parameter fluctuations are characterized by $z\nu = 1$ only at energy scales below Γ, while $z\nu = \frac{1}{2}$ behavior takes over at the intermediate energy scales between Γ and $\sqrt{\Gamma U}$. For all energies below $\sqrt{\Gamma U}$, and in finite, but large, dimensions, the action S in Eq. (1.1) is an excellent starting point for describing order parameter fluctuations and the crossover between $z\nu = 1$ and $z\nu = \frac{1}{2}$ criticality, as examined in Ref. 13. As Γ can be made small by moving towards phase D, there is a significant window of intermediate energies with $z\nu = \frac{1}{2}$ order parameter fluctuations. (For extremely small values of Γ, it may also be necessary to consider the energy range between $\sqrt{\Gamma U}$ and U—this regime also has $z\nu = \frac{1}{2}$ criticality, but with a significant nonuniversal renormalization of the parameter c_0 in S at the scale $\sqrt{\Gamma U}$.) These results suggest an intimate relationship between a low energy crossover to $z\nu = \frac{1}{2}$ behavior, heavy quasiparticle bands, and the removal of spectral weight to the lower and upper Hubbard bands—we conjecture that this relationship is more generally valid.

Finally, we mention that a recent study[25] of liquid ^{3}He considers a large dimensionality model whose phase diagram has many similarities to Fig. 1, and which also appeals to the proximity to a multicritical point closely anologous to M.

The infinite-dimensional model will be introduced in Sec. II and its ground states discussed in Sec. III. The main conclusions will be reiterated in Sec. IV.

II. THE MODEL

We motivate our model from the $d = 2$ spin-$\frac{1}{2}$ model considered in Sec. I. In the vicinity of the transition between phases A and B, we need only focus on the spin-density-wave order parameter and portions of the Fermi surface which are close to pairs of points that can be connected by the ordering wave vector $\vec{Q}$. Let $\vec{k}_1$ and $\vec{k}_2 = \vec{k}_1 + \vec{Q}$ be one such pair of points; in general, there will be other pairs of points, usually related to $\vec{k}_1$, $\vec{k}_2$ by symmetry operations of the square lattice—these can be treated in a similar manner and are not considered explicitly. We introduce two species of fermions $c_{1\alpha}$, $c_{2\alpha}$ ($\alpha = \uparrow, \downarrow$ is the spin index) representing Fourier components of the electron in the vicinity of $\vec{k}_1$ and $\vec{k}_2$. The low energy effective action for the vicinity of the boundary between A and B can be written as[13]

$$\tilde{S} = \int d^dx\, d\tau [(\vec{\nabla}\Psi_\mu)^2 + (\partial_\tau \Psi_\mu)^2/\tilde{c}_0^2 + \tilde{r}\Psi_\mu^2 + c_{1\alpha}^\dagger(\partial_\tau - \vec{v}_1\cdot\vec{\nabla})c_{1\alpha} + c_{2\alpha}^\dagger(\partial_\tau - \vec{v}_2\cdot\vec{\nabla})c_{2\alpha} - \lambda\Psi_\mu(c_{1\alpha}^\dagger\sigma^\mu_{\alpha\beta}c_{2\beta} + \text{H.c.})], \tag{2.1}$$

where $\vec{v}_1$, $\vec{v}_2$ are the Fermi velocities at $\vec{k}_1$, $\vec{k}_2$, and σ^μ are the Pauli matrices. After integrating out the fermions, the effective action for Ψ_μ should be of the form (1.1). The dissipative term is of the form $|\omega|$ as long as $\vec{v}_1$ and $\vec{v}_2$ are not antiparallel, i.e., there is no nesting.

We now abstract from $\tilde{S}$ the essential ingredients for a simple model of the ordering transition in large dimensions. First, we reduce the symmetry of the order parameter from $O(3)$ down to Z_2 (the symmetry of a charge-density-wave order parameter) by discarding the spin index α. Then, we replace the scalar field Ψ by an Ising spin τ_z—its "kinetic" term then becomes a transverse field, g. [For the model with $O(3)$ symmetry, the Ising spins in a tranverse field would be replaced by $O(3)$ quantum rotors.] Finally, we place the system on a lattice (not the same lattice for which $\tilde{S}$ was the continuum limit) and write down the Hamiltonian

$$H = -g\sum_i \tau_{xi} - \frac{1}{Z}\sum_{i>j} J_{ij}\tau_{zi}\tau_{zj} - \mu\sum_i (c_{1i}^\dagger c_{1i} + c_{2i}^\dagger c_{2i}) - \frac{1}{\sqrt{Z}}\sum_{ij}(t_{1ij}c_{1i}^\dagger c_{1j} + t_{2ij}c_{2i}^\dagger c_{2j}) - \lambda\sum_i \tau_{zi}(c_{1i}^\dagger c_{2i} + c_{2i}^\dagger c_{1i}). \tag{2.2}$$

We have introduced the two Pauli matrices τ_z, τ_x, an Ising spin exchange J_{ij}, a chemical potential μ, hopping matrix elements t_{1ij} and t_{2ij}, and a fermion-Ising coupling λ. The parameter Z has different meanings depending upon the particular large dimensionality limit chosen[16,19,20]—for a regular d dimensional lattice, $Z = d$; for the Bethe lattice, Z is the coordination number; and for a fully connected cluster with random hopping t_{1ij}, t_{2ij} between all pairs of site, Z is the total number of sites. The Hamiltonian H contains all low order terms consistent with the Z_2 symmetry,

$$\tau_z \to \tau_x\tau_z\tau_x = -\tau_z \quad , \quad \tau_x \to \tau_x\tau_x\tau_x = \tau_x \quad ,$$
$$c_1 \to c_1 \quad , \quad c_2 \to -c_2 \quad . \tag{2.3}$$

In the context of the original lattice model of electrons, this Z_2 symmetry is simply the sublattice interchange

symmetry which is broken by a charge-density-wave ordered state.

We will study in this paper the $Z = \infty$ limit of H. Further, we will focus only on solutions of the mean-field equations in which all sites are equivalent. This amounts to neglecting possibilities in which there is a staggered ordering of the Ising spins τ_z. Such solutions do occur, and are often lower in energy than the ones we consider;[19,23,26] however, we are not interested in them on physical grounds. One can also appeal to the fully connected random clusters for which the spatial uniform solutions are expected to be true ground states.[27,19,23,26]

We will make an additional, final, simplification. We will work with models in which $t_{1ij} = t_{2ij}$. Although there is no symmetry enforcing this equality, in finite-dimensional, regular lattice models such an assumption would drastically change the physics of the transition. This is because, as will become clear below, for $t_{1ij} = t_{2ij}$ there are additional conserved charges which have a significant effect on the critical theory.[1] However, at $Z = \infty$, all of the nontrivial critical behavior is in local correlators which are expected to behave in a similar manner for $t_{1ij} = t_{2ij}$ and $t_{1ij} \neq t_{2ij}$. The numerical analysis required to solve the mean-field equations becomes much simpler at $t_{1ij} = t_{2ij}$.

We conclude this section by writing down the mean-field equations. The equations take their simplest form after performing a rotation of the fermionic fields,

$$c_a = \frac{1}{\sqrt{2}}(c_1 + c_2), \quad c_b = \frac{1}{\sqrt{2}}(c_1 - c_2). \tag{2.4}$$

Under the Z_2 symmetry (2.4) we have $c_a \to c_b$ and $c_b \to c_a$; this makes it clear that we can simply think of the a and b fermions as moving predominantly on the two sublattices of the model underlying $\tilde{S}$. For $Z = \infty$, the model is mapped onto a single-site mean-field Hamiltonian supplemented by a self-consistency condition. Following Refs. 17, 19 and 20, for $t_{1ij} = t_{2ij} = t$ for nearest neighbors on the Bethe lattice, or for the fully connected cluster with $t_{1ij} = t_{2ij}$ random but J_{ij} uniform, the single-site mean-field Hamiltonian is

$$H_{\rm MF} = -g\tau_x - \mu(c_a^\dagger c_a + c_b^\dagger c_b) - Jm\tau_z - \lambda\tau_z(c_a^\dagger c_a - c_b^\dagger c_b) + \sum_k \left(\epsilon_{ak} f_{ak}^\dagger f_{ak} + \epsilon_{bk} f_{bk}^\dagger f_{bk} - V_{ak} c_a^\dagger f_{ak} - \text{H.c.} - V_{bk} c_b^\dagger f_{bk} - \text{H.c.}\right). \tag{2.5}$$

We have introduced fermions f_a, f_b to model the environment of the site of interest. The couplings of these fermions and the parameter m are determined by the self-consistency conditions[17,19,20,23]

$$\begin{aligned} m &= \langle \tau_z \rangle , \\ t^2 G_a(\omega) &= \sum_k \frac{|V_{ak}|^2}{i\omega - \epsilon_{ak}}, \\ t^2 G_b(\omega) &= \sum_k \frac{|V_{bk}|^2}{i\omega - \epsilon_{bk}}, \end{aligned} \tag{2.6}$$

where G_a is the Fourier transform of the a fermion Green's function $-\langle c_a(0) c_a^\dagger(\tau)\rangle$, and likewise for G_b.

Note that the total number of a fermions and b fermions is separately conserved. This is a consequence of the choice $t_{1ij} = t_{2ij}$; we reiterate that while such a choice and the additional conserved quantities would be dangerous in the finite-dimensional theory, its effect on local correlators in the $Z = \infty$ limit is expected to be innocuous.

III. GROUND STATES OF THE MODEL

This section will consider the solution of the $Z = \infty$ model $H_{\rm MF}$ in Eq. (2.5) along with the self-consistency conditions (2.6). We will consider in Sec. III A the exact solution in the atomic limit $t = 0$, $J = 0$, followed by a numerical solution of the $t \neq 0$, $J = 0$ case in Sec. III B. The most general $t \neq 0$, $J > 0$ case will be considered in Sec. III C.

A. Atomic limit, $t = 0$, $J = 0$

All of the sites are now independent. Each site can have either 0, 1, or 2 fermions and the eigenenergies of H can be easily determined. They are

$$\begin{aligned} &E_0 = \pm g, \quad 2 \text{ states} \\ &E_1 = -\mu \pm \sqrt{\lambda^2 + g^2}, \quad \text{both doubly degenerate, 4 states} \\ &E_2 = -2\mu \pm g, \quad 2 \text{ states.} \end{aligned} \tag{3.1}$$

A key observation is that if we take the lower eigenvalue for each particle number, the states map exactly onto those of the Hubbard model with $U/2 = \sqrt{\lambda^2 + g^2} - g$. Moving away from the atomic limit, the mapping of the low energy states to the Hubbard model will continue to hold as long as $t, J < g$. This mapping will be very useful to us in the subsequent discussion.

B. $J = 0$

We will study the ground states at fixed values of λ and t as a function of g. This corresponds to the y axis in Fig. 1 which presents results at $t = 1$ and $\lambda = 2.5$.

First consider the limits of large and small g. For large g, the Ising spin flips rapidly between its up and down states as a consequence of the $g\tau_x$ term. The value of τ_z averages out to zero, and the fermions effectively do not see the Ising spin. The fermion spectral function

$\rho_{a,b}(\Omega) = \mathrm{Im}G_{a,b}(\Omega)$ is then simply the semicircular density of states of free fermions:

$$\rho_a(\Omega) = \rho_b(\Omega) = \frac{1}{2t^2}\sqrt{4t^2 - (\Omega-\mu)^2}, \quad g \to, \infty \quad (3.2)$$

for $|\Omega - \mu| < 2t$ and zero otherwise.

The behavior at small g is a little more subtle. The Ising spin now fluctuates slowly between its up and down states and the fermions have plenty of time to respond to its instantaneous orientation: this yields fermion bands centered around $\pm\lambda$. As the Ising spin is equally likely to be up or down, the fermion spectral function is an equal superposition of the two possibilities

$$\rho_a(\Omega) = \rho_b(\Omega) \approx \frac{1}{4t^2}[\sqrt{4t^2 - (\Omega-\lambda-\mu)^2} + \sqrt{4t^2 - (\Omega+\lambda-\mu)^2}], \quad g \text{ small} \quad (3.3)$$

where it is assumed that the square roots vanish when their arguments are negative. For $\lambda > 2t$ there is a window of energies where (3.3) predicts a gap; in reality, we will only have a pseudogap whose origin is related to the phenomenology discussed by Kampf and Schrieffer.[28] For $g > t$ (see Sec. III A) it is more appropriate to think of the pseudogap as arising from the formation of the "upper and lower Hubbard bands;" there is, however, no fundamental distinction between the two mechanisms and they continuously evolve into each other.

One might also wonder why, for small g, we do not expect the Z_2 symmetry to be broken, thus causing the Ising spin to pick a definite orientation and $\rho_a \neq \rho_b$. This, however, does not happen for the same reason that the insulating solution of the Hubbard model in Refs. 19, 20, and 23 is not ferromagnetic. One can test instability towards "ferromagnetism" by measuring the response to an external field—even though the local susceptibility is infinite in the insulating solution, there is an internal field from the neighboring fermions which causes the net local effective field to vanish,[23] and the uniform susceptibility remains finite; the reader is referred to the discussion in Refs. 23 and 29 for more discussion on this important point in the context of the Hubbard model.

We have numerically studied the crossover from small to large g by solving Eqs. (2.6) using the exact diagonalization method.[30,31] We used as many as eight sites each for the a and b fermions and worked at half-filling. The results were very similar to those obtained in the Hubbard model.[19,20,23] We obtained two classes of solutions, a metallic solution present for $g > g_{c2}$ and an insulating solution present for $g < g_{c1}$ with $g_{c1} > g_{c2}$. For $\lambda = 2.5$ and $t = 1$ (the parameters used in Fig. 1), the energies of the two solutions crossed each other at a value of $g \approx 0.7$, which was quite close to $g = g_{c2}$. We are therefore uncertain as to whether the metal-insulator transition was first or second order. However, this issue is really peripheral to what we are interested in here, and so we did not do the necessary investigation of numerical fine structure to resolve it.

What we do care about is the behavior of the metallic solution for g close to but greater than g_{c2}—i.e., the shaded region of the strongly correlated metal in Fig. 1. In this region, it is appropriate to use the continuous transition at $g = g_{c2}$ to obtain a scaling description of the response functions. There is a low energy scale, which we denote by Γ, which vanishes as g approaches g_{c2} as[23]

$$\Gamma \sim g - g_{c2}. \quad (3.4)$$

The scale Γ controls the width of the quasiparticle band ($\sim \Gamma$) or the effective mass ($\sim 1/\Gamma$). Our main interest here is in the behavior of dynamic correlations of the order parameter τ_z. Its scaling properties can be deduced from the elegant critical theory of the Mott transition provided recently by Moeller *et al.*[24] (Our model H has only a Z_2 symmetry and so the critical theory will be a self-consistent Kondo-like model[24] but with a planar anisotropy in the exchange constants.) For the response, χ_{loc}, to a local field coupling to τ_z

$$\chi_{\mathrm{loc}}(\omega) = \int d\tau\, e^{-i\omega\tau} \langle \tau_z(0)\tau_z(\tau)\rangle, \quad (3.5)$$

we have[24]

$$\chi_{\mathrm{loc}}(\omega) = \frac{1}{\Gamma}\phi\left(\frac{\omega}{\Gamma}\right) + X_1 - X_2\omega^2 + \cdots, \quad |\omega| < \Lambda, \quad (3.6)$$

with ϕ a universal scaling function; Λ is an upper cutoff of order λ or g, and constants X_1, X_2 contain the corrections to scaling contributions of the higher energy excitations associated with lower and upper Hubbard bands. The latter excitations have an energy $\sim \Lambda$ and hence their contribution can be expanded in a smooth power series in even powers of ω. On dimensional grounds we expect $X_1 \sim 1/\Lambda$ and $X_2 \sim 1/\Lambda^3$.

We show in Fig. 2 a test of the scaling form (3.6) using

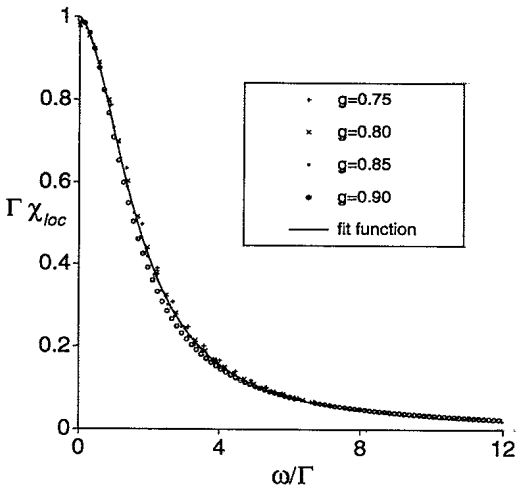

FIG. 2. Scaling plot of the local Ising spin correlation function χ_{loc} for $t = 1$, $\lambda = 2.5$ in phase A of Fig 1. The values of Γ with their respective values of g are $g = 0.75$, $\Gamma = 0.0056$; $g = 0.8$, $\Gamma = 0.0090$; $g = 0.85$, $\Gamma = 0.0128$; $g = 0.0$, $\Gamma = 0.0179$. The fit function ϕ is defined in Eq. (3.8), and the values of the fitting parameters are quoted below it.

the numerically computed value of $\chi_{\rm loc}$ at four values of $g > g_{c2}$—the collapse of the data onto a single scaling curve is quite reasonable. The scaling function ϕ can be chosen such that $\phi(0) = 1$ and must satisfy the asymptotic limits

$$\phi(x) = \begin{cases} 1 - \tilde{c}_1|x|, & \text{for } |x| \to 0 \\ \tilde{c}_2/x^2, & \text{for } |x| \to \infty \end{cases} \tag{3.7}$$

for some positive constants $\tilde{c}_1, \tilde{c}_2$. The nonanalytic $|x|$ behavior at small frequencies is a consequence of the damping of spin excitations from the finite density of states at the Fermi level in the metal, while the x^2 behavior at large frequencies follows simply from the spectral representation of the response functions in the critical theory. These asymptotic limits suggest the simple interpolation form

$$\phi(x) \approx \frac{1}{1 + c_1|x| + c_2x^2}, \tag{3.8}$$

which satisfies (3.7). We also show in Fig. 2 a fit of the measured scaling functions to (3.8). It is apparent that the interpolation form works rather well, and that the accuracy of the numerical results is not sufficient to distinguish between the true ϕ and the approximate form (3.8). For the parameters chosen, the best fit values were $c_1 \approx 0.07$ and $c_2 = 0.32$; the value of c_2 is quite reliable, but the same cannot be said of c_1— slightly different choices in the fitting process gave values of c_1 differing by a factor of 2, but only a few percent changes in c_2. However, c_1 always remained significantly smaller than c_2—indeed, the linear $|\omega|$ dependence of ϕ is barely visible in Fig. 2. We had to compute $\chi_{\rm loc}$ at fairly large values of g ($g > 2.0$), lying well within phase A, before the metallic $|\omega|$ behavior was clearly evident.

The scaling behavior of the $q = 0$ susceptibility, $\chi_{q=0}(\omega)$, which determines the dynamic response of the τ_z to a spatially uniform but time-dependent field acting on the τ_z, is somewhat more complicated. (Note that since τ_z mimics the density-wave order parameter at a wave vector $\vec{Q}$ in the physical system, the $q = 0$ susceptibility of H is really the physical staggered susceptibility.) Unlike $\chi_{\rm loc}$, this susceptibility is finite at the transition at $g = g_{c2}$;[19,20,23] as a result the interesting frequency dependence of $\chi_{q=0}$ is really a correction to scaling contribution. With the limited accuracy of the numerical method we are using, it would be quite difficult to obtain the scaling results from the data. We therefore restrict ourselves here to a qualitative discussion, which will be sufficient to extract the physics we are interested in. Because of the similarity in the low energy structure of H to the Hubbard model [in particular, the twofold degeneracy of the lowest energy state E_1 in (3.1) in the atomic limit], we expect that $\chi_{q=0}$ will behave in a manner similar to the uniform spin susceptibility near the Mott transition. From arguments similar to those in Ref. 23 we may then deduce that $\chi^{-1}_{q=0}$ behaves roughly like

$$\chi^{-1}_{q=0} \sim X + c_3\chi^{-1}_{\rm loc}, \tag{3.9}$$

where the constant $X \sim \Lambda$ and c_3 is a dimensionless constant of order unity (on the hypercubic lattice, the above equation actually requires $t_{1ij} \neq t_{2ij}$). Combining (3.6), (3.7), and (3.9), we can now deduce the frequency dependency of the uniform dynamic susceptibility:

$$\chi^{-1}_{q=0}(\omega) \sim X + \begin{cases} c_3(\Gamma + c_1|\omega| + c_2\omega^2/\Gamma), & \text{for } |\omega| < \sqrt{\Gamma\Lambda} \\ c_3(1/X_1 + X_2\omega^2/X_1^2 + \cdots), & \text{for } \sqrt{\Gamma\Lambda} < |\omega| < \Lambda. \end{cases} \tag{3.10}$$

The first of these results in the energy range $|\omega| < \sqrt{\Gamma\Lambda}$ will be used below to reach the main conclusions of this paper.

C. $J > 0$

The exchange coupling J plays a very simple role in the $Z = \infty$ mean-field theory. It is apparent from Eqs. (2.6) that in phases with $m = \langle\tau_z\rangle = 0$ the single-particle Green's functions are in fact independent of J. The results at $J = 0$ thus continue to apply for a finite range of values of J.

There is, however, a change in the τ_z correlation functions. It is not difficult to show, using an argument quite similar to that in the original Curie-Weiss mean-field theory, that

$$\chi^{-1}_{q=0}(\omega)\big|_{J\neq 0} = \chi^{-1}_{q=0}(\omega)\big|_{J=0} - J. \tag{3.11}$$

The finite J uniform susceptibility therefore diverges at $J = \chi^{-1}_{q=0}(\omega)\big|_{J=0}$, which is the point we have onset of a nonzero $\langle\tau_z\rangle$. The phase boundary between phases A and B and between D and C in Fig. 1 was determined in this manner. The phase boundary between phases C and D requires computations in the phase with $\langle\tau_z\rangle \neq 0$; as this phase boundary is of no interest to us here, we did not carry out the rather involved computations required—the boundary between C and D, shown in Fig. 1, is just an educated guess.

Figure 1 also shows a multicritical point M, which is the point where all four phases would meet if the metal-insulator transition was second order. The correlation functions on the $\langle\tau_z\rangle = 0$ side of this critical point are, however, simply related to those at the $g = g_{c2}$, $J = 0$ critical point discussed in Sec. III B: the single-particle correlators are unchanged, while the relationship in the spin susceptibility follows from (3.11).

The central interest of this paper is in the nature of the order parameter fluctuations near the phase boundary between A and B, at a point not too far from M (Fig. 1). From (3.11) and (3.10) we see that the static uniform susceptibility diverges at $J = X$, and the Lan-

dau parameter $r = X+\Gamma-J$. The nature of the dynamic susceptibility near the phase boundary between A and B also follows from (3.11) and (3.10). From these equations we see that the infinite-dimensional transition has $z\nu = 1$ at the lowest energies; however, this behavior is only present for energies smaller than Γ, and $z\nu = \frac{1}{2}$ criticality takes over for larger energy scales. Observe, however, by comparing the two equations in (3.10), that there is a significant change in the coefficient of the ω^2 term at a scale $\sqrt{\Gamma\Lambda}$.

We can, in fact, also make a crude connection between the dynamic susceptibility computed here and the finite-dimensional action S discussed in Sec. I. One perspective on the meaning of the results for dynamic correlators in the infinite-dimensional model is that these specify the input form of the effective action that must then be used to understand fluctuations in finite dimensions. With this point of view, our results allow us to deduce the following effective action for the order parameter Ψ_μ in finite dimensions:

$$S = \int d^d q\, d\omega |\Psi_\mu(q,\omega)|^2 (q^2 + \chi^{-1}_{q=0}(\omega)) + \cdots, \quad (3.12)$$

where the q^2 has been added on phenomenological grounds and, as in (1.1), the ellipsis represents nonlinearities not explicitly displayed. From (3.10) and (3.11) we see again that $r = X+\Gamma-J$, and that the two actions (1.1) and (3.12) have identical frequency dependencies in the frequency range $|\omega| < \sqrt{\Gamma\Lambda}$ where

$$S = \int d^d q\, d\omega |\Psi_\mu(q,\omega)|^2 (r + q^2 + c_3 c_1 |\omega| + c_3 c_2 \omega^2/\Gamma) + \cdots . \quad (3.13)$$

The insight gained from the present approach is that we now have an estimate of the scale at which the crossover from $z\nu = 1$ to $z\nu = \frac{1}{2}$ behavior occurs—it is the small energy Γ, as had been claimed earlier in the paper. The crossover itself is described by the action S in (3.13), which is an excellent approximation for energies below $\sqrt{\Gamma\Lambda}$. In the higher energy range $\sqrt{\Gamma\Lambda} < |\omega| < \Lambda$ we should use instead the second result for $\chi^{-1}_{q=0}$ in (3.10)—this range still has $z\nu = \frac{1}{2}$ behavior, but there is a nonuniversal crossover in the coefficient of the ω^2 term at the boundary $|\omega| \sim \sqrt{\Gamma\Lambda}$. So if Γ is extremely small, this second regime of $z\nu = \frac{1}{2}$ behavior will be the most important, and the very low energy regime of $z\nu = 1$ behavior will be unobservable.

Before concluding, we also note that a similar approach can be used to describe the ordering transition between the insulating phases D and C. In this case, $\Gamma = 0$ and we are always in the second of the regimes in (3.10)—the transition therefore has $z\nu = \frac{1}{2}$ down to the lowest energy scales.

IV. CONCLUSIONS

This paper has examined a simple, infinite-dimensional model for spin- or charge-density-wave ordering transitions in strongly correlated metals. We were interested in the case, originally considered by Hertz,[1] in which Fermi surface geometry was such as to induce a $|\omega|$ damping in effective action for the critical modes of the order parameter. As a result, the order parameter fluctuations have $z\nu = 1$ at the lowest energy scales. We examined the conditions under which there is a well-defined crossover at intermediate energy scales to $z\nu = \frac{1}{2}$ criticality. We showed that, under suitable conditions, it was indeed possible to have a low energy scale Γ such that the $z\nu = 1$ behavior was restricted to $|\omega| < \Gamma$, and universal $z\nu = \frac{1}{2}$ behavior appeared in the energy range $\Gamma < |\omega| < \sqrt{\Gamma\Lambda}$; here Λ is an upper cutoff of order of the repulsion energy between the electrons—$\Lambda \sim U$. For all energies smaller than $\sqrt{\Gamma\Lambda}$ the order parameter fluctuations in large, but finite, dimensions are expected to be well described by the action S in Eq. (1.1) or Eq. (3.13): a detailed analysis of the finite temperature crossovers and fluctuations in a $d = 2$ system controlled by S has already been presented in Ref. 13. For frequencies larger than $\sqrt{\Gamma\Lambda}$, the order parameter fluctuations still have $z\nu = \frac{1}{2}$—the main caveat to keep in mind is that there is nonuniversal change in the value of c_0 [see (1.1)] around $\omega \sim \sqrt{\Gamma\Lambda}$ which is not describable by the simple frequency dependence in S.

The key feature of the above scenario is of course the presence of the low energy scale Γ in a strongly correlated metal. In infinite dimensions, Γ vanishes at the transition to a Mott-Hubbard insulator, which we assume (see Fig. 1) is in the vicinity of the strongly correlated metal. In this same region,[19,20,23] the single-particle spectral function has a narrow quasiparticle band of width Γ, and additional spectral weight at the energies $\sim \Lambda$ which form the analogs of the upper and lower Hubbard bands. This window of energy between the quasiparticle excitations and the localized Hubbard excitations is directly responsible for the $z\nu = \frac{1}{2}$ criticality in the order parameter fluctuations.

ACKNOWLEDGMENTS

S.S. would like to thank T. Senthil for his interest, probing questions, and many helpful remarks on the subject matter of this paper. We also had beneficial discussions with M. Caffarel, A. Chubukov, W. Krauth, M. Rozenberg, R. Shankar, Q. Si, and A. Sokol. The research was supported by NSF Grant No. DMR-92-24290.

[1] J.A. Hertz, Phys. Rev. B **14**, 525 (1976).
[2] S. Chakravarty, B.I. Halperin, and D.R. Nelson, Phys. Rev. B **39**, 2344 (1989).
[3] S. Sachdev and J. Ye, Phys. Rev. Lett. **69**, 2411 (1992).
[4] A.V. Chubukov and S. Sachdev, Phys. Rev. Lett. **71**, 169 (1993); **71**, 2680(E) (1993); A.V. Chubukov. S. Sachdev, and J. Ye, Phys. Rev. B **49**, 11 919 (1994).
[5] A.J. Millis, Phys. Rev. B **48**, 7183 (1993).

[6] A. Sokol and D. Pines, Phys. Rev. Lett. **71**, 2813 (1993).
[7] A. Sokol, R.L. Glenister, and R.R.P. Singh, Phys. Rev. Lett. **72**, 1549 (1994); N. Elstner, R.L. Glenister, R.R.P. Singh, and A. Sokol, Phys. Rev. B **51**, 8984 (1995).
[8] S. Sachdev, Phys. Rev. B **49**, 6770 (1994).
[9] V. Barzykin, D. Pines, A. Sokol, and D. Thelen, Phys. Rev. B **49**, 1544 (1994).
[10] P. Monthoux and D. Pines, Phys. Rev. B **50**, 16 015 (1994); **49**, 4261 (1994).
[11] Y.-L. Liu and Z.-B. Su (unpublished).
[12] L. Ioffe and A.J. Millis, Phys. Rev. B (to be published).
[13] S. Sachdev, A. Chubukov, and A. Sokol, Phys. Rev. B **51**, 14 874 (1995).
[14] V. Barzykin and D. Pines, Phys. Rev. B (to be published).
[15] A. Sokol, in *Strongly Correlated Electronic Materials*, edited by K. S. Bedell, Z. Wang, D. E. Meltzer, A. V. Balatsky, and E. Abrahams (Addison-Wesley, Reading, MA, 1994).
[16] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[17] A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992).
[18] M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992); Th. Pruschke, D.L. Cox, and M. Jarrell, Europhys. Lett. **21**, 5 (1993); Phys. Rev. B **47**, 3553 (1993).
[19] A. Georges and W. Krauth, Phys. Rev. Lett. **69**, 1240 (1992); Phys. Rev. B **48**, 7167 (1993).
[20] M.J. Rozenberg, X.Y. Zhang, and G. Kotliar, Phys. Rev. Lett. **69**, 1236 (1992); X.Y. Zhang, M.J. Rozenberg, and G. Kotliar, *ibid.* **70**, 1666 (1993);
[21] E. Dagotto and A. Moreo, Phys. Rev. Lett. **63**, 2148 (1989); R.R.P. Singh and R. Narayan, *ibid.* **65**, 1072 (1990); A. Moreo, E. Dagotto, T. Joliceour, and J. Riera, Phys. Rev. B **42**, 6283 (1990).
[22] N. Read and S. Sachdev, Phys. Rev. Lett. **62**, 1694 (1989); Phys. Rev. B **42**, 4568 (1990); Phys. Rev. Lett. **66**, 1773 (1991); Int. J. Mod. Phys. B **5**, 219 (1991).
[23] M.J. Rozenberg, G. Kotliar, and X.Y. Zhang, Phys. Rev. B **49**, 10 181 (1994).
[24] G. Moeller, Q. Si, G. Kotliar, M. Rozenberg, and D.S. Fisher, Phys. Rev. Lett. **74**, 2082 (1995).
[25] L. Laloux and A. Georges (unpublished).
[26] L. Laloux, A. Georges, and W. Krauth, Phys. Rev. B **50**, 3092 (1994).
[27] A. Georges and S. Sachdev (unpublished).
[28] A.P. Kampf and J.R. Schrieffer, Phys. Rev. B **41**, 6399 (1990); **42**, 7967 (1990).
[29] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg (unpublished).
[30] M. Caffarel and W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994).
[31] Q. Si, M.J. Rozenberg, G. Kotliar, and A.E. Ruckenstein, Phys. Rev. Lett. **72**, 2761 (1994).