ARTICLES

Critical behavior of the $T = 0$ $2k_F$ density-wave phase transition in a two-dimensional Fermi liquid

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We study $T = 0$ spin-density-wave transitions in two-dimensional Fermi liquids in which the ordering wave vector $\mathbf{Q}$ is such that the tangents to the Fermi line at the points connected by $\mathbf{Q}$ are parallel (e.g., $Q = 2p_F$ in a system with a circular Fermi line) and the Fermi line is not flat. We show that the transition is first order if the ordering wave vector $\mathbf{Q}$ is not commensurate with a reciprocal lattice vector $\mathbf{G}$, i.e., $\mathbf{Q} \neq \mathbf{G}/2$. If $\mathbf{Q}$ is close to $\mathbf{G}/2$ the transition is weakly first order and an intermediate scaling regime exists; in this regime the $2p_F$ susceptibility and observables such as the NMR rates T_1 and T_2 have scaling forms which we determine.

I. INTRODUCTION

Quantum phase transitions have attracted substantial recent interest. Antiferromagnet-singlet transitions in insulating magnets[1–4] and ferromagnetic and antiferromagnetic transitions in Fermi liquids[5,6] have been studied in detail, and the crossover between the insulating and Fermi liquid critical points in two spatial dimensions has also been studied.[7] Here we consider an important case which has not so far been discussed in the literature, namely, what we call the "$2p_F$" spin- or charge-density-wave transition of a fermion system. By "$2p_F$" we mean an ordering wave vector $\mathbf{Q}$ which connects two points on the Fermi line with parallel tangents (see Fig. 1).[8] For a circular Fermi line any vector $\mathbf{Q}$ of magnitude $2p_F$ connects two such points. In this paper we consider explicitly the spin-density-wave case, but our results can be applied with only minor modifications to the charge-density-wave case. We assume that the Fermi line is not straight. We also assume that Fermi liquid theory adequately represents the noncritical properties of the fermions. If it does not, our results do not apply. We briefly discuss one non-Fermi-liquid scenario in the conclusion. One important motivation for studying the $2p_F$ case is the high T_c superconducting material $La_{2-x}Sr_xCuO_4$, in which strong magnetic fluctuations have been observed;[9] the fluctuations are peaked at an x-dependent wave vector $Q(x)$ which is claimed to be a "$2p_F$" wave vector of the Fermi line calculated by standard band-structure techniques for this material.[10] Our results may also be relevant for quasi-two-dimensional materials such as $(TMTSF)_2PF_6$.[11]

In order to study critical phenomena analytically, one expands about a mean field solution. If Fermi liquid theory is a good starting point, then the appropriate mean field theory is the random phase approximation (RPA), in which the susceptibility $\chi(\omega, \mathbf{q})$ is given in terms of the interaction constant g and the polarizability of noninter-

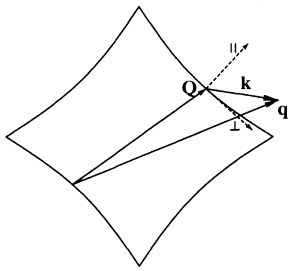


FIG. 1. Sketch of Fermi line and important wave vectors. The Fermi line shown here is similar to that claimed to be appropriate to $La_{1.8}Sr_{0.14}CuO_4$. The ordering wave vector $\mathbf{Q}$ for spin fluctuations connects two points on the Fermi line. It is assumed that the tangent to the Fermi line at one end of the vector $\mathbf{Q}$ is parallel to the tangent to the Fermi line at the other end. We have also shown a typical momentum of a spin fluctuation $\mathbf{q}$. We parametrize the vector $\mathbf{k} = \mathbf{q} - \mathbf{Q}$ by its Cartesian components $k_\perp$ and $k_\parallel$ in the coordinate system (shown by dashed lines) associated with the Fermi line at the points connected by $\mathbf{Q}$.

acting fermions, $\Pi_0(\omega,\mathbf{q})$, by $\chi(\omega,\mathbf{q}) = \Pi_0(\omega,\mathbf{q})/[1 - g^2\Pi_0(\omega,\mathbf{q})]$. The transition occurs at the wave vector $\mathbf{Q}$ as g is increased to the point at which $g^2\Pi_0(0,\mathbf{Q}) = 1$. In three spatial dimensions, $\Pi_0(0,\mathbf{q})$ is not maximal at any $2p_F$ wave vector; moreover, $d\Pi_0(0,\mathbf{q})/dq$ is logarithmically divergent as $q \to 2p_F$. Therefore a "$2p_F$" transition is impossible in $d = 3$ and so we focus on $d = 2$ in this paper.

In the two-dimensional case, $\Pi_0(0,\mathbf{q})$ is so strongly peaked at $q = 2p_F$ that it is natural to assume that the spin-density instability happens at "$2p_F$." The "$2p_F$" case is difficult to treat by the methods used previously to study phase transitions at other momenta.[5,6] In these works the fermions are "integrated out" and the problem is reduced to a model of interacting bosonic spin fluctuations. In the "$2p_F$" case the action functional obtained by integrating out the fermions has coefficients which are singular and nonanalytic because the fermion response functions are nonanalytic for $Q = 2p_F$. These nonanalyticities lead to divergences in the action as $T \to 0$ and make it difficult to apply the conventional approach.[5,6] Instead, in this paper we apply a perturbative renormalization group technique to a model which includes both spin fluctuations and fermions.

Our perturbation parameter is $1/N$, the fermion spin degeneracy. The leading order of the perturbation theory is the familiar RPA approximation. The next order is a theory of electrons interacting by exchanging RPA fluctuations. We show that this theory is infrared divergent. We sum the leading infrared divergent contributions using the renormalization group.

The behavior of spin fluctuations changes dramatically if their wave vectors are close to half of a reciprocal lattice vector $\mathbf{G}$. The important parameter is $\Delta G = |\mathbf{Q} - \mathbf{G}/2|$. If ΔG is sufficiently small we must distinguish two regimes in the renormalization group flow: large momenta, where the infrared cutoff is greater than ΔG, and small momenta, where it is less. For large momenta the divergences are logarithmic; the logarithms may be summed by the renormalization group to power laws and we use the $1/N$ expansion to find the exponents. Although the physical value of $N = 2$, the small value of the numerical coefficients in front of these logarithms suggests that the exponents obtained in the first order in $1/N$ are close to their exact values at $N = 2$. For small momenta, the divergences are much stronger and, we show, drive the transition first order as soon as the regime of small momenta is reached.

The outline of this paper is as follows. In Sec. II we define the model, derive the RPA theory, and make a convenient scaling of variables. In Sec. III we analyze the fluctuation corrections and derive renormalization group (RG) equations in the regime of large momenta. In Sec. IV we derive analogous equations in the regime of small momenta and show that they imply that the transition is first order. In Sec. V we discuss the physical consequences of our results. Section VI contains a summary of the results, a discussion of their relation to previous work on quantum critical phenomena and correlated electrons, a note on the extension of our results to a charge-density-wave transition, and a conclusion.

II. MODEL AND RANDOM PHASE APPROXIMATION

Our starting point is a Hamiltonian H describing fermions moving in a lattice and interacting with each other via a short range four-fermion interaction W:

$$H = \sum_{p\alpha} \epsilon(p) c^\dagger_{p,\alpha} c_{p,\alpha} + W \sum_{p,p',q,\alpha,\beta} c^\dagger_{p,\alpha} c_{p+q,\alpha} c^\dagger_{p',\beta} c_{p'-q,\beta}. \quad (1)$$

We assume that a $T = 0$ spin-density-wave transition to a state with long range order at wave vector $\mathbf{Q}$ occurs as W is increased to a critical value W_c. Because we expect the physics in this region to be determined by the exchange of spin-density fluctuations we use a Hubbard-Stratonovich transformation to recast Eq. (1) as a theory of fermions coupled to spin fluctuations $\mathbf{S_q}$. The theory is described by the action

$$\mathcal{A}\{c,S\} = \sum_{p\alpha} G^{-1}(\epsilon,p) c^\dagger_{\epsilon,p,\alpha} c_{\epsilon,p,\alpha} + \sum_{\omega,q} D^{-1}(\omega,q) \mathbf{S}_{\omega,q} \mathbf{S}_{-\omega,q} + g_b \sum_{p,q,\epsilon,\omega} c^\dagger_{\epsilon,p,\alpha} \vec{\sigma}_{\alpha\beta} c_{\epsilon+\omega,p+q,\beta} \vec{S}_{-\omega,-q}. \quad (2)$$

Here $G(\epsilon,p)$ is the fermion Green function, $D(\omega,q)$ is the spin fluctuation propagator, and g_b is a bare coupling constant derived from W. When Hubbard-Stratanovich transformation is applied to Eq. (1), the result is $D_b(\omega,q) = 1$, $g_b^2 = W$, and $G_b(\epsilon,p)$ is the noninteracting fermion Green function, i.e.,

$$G_b(\epsilon,p) = \frac{1}{i\epsilon - \epsilon(p)}. \quad (3)$$

The interaction between spin fluctuations and fermions changes the form of the fermion Green function and spin fluctuation propagator. We assume that the effects of the short scale fluctuations which do not become singular at the critical point can be described by conventional Fermi liquid renormalizations.

The action, Eq. (2), has two dimensionless parameters: the number of spin components, n, and the fermion degeneracy, N. In the physical situation $n = 3$ and $N = 2$. We will expand about the limit $n/N \to 0$. We will argue that the expansion parameter is $(n-2)/N$ and, moreover, the numerical coefficients of this expansion are small, so that this expansion leads to a physically reasonably results, even for $n = 3$ and $N = 2$. To formally justify our expansion we assign the fermions an extra index $a = 1, \ldots, M$ and assume that the fermions transform as SU(2)×U(M) with $N = 2M$.

The action, Eq. (2), describes an $O(3)$ vector field $\mathbf{S}$ coupled to SU(2) symmetric fermions. Because it has no natural small parameter, we will consider the theory in the limit of large fermionic degeneracy. The simplest possibility would be to consider an m-component field $\mathbf{S}$ ($m = 3$ in the physical problem) coupled to k-

fold degenerate fermions transforming as SU(k). However, the most natural generalization of Eq. (2) to SU(k) fermions involves coupling them to $n = k^2 - 1$ degenerate spin field $\mathbf{S}$ transforming as the vector representation of SU(k). The combinatoric factors associated with loops in this theory involve n/k, so a large k expansion is not possible. Instead, we assign the fermions an additional flavor index $a = 1, ..., M$ and assume that fermions transform as SU(k)×SU(M). The total fermion degeneracy is $N = kM$; $\mathbf{S}$ has $n = k^2 - 1$ components, and the large M limit at fixed k generates an expansion. We argue that this expansion provides useful information about the physical case $n = 3$ (i.e., $k = 2$), $N = 2$ (i.e., $M = 1$) because the renormalization of the charge of this theory is controlled by $(n-2)/N$ and, moreover, the numerical coefficents are small. We will write our results in terms of n and N; however, they are valid only for $n = k^2 - 1$ and $N = kM$.

The large N expansion is a loop expansion; the leading order of perturbation theory for the action (2) is the random phase approximation (RPA) which takes into account the renormalization of the spin propagator by the electron polarization bubble, $D_0^{-1}(\omega, q) = D_b^{-1}(\omega, q) - \Pi_0(\omega, q)$.

We shall be interested in momenta close to the momentum Q at which $\Pi_0(0, q)$ is maximal. For wave vectors near Q the momentum and frequency dependences of $\Pi_0(0, q)$ are nonanalytic and controlled by Fermi line singularities. Because the singular behavior of $\Pi_0(\omega, q)$ is controlled by the distance from $\mathbf{q}$ to the Fermi line, it will be convenient to parametrize the momentum $\mathbf{q}$ in terms of the variables $k_\parallel$ and $k_\perp$ shown in Fig. 1.

The fermion polarizability $\Pi_0(\omega, q)$ can be calculated by summing all diagrams which are irreducible with respect to the fermion-fermion interaction and have two external $S_{\omega,\mathbf{q}}$ legs. This generalizes the RPA by including Fermi liquid corrections. This sum has contributions from short length scale processes which give $\Pi_0(\omega, q)$ an analytic dependence on q and ω and also contributions from Fermi line singularities, which lead to a nonanalytic dependence of $\Pi_0(\omega, q)$ on q and ω. Thus we write $\Pi_0(\omega, q) = \Pi^{\text{anal}}(\omega, q) + \Pi^{\text{sing}}(\omega, q)$; within Fermi liquid theory singularities come from the diagram shown in Fig. 2. The analytic expression corresponding to this diagram is

$$\Pi^{\text{sing}}(\omega, q) = -g_0^2 \sum_{\epsilon, p} G(\epsilon + \omega, p + q) G(\epsilon, p), \tag{4}$$

where g_0 represents the interaction constant renormalized by Fermi liquid corrections. To obtain the form of Fermi line singularities we expand the spectrum of the fermions in the vicinity of the points $\pm\mathbf{Q}/2$, obtaining for the fermion Green function

$$G(\epsilon, p) = \frac{1}{iz\epsilon - v_F p_\parallel + \frac{v_F p_\perp^2}{2p_0}}. \tag{5}$$

Here v_F is the renormalized Fermi velocity, p_0 is the radius of curvature of the Fermi line, $p_\parallel$ ($p_\perp$) are momentum components normal (tangential) to the Fermi line as measured from the points $\pm\mathbf{Q}/2$, and z is the quasiparticle residue. Note that coordinates $p_\parallel$ and $p_\perp$ are compatible with the spin fluctuation coordinates $k_\parallel$ and $k_\perp$.

All dominant infrared contributions come from processes in which an electron is scattered from one small region of fermion momenta around $\mathbf{Q}/2$ to another around $-\mathbf{Q}/2$. It is convenient to introduce dimensionless momenta parametrizing these regions and rescale all fields so that the resulting action does not contain dimensioned variables. We choose

$$\begin{aligned} &p_\perp \to \sqrt{p_0 p_F}\, p_\perp\,, \quad c_{\epsilon,p} \to v_F^{-1} p_F^{-5/2} p_0^{-1/2} c_{\epsilon,p}, \\ &p_\parallel \to p_F p_\parallel\,, \quad S_{\omega,k} \to g_0^{-1} p_0^{-1/2} p_F^{-3/2} S_{\omega,k}, \\ &\epsilon \to v_F p_F \epsilon, \quad g_0 \to 1. \end{aligned} \tag{6}$$

After this transformation we may assume we are dealing with a circular Fermi surface of unit radius but with an upper cutoff on angular integrals of the order of p_F/p_0 and an upper cutoff on radial integrals of the order of 1; the dimensionless parameter controlling the incommensurability becomes

$$\Delta G \to \frac{|\mathbf{G}|}{2p_F} - 1.$$

In the new variables the action retains the general form (2) but the Green function of the fermions changes to

$$G(\epsilon, p) = \frac{1}{iz\epsilon - p_\parallel + p_\perp^2/2}, \tag{7}$$

while the bare spin fluctuation propagator becomes

$$D_b(\omega, q) = g^2 \frac{\sqrt{p_0 p_F}}{v_F}.$$

Evaluating the diagram shown in Fig. 2 yields the

FIG. 2. Diagram yielding the nonanalytic momentum and frequency dependence of the polarizability $\Pi_0(\omega, q)$ in Fermi liquid theory. The solid lines are fermion propagators.

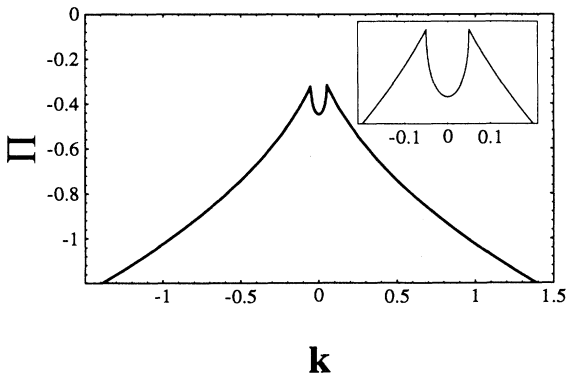


FIG. 3. The qualitative form of fermion polarization $\Pi(0, k)$ in the RPA approximation. $k = 0$ corresponds to the commensurate vector $\mathbf{G}/2$; peaks occur at k corresponding to $\mathbf{q} = \mathbf{Q}$ and $\mathbf{q} = \mathbf{G} - \mathbf{q}$. The inset shows the enlarged structure of the double peak maximum.

singular part of the fermion polarizability in $d = 2$:

$$\Pi^{\rm sing}(\omega, \mathbf{q}) = -\frac{N}{2\pi z}\mathrm{Re}\sqrt{k_\parallel + \frac{1}{4}k_\perp^2 - i\omega}. \quad (8)$$

Here and below we are use Matsubara frequencies $\omega = 2\pi nT$ so that $\Pi(\omega, \mathbf{q})$ is purely real. $\Pi^{\rm sing}(\omega, \mathbf{q})$ depends only on the combination $k_\parallel + \frac{1}{4}k_\perp^2$ because for a circular Fermi line $\Pi^{\rm sing}(\omega, \mathbf{q})$ is a function only of $|\mathbf{q}| - 2\mathbf{p}_F$.

For electrons on a lattice there are additional images of $\Pi^{\rm sing}(\omega, \mathbf{q})$ coming from fermion transitions with momenta shifted by reciprocal lattice vectors. The most important of these is the transition with momentum $\mathbf{G} - \mathbf{q}$ which might also be close to $\mathbf{Q}$ in a typical situation. Generally, we expect that the singular contribution to fermion polarizability comes from the transitions with momenta transfer $\mathbf{q}$ and $\mathbf{G} - \mathbf{q}$:

$$\Pi_0(\omega, \mathbf{q}) = \Pi^{\rm sing}(\omega, \mathbf{q}) + \Pi^{\rm sing}(\omega, \mathbf{G} - \mathbf{q}) + \Pi^{\rm anal}(\omega, \mathbf{q}). \quad (9)$$

Here $\Pi^{\rm anal}(\omega, \mathbf{q})$ is the analytical contribution to fermion polarizability coming from fermion momenta far from $\mathbf{Q}/2$; its dependence on the momenta and frequency is negligible relative to the strong dependence coming from the singular parts.

There are two regimes of $\mathbf{q}$ at $T = 0$. For $k \gg \Delta G$, $\Pi_0(\omega, \mathbf{q})$ has a symmetric square root peak at a wave vector indistinguishable from $\mathbf{G}/2$. At smaller scales, $k \ll \Delta G$, the peaks separate and each peak acquires asymmetric form: $\Pi(0, k) \sim -\sqrt{k}$ at $k > 0$ and $\Pi(0, k) \sim -|k|/(\Delta G)^{1/2}$ at $k < 0$. The qualitative form of $\Pi(0, k)$ is shown in Fig. 3.

After RPA corrections are included, the spin fluctuation propagator entering the action (2) becomes

$$D_0(\omega, \mathbf{q}) = \frac{1}{D_b^{-1} - \Pi_0(\omega, \mathbf{q})}. \quad (10)$$

Within the RPA, a second order phase transition occurs when the interaction constant g_0 controlling the value of D_0^{-1} is increased through the critical value

$$g_c^2 = \frac{v_F}{\sqrt{p_0 p_F}\Pi(0, 0)}.$$

For $g = g_c$, $D(\omega, \mathbf{q})$ diverges as $\mathbf{q} \to \mathbf{Q}$ and $\omega \to 0$. For $g \le g_c$ the divergence is cut off. It is convenient to define a bare dimensionless cutoff Δ_0 by

$$D_0(0, \mathbf{Q}) = \frac{1}{\Delta_0}. \quad (11)$$

Within the RPA, $\Delta_0 \propto g_c - g$.

Corrections to the RPA involve diagrams in which electrons interact by exchange of spin fluctuations. These corrections may be organized in a $1/N$ expansion because the spin fluctuation propagator is proportional to $1/N$ and each fermion loop contains a factor of N. The leading diagrams in $1/N$ are the self-energy correction shown in Fig. 4 and the vertex correction shown in Fig. 5. These diagrams are infrared divergent; the divergence is logarithmic if the external momentum is larger than ΔG and power law if the external momentum is less than ΔG. These two cases require separate discussions.

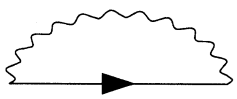


FIG. 4. Leading contribution to the self-energy. Solid line denotes fermion; wavy line denotes spin fluctuations.

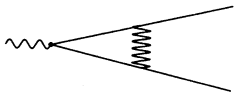


FIG. 5. Leading contribution to the vertex renormalization. Solid lines denote fermions; wavy lines denote spin fluctuations.

III. SCALING AT LARGE MOMENTA

At large momentum the small difference between the $\mathbf{Q}$ and $\mathbf{G}/2$ is unimportant and we may write

$$D(\omega, \mathbf{k}) = \frac{1}{\frac{g^2 N}{2\pi z}\mathrm{Re}\left[\sqrt{\frac{k_\perp^2}{4} + iz\omega + k_\parallel} + \sqrt{\frac{k_\perp^2}{4} + iz\omega - k_\parallel}\right] + \Delta} \quad (12)$$

for the spin fluctuation propagator. We use this and the fermion Green function (7) to calculate leading corrections to the fermion self-energy, the fermion-spin fluctuation vertex, and the spin fluctuation propagator. We find that the fermion self-energy and fermion-spin fluctuation vertex are logarithmically divergent, while the polarization bubble itself which controls spin fluctuations is not divergent. We argue that these logarithms sum to a power law and we calculate this power law to order $1/N$.

We begin with the self-energy. The leading contribution is shown in Fig. 4 and corresponds to

$$\Sigma(\epsilon, \mathbf{p}) = g^2 \int G(\epsilon + \omega, \mathbf{p}')D(\omega, \mathbf{p} - \mathbf{p}')d\omega d^2p'. \quad (13)$$

The form of the fermion Green function implies that the energy of the scattered electron is small ($\sim \epsilon$), so the frequency transferred to the spin fluctuations is small and the scattered electron remains near the Fermi line. Although $\mathbf{p}$ and $\mathbf{p}'$ must both be near the Fermi line, the angle between them may be large; thus it will be convenient to parametrize the momenta $\mathbf{p}$ and $\mathbf{p}'$ by their polar coordinates p, θ, p', and θ'. Moreover, since the momentum $\mathbf{p} - \mathbf{p}'$ transferred to the spin fluctuation is large, we may neglect the frequency dependence of the spin propagator except as a lower cutoff and estimate the large momentum $\mathbf{p} - \mathbf{p}'$ neglecting the small differences $|p| - 1$ and $|p'| - 1$. For electrons near the Fermi line the difference $\mathbf{p} - \mathbf{p}'$ is always smaller than 2, so the

main contribution to the spin fluctuation propagator (10) comes from the term $\Pi^{\rm sing}(\omega, \mathbf{G}-\mathbf{q})$ in (9), yielding

$$D(\omega, \mathbf{p}-\mathbf{p}') = \frac{4\pi z}{N\sqrt{3\theta^2+3\theta'^2+2\theta\theta'}}. \tag{14}$$

The $1/|\theta'|$ dependence of $D(\omega, \mathbf{p}-\mathbf{p}')$ at large θ' leads to a logarithmic contribution to the self-energy and justifies our assumption that angular deviations are typically large. The logarithm is cut off by Λ which is the largest of $|\epsilon|$, $p-1$, and θ^2. Substituting Eq. (14) into (13) we get

$$\Sigma(\epsilon,\theta) = -iz_0\epsilon\frac{n}{\sqrt{3}N\pi}\ln(1/\Lambda). \tag{15}$$

Here $n=3$ is the number of spin components and z_0 is the usual Fermi liquid wave-function renormalization. We emphasize again that this expression is only correct if the infrared cutoff Λ is larger than ΔG.

Note that Σ is a function only of energy and θ, so the Fermi velocity is not renormalized and the structure (7) that we assumed for the Green function is not changed. Note also that the relative value of the renormalization $\Sigma(\epsilon)/(z\epsilon)$ does not depend on the value of the coupling constant g or indeed on any other parameter of the theory except for the number of electron components N and spin components n. Thus, even though g is renormalized by the interaction, this renormalization is not important for the calculation of $\Sigma(\epsilon)$ and we may expect that the logarithms sum up to a power law and that the exponent depends only on n and N. We express the renormalization of the self-energy as a scale-dependent wave-function renormalization $z(\Lambda)$ and find

$$z \sim (1/\Lambda)^{\alpha} \tag{16}$$

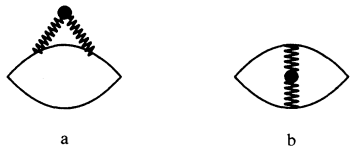
with $\alpha = n/(N\sqrt{3}\pi)$ in the large N limit. Note that even at $N=2$ and $n=3$ $\alpha \approx 0.27$ is a small number, suggesting that the leading logarithm approximation is reasonably accurate even in this case.

We now consider the renormalization of the interaction vertex g. At leading order in $1/N$ this is given by the diagram shown in Fig. 5. The evaluation proceeds differently from the evaluation of the self-energy because the momenta of the particle and hole are on the opposite sides of the Fermi line and the frequency of the spin fluctuation ω is not small. It is convenient to use the Cartesian coordinates $p_{\|}$ and $p_{\perp}$, introduced in (7) and Fig. 1. The expression corresponding to Fig. 5 is

$$\frac{\delta g}{g} = \frac{2\pi(2-n)}{N}\int \frac{d\epsilon dp_{\|}dp_{\perp}}{(2\pi)^3}\frac{1}{i\epsilon - p_{\|}-\frac{p_{\perp}^2}{2}}\frac{1}{i\epsilon+p_{\|}-\frac{p_{\perp}^2}{2}} \times \frac{1}{\mathrm{Re}\left[\sqrt{i\omega+\frac{p_{\perp}^2}{4}+p_{\|}}+\sqrt{i\omega+\frac{p_{\perp}^2}{4}+p_{\|}}\right]}.$$

This integral is logarithmic. The coefficient of the logarithm may be obtained by scaling ϵ and $p_{\|}$ by $p_{\perp}^2$ and evaluating the integral over the rescaled ϵ and $p_{\|}$ numerically. We find

$$\frac{\delta g}{g} = a\frac{n-2}{N\pi}\ln(1/\Lambda) \tag{17}$$



a b

FIG. 6. Leading contribution to the mass, Δ, renormalization. Solid line denotes fermion, wavy lines denote spin fluctuations. Heavy dot denotes mass operator Δ.

with $a \approx 0.75$. As in the case of the self-energy this expression exponentiates, leading to

$$g(\Lambda) = (1/\Lambda)^{\beta} g_0 \tag{18}$$

with $\beta = a\frac{n-2}{N\pi}$, which in the physically relevant case $n=3$ and $N=2$ becomes $\beta \approx 0.08$, so the corrections to the vertex are very small and we may assume that the one-loop approximation of the vertex corrections is reasonably accurate in the physical situation.

Note that both exponents α and β depend only on n and N but not on any other parameter. This can also be seen directly from the action (2) because one can always scale away the interaction constant g and the wave-function renormalization z changing the scales of the S fields and frequencies. This shows that the effective charge controlling the RG flow depends only on the parameters n and N and is not renormalized.

We finally consider the renormalization of the spin fluctuation propagator $D(\omega, q)$. To order $1/N$ there are two diagrams; a self-energy and a vertex correction. Power counting shows that the frequency- and momentum-dependent terms in $\Pi(\omega, q)$ acquire no additional renormalization beyond the one imposed by the momentum-dependent z and g, so $D(\omega, q)$ is given by Eq. (12) with z and g replaced by their running values. However, there are logarithmic contributions to the mass Δ_0. These come from the diagrams shown in Fig. 6.

The analytic expression corresponding to the diagram in Fig 6(a) is

$$\frac{\delta\Delta}{\Delta} = \int G(\epsilon, \mathbf{p}+\mathbf{Q})G(\epsilon,\mathbf{p})^2 \times G(\epsilon-\omega, \mathbf{p}-\mathbf{q})D^2(\omega,\mathbf{q})\frac{d^2pd^2qd\omega d\epsilon}{(2\pi)^6}. \tag{19}$$

The self-energy part of this diagram [second line in (19)] has an ultraviolet divergence which leads to a trivial shift of the fermion chemical potential, which we subtract, and a logarithmic divergence which we obtain by performing the integrations in the following order. We integrate first over $p_{\|}$, then over ϵ, and finally over $p_{\perp}$, obtaining an integral over ω, $k_{\perp}$, and $k_{\|}$. We then find that $k_{\perp}$ can be scaled out of the integrals, leading to

$$\frac{\delta\Delta}{\Delta} = -\frac{n}{N}c_a\int\frac{dk_{\perp}}{|k_{\perp}|} = -\frac{n}{N}c_a\ln(1/\Lambda). \tag{20}$$

Here the coefficient

$$c_a = \pi^2\int \frac{dxd\tilde{\omega}}{\left[\mathrm{Re}\left(\sqrt{\frac{1}{4}+x+i\tilde{\omega}}+\sqrt{\frac{1}{4}-x+i\tilde{\omega}}\right)\right]^2} \times \mathrm{Im}\left(\frac{\zeta^{-1}\mathrm{sgn}(\tilde{\omega})}{2i\tilde{\omega}-2x+\zeta\mathrm{sgn}\tilde{\omega}}\right) \approx 0.20, \tag{21}$$

where $\zeta = \sqrt{4i\tilde{\omega} - 4x - 1}$.

The contribution of the diagram shown in Fig. 6(b) may be evaluated similarly, but in this case no subtraction is necessary. We find ultimately a logarithmic divergence from the last $q_\perp$ integral. As was the case for the diagram shown in Fig. 6(a), the coefficient of the logarithm is independent of g and z:

$$\frac{\delta\Delta}{\Delta} = \frac{n-2}{N} c_b \ln(1/\Lambda) \tag{22}$$

with $c_b \approx 0.45$. By combining the results of these two diagrams and integrating the resulting scaling equation we find

$$\Delta(\Lambda) = \Delta_0 \Lambda^\eta \tag{23}$$

with exponent $\eta = 2\frac{c_a n - c_b(n-2)}{N} + O(1/N^2)$. Evaluating this formula at $N = 2$ gives $\eta \approx 0.15$. The formula for $\Delta(\Lambda)$ implies that the mass term becomes important at a scale set by equating the renormalized kinetic term to the renormalized mass term, i.e., at

$$g^2(\Lambda)\frac{1}{z(\Lambda)}\sqrt{z(\Lambda)\Lambda} = \Delta_0 \Lambda^\eta. \tag{24}$$

Solving for the scale Λ we get

$$\Lambda_\Delta = \Delta_0^{\frac{2}{1+\alpha-4\beta}}. \tag{25}$$

This result is meaningful only if $\Lambda_\Delta > \Delta G$. At energy smaller than Λ the infrared divergences are absent and the renormalization flow stops. One expects that Δ_0 is linear in some external control parameter such as pressure (which would vary the interaction constant); thus if $p - p_c > \Delta G$ we would expect that $\chi(0, \mathbf{Q})$ would vary with pressure as

$$\chi(0, \mathbf{Q}) \propto (p - p_c)^{-\frac{2\eta}{1+\alpha-4\beta}}. \tag{26}$$

IV. SCALING AT SMALL MOMENTA

For small energy and momentum the splitting ΔG between the peaks in $\Pi(0, \mathbf{q})$ becomes important. To treat this regime it is convenient to expand $\Pi(0, \mathbf{q})$ for momenta small compared to ΔG. It is also convenient to measure parallel momenta in the units of ΔG and frequencies in the units of $z(\Delta G)\Delta G$. In these units the spin fluctuation propagator

$$D(\omega, \mathbf{q}) = \frac{2\pi}{N\left[\mathrm{Re}\sqrt{k_\parallel + \frac{k_\perp^2}{4} + i\omega} - b\left(k_\parallel - \frac{k_\perp^2}{4}\right) + \Delta\right]} \tag{27}$$

contains a new parameter b, which, as we show below, controls the renormalization group flow and which itself is renormalized. In our units the initial value of b is $1/2$.

We analyze the model in the same way as in the previous section. The spin fluctuation propagator is more singular in the region of large and negative $k_\parallel + \frac{k_\perp^2}{4}$ when the real part of the square root in Eq. (27) is small. The more singular propagator leads to infrared divergences which are stronger than logarithmic, and, we shall show, to a first order transition.

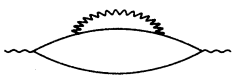


FIG. 7. Leading contribution to the renormalization of the spin fluctuation propagator. Solid lines denote fermions; wavy lines denote spin fluctuations.

As before, we may consider the renormalization of the electron self-energy, the interaction constant, and the polarization bubble. Also as before, the renormalization of the self-energy does not affect the renormalization of other quantities; we do not discuss it further. Unlike the situation at large momenta, there is no renormalization of the interaction constant in the leading order in $1/N$ because in the diagram of Fig. 5 it is not possible to put all fermion lines on the Fermi line and simultaneously have the wavy line carry momentum close to $\mathbf{Q}$. The leading corrections to both Δ and b thus come only from the self-energy insertion in the polarization bubble, as shown in Fig. 6(a).

The dominant scattering processes contributing to the electron self-energy are those in which the electron momentum remains close to the Fermi line. Note that for such processes the momentum transfer is such that $k_\parallel + \frac{k_\perp^2}{2} \approx 0$, so the spin propagator is large. To discuss these processes it is convenient to use the radial and angle coordinates used in the discussion of the electron self-energy in the previous section. It further develops that the dominant contribution comes from processes in which the angle θ pertaining to initial momentum $\mathbf{p}$ is small relative to the angle θ' pertaining to $\mathbf{p}'$. In this limit we may approximate

$$D(\omega, \mathbf{q}) = \frac{2\pi}{N}\frac{1}{\frac{|\omega|}{|\theta'|} + \frac{3}{4}b\theta'^2}. \tag{28}$$

Using this expression for $D(\omega, \mathbf{q})$ and evaluating the diagram shown in Fig. 6(a) gives

$$\frac{\delta\Delta}{\Delta} = -\frac{2n}{27\pi N}\frac{1}{b}\frac{\ln(1/\Lambda)}{\Lambda^{1/2}}. \tag{29}$$

The leading correction to b comes from the diagram shown in Fig. 7 and may be evaluated similarly. We obtain

$$\frac{\delta b}{b} = -\frac{3^{5/6} n}{10N(2b)^{2/3}}\frac{1}{\Lambda^{5/6}}. \tag{30}$$

Equation (29) implies that Δ decreases exponentially as Λ is decreased. This means that it is not possible to find a self-consistent solution along the lines of Eq. (25) for Λ less than a number of order 1.

Arguments originally developed by Brazovskii[12] in a slightly different context show that the minimal value of Λ implies a first order transition. The physical reason is that fluctuations lead to such a large increase in the energy of the critical state that at some point it is favorable to discontinuously open a gap, gaining condensation energy and suppressing fluctuations. In the present problem, the fluctuations are so strong that for physical values of n, N, and b the first order transition happens almost

immediately as the scale ΔG is reached and we expect that the discontinuities in physical quantities are on the scale set by ΔG.

V. PHYSICAL CONSEQUENCES

In this section we describe the implications of our results for observables. We focus on the intermediate scaling regime discussed in Sec. III. The observables are determined by the spin susceptibility which is, restoring units,

$$\chi(\omega,\mathbf{q}) = \frac{g_0^{-2}}{g^2(\Lambda)\left[\Pi(\omega,\mathbf{q})+\Pi(\omega,\mathbf{Q}-\mathbf{q})\right]+\Delta}, \tag{31}$$

$$\Pi(\omega,\mathbf{q}) = \frac{N\sqrt{p_0 p_F}}{2\pi z(\Lambda) v_F}\mathrm{Re}\sqrt{\frac{|q|-2p_F}{p_F}+\frac{iz(\Lambda)\omega}{v_F p_F}}. \tag{32}$$

Here $g^2(\Lambda)$ and $z(\Lambda)$ are slow power law functions of momentum and energy; explicit formulas are given in Eqs. (16) and (18). We emphasize that these formulas only apply at scales larger than the peak splitting ΔG. This form for $\chi(\omega,\mathbf{q})$ is essentially the RPA form with small modifications due to the momentum and frequency dependence of g^2 and z. The Eq. (31) is written in Matsubara frequencies. The imaginary part of the analytic continuation of $\chi(\omega,\mathbf{q})$ is measurable in neutron scattering experiments. The actual form of this imaginary part is somewhat complicated, due to the structure associated with the boundaries of the particle-hole continuum, so we do not write it here. We do discuss in more detail the predictions for NMR relaxation rates $1/T_1$ and $1/T_2$, which involve the low-frequency limits of the real and imaginary parts of $\chi(\omega,\mathbf{q})$, respectively.

The static limit of the real part of $\Pi(\omega,\mathbf{q})$ is easily obtained from Eq. (32) and is

$$\mathrm{Re}\Pi(0,\mathbf{q}) = \frac{N\sqrt{p_0 p_F}}{2\pi z(T) v_F}\mathrm{Re}\sqrt{\frac{|q|-2p_F}{p_F}}. \tag{33}$$

There are different regimes for the imaginary part of $\Pi(\omega,\mathbf{q})$ at small frequency $\omega \ll T$. We find it more convenient to evaluate $\mathrm{Im}\Pi$ directly from the diagram shown in Fig. 2 using renormalized Green functions and vertices than to analytically continue Eq. (32). The general expression

$$\lim_{\omega\to 0}\frac{\mathrm{Im}\Pi(\omega,\mathbf{q})}{\omega} = \int \mathrm{Im}G_R(\epsilon,\mathbf{p}+\mathbf{q})\mathrm{Im}G_R(\epsilon,\mathbf{p})\frac{d^2p d\epsilon g^2(\epsilon,\mathbf{p})}{(2\pi)^3 2T\cosh^2[\epsilon/(2T)]}$$

is obviously dominated by frequencies of the order of T and momenta T/v_F so for this calculation we can use $g^2(\Lambda)$ and $z(\Lambda)$ evaluated at $\Lambda = T$. If $v_F(|q|-2p_F) < z(T)T$ we get

$$\lim_{\omega\to 0}\frac{\mathrm{Im}\Pi(\omega,\mathbf{Q})}{\omega} = \frac{N c_1 p_0^{1/2} g^2(T)}{2\pi z^{1/2}(T) v_F^{3/2} T^{1/2}}, \tag{34}$$

where $c_1 \approx 0.23$. If $v_F(|q|-2p_F) > z(T)T$ the integral is cut off by the external momentum and is

$$\lim_{\omega\to 0}\frac{\mathrm{Im}\Pi(\omega,\mathbf{q})}{\omega} = \frac{N p_0^{1/2} g^2(T)}{4\pi v_F^2 (|q|-2p_F)^{1/2}}. \tag{35}$$

We may now calculate the relaxation rates by combining the results above with the general relation of the real and imaginary parts of the susceptibility to the polarization operator

$$\chi'(0,\mathbf{q}) = \frac{1}{g_0^2\left[g^2\mathrm{Re}\Pi(0,\mathbf{q})+\Delta\right]},$$

$$\lim_{\omega\to 0}\frac{\chi''(\omega,\mathbf{q})}{\omega} = \lim_{\omega\to 0}\frac{g^2\mathrm{Im}\Pi(\omega,\mathbf{q})}{\omega g_0^2\left[g^2\mathrm{Re}\Pi(0,\mathbf{q})+\Delta\right]^2},$$

and inserting the results into the general expressions for relaxation rates

$$\frac{1}{T_1 T} = \sum_q A_q \lim_{\omega\to 0}\frac{\chi''(\omega,\mathbf{q})}{\omega},$$

$$\frac{1}{T_2} = \sqrt{\sum_q \left[A_q \chi'(0,\mathbf{q})\right]^2},$$

where A_q is determined by hyperfine couplings. We see that the T_2 rate behaves as

$$\frac{1}{T_2} = A - BT^{\frac{1}{4}+\frac{5}{4}\alpha-2\beta} \tag{36}$$

or, using our previous results $\alpha \approx 0.27$, $\beta \approx 0.08$,

$$\frac{1}{T_2} = A - BT^{0.05}.$$

Of course, our estimates for α and β come from a $1/N$ expansion, so for the $N = 2$ case we may conclude that the $1/T_2$ rate is either weakly divergent or nondivergent but with anomalously rapid T dependence at low temperatures. Evaluating $1/T_1 T$ similarly we find

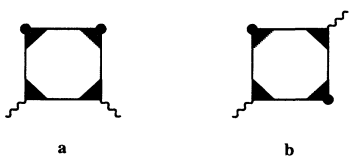
$$\frac{1}{T_1 T} = CT^{-\frac{3}{2}\alpha+2\beta} \approx CT^{-0.25}, \tag{37}$$

i.e., we expect the $1/T_1 T$ rate to be weakly divergent assuming (as was found at large N) $\alpha > 4\beta/3$.

Proximity to the antiferromagnetic transition also has an effect on the uniform susceptibility. We have shown elsewhere[13] that the leading low-T behavior of $\chi(\mathbf{q},0)$ in the limit $\mathbf{q}\to\mathbf{0}$ is given by

$$\chi_U = \lim_{\mathbf{k}\to\mathbf{0}}\chi(0,\mathbf{k}) = \sum_{q,\nu} B(k,\nu)D(\nu,\mathbf{q}), \tag{38}$$

where the coefficient B is given by the diagrams in Fig.



a b

FIG. 8. Leading contributions to the renormalization of the uniform susceptibility. Solid lines denote fermions; wavy lines denote spin fluctuations, and solid dot denotes coupling g_e to the external magnetic field.

8, in which the fermion mediates interaction between the spin fluctuations and the external magnetic field. We denote the bare vertex coupling fermions to the external magnetic field by g_e.

In order to calculate B we use renormalized fermion Green functions and renormalized fermion spin fluctuation vertices g. The coupling to the uniform external field is not renormalized; this follows mathematically from the fact that in any vertex correction diagram the poles in the Green function lines are in the same half plane, so in the limit of vanishing external frequency the low-energy contribution vanishes. Alternatively, one can show that the absence of logarithmic g_e renormalization follows from the fact that the logarithmic renormalization given in (16) does not affect the fermion density of states. Estimating the diagrams in Fig. 8 we get

$$B \sim z^{-5/2}(\epsilon) g^2(\epsilon) \epsilon^{-3/2}. \tag{39}$$

Combining this with our result for $D(\omega, \mathbf{q})$ gives

$$\chi_U \sim c_1 + c_2 T^{\frac{1+\alpha}{2}}. \tag{40}$$

Finally, we note that this scaling regime only exists for energy, temperature, and momenta cutoff greater than ΔG. As soon as the relevant scales fall below ΔG, the $T = 0$ transition becomes first order. This transition happens at some value Δ_0^c of the controlling parameter Δ. At small but nonzero temperatures the transition remains first order but it occurs at a somewhat different value of $\Delta(T)$. We may estimate this transition line from the argument that if $\Delta < \Delta_0^c$ then the ordered phase has lower energy than the disordered phase, so $\Delta E = E_0(\Delta_0^c - \Delta_0)$. However, the disordered phase has greater entropy, because there is no gap on the Fermi line; thus $\Delta F = -T^2 S_0$. Equating the two gives

$$T_{c1} = T_0(\Delta_0^c - \Delta)^{1/2}. \tag{41}$$

We expect that at scales greater than ΔG the line of first order transitions terminates at a critical point T_c. We estimate $T_c(T_c/E_F)^\alpha \sim v_F \Delta G$.

VI. CONCLUSION

We have presented arguments suggesting that the $2p_F$ density-wave transition is first order in $d = 2$ spatial dimensions. By way of conclusion we place our results in the context of quantum critical phenomena and of theories of strongly correlated electrons, and discuss some implications of our conclusions for the physics of high-T_c superconductors.

One may divide quantum critical phenomena in metals into two classes: those in which fluctuations of the order parameter are strongly coupled to the particle-hole continuum (and in particular may decay into a particle-hole pair) and those in which the coupling to fermions is irrelevant. If the coupling to fermions is irrelevant, then the critical phenomena are described by a theory of propagating bosons which may be studied by conventional methods.[14,15,3] If decay into a particle-hole pair is possible, then in most cases it is still possible to describe the critical phenomena by a theory of bosons, albeit with overdamped dynamics.[5,6,16] The description in terms of a purely bosonic theory is possible in these cases because the effect of the critical fluctuations on the fermions is small enough so renormalization of the fermions does not feed back into the properties of critical fluctuations.

The one exceptional case is the two-dimensional $2p_F$ transition. Here the large phase volume available for scattering across the Fermi line implies that the critical fluctuations have a strong effect on the electrons; further, the $2p_F$ singularities in electron response functions mean that electrons near the Fermi line, which are strongly affected by critical scattering, have a large effect on the critical fluctuations. This physics leads to apparently intractable difficulties in the bosonic model generated by formally integrating out the electrons. Specifically, in the resulting bosonic model nonlinear terms of all orders have divergent coefficients and are all relevant in the renormalization group sense. Therefore we used a model in which both electrons and spin fluctuations are retained. We assumed that the bare propagators and the susceptibilities have the Fermi liquid form and that the Fermi line is not straight near the points connected by the ordering wave vector $\mathbf{Q}$. The structure of the $2p_F$ singularities enabled us to construct a renormalization group transformation under which we could treat fermions and spin fluctuations on the same footing.

The solution of the resulting renormalization group equations implies that the transition is generically first order, because the critical fluctuations are so strong that they completely suppress the second order transition. There is one special case where the transition is not first order. If twice the ordering vector $\mathbf{Q}$ is commensurate with a reciprocal lattice vector $\mathbf{G}$, i.e., $2\mathbf{Q} = \mathbf{G}$, then the spin fluctuation propagator is less singular, the fluctuations are weaker, and the transition turns out to be second order and characterized by the exponents which we calculate in a $1/N$ expansion. If $|2\mathbf{Q} - \mathbf{G}|$ is small, the $T = 0$ transition is ultimately first order but a broad scaling regime exists.

Our explicit calculations were performed for a model of a spin-density-wave (SDW) transition. Most of our results carry over to the charge-density-wave case, if the number of spin components, n, is set to 1. There is one important caveat. If the system is sufficiently symmetric, e.g., if the Fermi line is circular, cubic terms (forbidden in the SDW case by time reversal) may exist in the Landau free energy. Cubic terms lead also to a first order transition but their presence would also complicate the analysis given above.

We now place our results in the context of theories of interacting electrons in two spatial dimensions. To produce a quantum phase transition one must increase an interaction parameter to a critical value which is generally large. One must therefore consider the effect of the interaction on the noncritical state of the electrons. There are two possibilities: One is Fermi liquid theory in which it is assumed that perturbation theory may be resummed to all orders. Within this assumption one may show that away from any critical point the low-energy properties are

not qualitatively changed from those of free electrons, so the transition takes place against a Fermi liquid background and one may use the theory given here to calculate the extra effects due to criticality.

An alternative possibility is that Fermi liquid theory is not a correct description of the low-energy properties even far from criticality. For example, it has been argued that in strongly correlated two-dimensional models the spin degrees of freedom form a "spin liquid."[17,18] A spin liquid possesses a Fermi surface, spin 1/2 fermionic excitations with constant density of states at low energies, and a particle-hole continuum, but the fermions interact via a singular interaction which, among other things, changes substantially $2p_F$ singularities.[19] The singular interaction causes anomalous temperature dependence of susceptibility and NMR relaxation rates even away from the criticality[16] and changes the critical properties. The spin-liquid to antiferromagnet transition has been studied elsewhere.[16]

The high-temperature superconductors are quasi-two-dimensional materials with spin dynamics which have been claimed to be controlled by a quantum critical fixed point. It is still controversial whether Fermi liquid theory is the correct starting point for a description of the low-energy electron physics. It is therefore interesting to compare our theoretical results to the known magnetic properties of high-T_c materials.

For a two-dimensional Fermi liquid the bare polarizability is so strongly peaked at $2p_F$ that it is most natural to assume that the transition occurs at $Q = 2p_F$. This is consistent with neutron scattering data on $La_{2-x}Sr_xCuO_4$, in which strong and temperature-dependent peaks were observed. These peaks are centered at x-dependent wave vectors $\mathbf{Q}(x)$ which are claimed to be $2p_F$ wave vectors of the local density approximation (LDA) band structure.[10] Therefore, if a Fermi liquid picture is appropriate, it is natural to expect our results to describe experiments on $La_{2-x}Sr_xCuO_4$.

In fact, they do not. There is no sign of a first order transition; the magnetic properties apparently evolve smoothly with doping. It is conceivable that disorder due to random positions of the Sr dopants masks the first order transition. However, for all Sr concentrations including $x = 0.14$ there is a wide temperature regime in which the NMR relaxation rates and uniform susceptibility vary with temperature. Roughly, the copper $1/(T_1T)$ and $1/T_2$ are inversely proportional to $1/T$,[20,21] while $\chi_U \sim A + BT$.[22] These temperature dependences are not consistent with our results, Eqs. (37), (36), and (40). We conclude that the magnetic properties of $La_{2-x}Sr_xCuO_4$ are not well described within a Fermi liquid approach. Two alternatives have been proposed: one is that the fermions are in the "spin-liquid" regime described above;[16] another is that the critical behavior is due to propagating spin waves only weakly coupled to the electrons.[4,23]

Another class of materials to which our results might be relevant are the low-dimensional organics such as $(TMTSF)_2PF_6$. These materials have strongly anisotropic transfer integrals $t_a \gg t_b \gg t_c$, leading typically to an open Fermi line, but with nonnegligible curvature. The curvature implies that the physics of these materials is not strictly one dimensional and makes it possible that the theory developed here is relevant and explains the experimental observation that the spin-density-wave transition produced by lowering the temperature is weakly first order.[11]

We recently received unpublished results from Chubukov[24] analyzing the spin-density-wave transition with $\mathbf{Q} = \mathbf{G}/2$ but $\mathbf{Q} \neq 2p_F$. He found a logarithmic renormalization very similar to the one we found in the intermediate scaling regime discussed in Sec. III and showed that this implies that the exponents characterizing the critical point he analyzed differ from the exponents characterizing the general case in which $\mathbf{Q} \neq \mathbf{G}/2$ and $\mathbf{Q} \neq 2p_F$ analyzed by previous authors.[5,6]

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