Overscreening of magnetic impurities in $d_{x^2-y^2}$ -wave superconductors

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We consider the screening of a magnetic impurity in a $d_{x^2-y^2}$ -wave superconductor. The properties of the $d_{x^2-y^2}$ state lead to an unusual behavior in the impurity magnetic susceptibility, the impurity specific heat, and in the quasiparticle phase shift which can be used to diagnose the nature of the condensed state. We construct an effective theory for this problem and show that it is equivalent to a multichannel (one per node) nonmarginal Kondo problem with linear density of states and coupling constant J. There is a quantum phase transition from an unscreened impurity state to an overscreened Kondo state at a critical value J_c which varies with Δ_0 , the superconducting gap away from the nodes. In the overscreened phase, the impurity Fermi level ϵ_f and the amplitude Δ of the ground state singlet vanish at J_c like $\Delta_0 \exp(-\text{const}/\Delta)$ and $J-J_c$, respectively. We derive the scaling laws for the susceptibility and specific heat in the overscreened phase at low fields and temperatures. [S0163-1829(97)01341-6]

I. INTRODUCTION

The problem of magnetic impurities in *d*-wave superconductors has been a subject of intense research.¹⁻⁴ It is known that in anisotropic superconductors, such as a $d_{x^2-y^2}$ state, magnetic impurities act as pair-breaking centers⁵ and hence reduce the amplitude of the condensate. Experimentally, the main effect of these impurities is to reduce the critical temperature T_c of the superconducting state.^{6,7}

Quantum-mechanical fluctuations of magnetic impurities give rise other important effects particularly when coupled to the fermionic quasiparticles of the superconducting state. In a normal metal these correlations lead to the Kondo screening of the impurity and to the generation of dynamical energy scales such as the Kondo temperature. In hightemperature superconductors, the effects of the magnetic impurities appear to depend significantly not only on the nature of the impurity but also on where the magnetic impurity is located. The conventional interpretation of the role of magnetic impurities in high-temperature superconductors relies, for the most part, on the chemical differences of the impurities (mainly Zn and Ni) and on the actual location of the impurities on the lattice relative to the CuO planes. The main focus of recent work on this subject has focused on how much different impurities are able to depress T_c (Ref. 7) and on the power laws that static (or clasical) impurities induce on low-tempreture properties.

In this paper we investigate the physics that results from the exchange coupling between isolated magnetic impurities and the quasiparticles of the superconducting state. In particular we will be interested in finding out under what circumstances there is a Kondo-like dynamical screening of the magnetic impurity by the quasiparticles. The mechanism that we have in mind is analogous to the exchange coupling between magnetic impurities and the electrons of a Fermi liquid that causes the Kondo effect. However, unlike the Kondo effect in metals, because the density of states of normal quasiparticles in a *d*-wave superconductor vanishes at the Fermi energy, screening is absent in perturbation theory and a critical exchange coupling between the quasiparticles and the magnetic impurity is necessary for Kondo screening to take place. Thus, magnetic impurities which couple strongly to the quasiparticles, such as Zn which substitute for Cu is the planes, may actually be Kondo screened at very low temperatures while Ni, which appears to couple more weakly, may not get to be in a Kondo screening regime. Likewise, magnetic impurities on sites away from the CuO planes are weakly coupled and therefore are less likely to undergo Kondo screening. We will see below that the critical coupling (which we will only estimate very roughly in this work) is controlled by Δ_0 , the size of the gap away from the nodes at zero temperature, and typically it is a fraction of Δ_0 .

The onset of Kondo screening at a critical value of the exchange coupling constant is a quantum critical point. We will show in this work that the behavior of the magnetic impurity, both near and beyond the phase transition, has unique signatures which follow from the nature of the condensate and hence can be used to investigate its nature. Among its most salient features are the temperature and magnetic field dependence of the impurity magnetic susceptibility and specific heat which exhibit strong deviations from Fermi-liquid behavior. We will also show that the quasiparticle phase shift exhibits a strong frequency dependence and a broad resonance and that the structure of the quasiparticle scattering matrix has detailed information on the phases and signs associated with *d*-wave superconductivity. Thus, the physics of magnetic impurities in a *d*-wave supercon-

<u>56</u> 11 246

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ductor can be used to diagnose the nature of the superconducting order. The purpose of this paper is to describe these effects in detail.

The Kondo problem in metals⁸ has been intensively and extensively studied and it is by now very well understood. It is described in terms of a *smooth* crossover from a marginally unstable fixed point at zero exchange coupling to a stable Fermi-liquid fixed point with a screend impurity.^{9–11} The validity of this picture has been confirmed by the exact solution by the Bethe ansatz^{12,13} and by large-*N* methods.¹⁴ We will refer to this case as to the *marginal* Kondo problem since it bears a strong resemblance to a critical system at its low critical dimension.

In a conventional *s*-wave superconductor the Kondo effect is suppressed by the formation of the superconducting gap, as shown by the classic theory of Abrikosov and Gorkov.¹⁵ However, in the case of a *d*-wave superconductor, there are quasiprticle states inside the superconducting gap which concentrate near the nodes of the order parameter. Although the density of states vanishes at the Fermi energy, for strong enough exchange coupling it may still be possible that isolated magnetic impurities may still be screend by the quasiparticles. The central idea of this work is that the way this screening happens may be used as a tool to study the superconducting order.

Impurities cause many different effects in superconductors. In the case of a d-wave symmetry, any sort of scattering breaks pairs⁵ and, for instance, static magnetic impurities produce quasiparticle bound states in the gap of the superconductor. However, the binding energy of these states vanishes in the vicinity of the nodes of the d-wave superconductor.^{3,4,16} Random potential scattering also leads to interesting effects, in particular close to the nodes of the superconductor where the density of states (DOS) of quasiparticle states, which behave like Dirac fermions near the nodes, vanishes linearly with the energy (measured from the Fermi energy). It has also been shown that random potential scattering should generally lead to a *finite* DOS at the Fermi energy (zero) for Dirac fermions in random potentials^{17–19} and in *d*-wave superconductors.^{20,2,21} The precise behavior of the DOS appears to depend on how many nodes are coupled and on what channels are mixed by the scattering processes.^{2,19,22,23} However, if the superconductor is sufficiently clean, the effective DOS induced by the disorder is *exponentially* small^{17,18} and its effects can be neglected. Notice, however, that the combined effects of Kondo screening and random scattering is a problem that is still not undertood, even in metals.^{24,25}

The problem of a quantum magnetic impurity coupled to fermions with a vanishing DOS at the Fermi energy was discussed by Withoff and Fradkin.²⁶ In contrast with the Fermi liquid which has a finite DOS at the Fermi energy, Kondo screening of the magnetic impurity could only happen for values of the exchange coupling constant J larger than some critical value. If the DOS vanishes with a power of the energy with exponent r, the fixed point at J=0 is stable for r>0 and a new unstable fixed point appears at $J_c>0$, signaling a quantum phase transition. We will refer to this problem as the nonmarginal Kondo problem and r measures the deviation from marginality. Using a close analogy with the theory of critical phenomena, Withoff and Fradkin developed a large-*N* theory for this problem and found that the essential singularity of the Kondo temperature is replaced by power law singularities determined by the DOS exponent *r*. However, in that work only the regime $0 < r \le \frac{1}{2}$ was considered. The behavior of these systems for small *r* was also exlored by Chen and Jayaprakash²⁷ and by Ingersent²⁸ who used a generalization of Wilson's numerical renormalization group (RG) for this problem. The case of interest for a *d*-wave superconductor is r=1 which turns out to be special in several ways. In Ref. 29 we discussed recently the closely related problem of a magnetic impurity in a flux phase which is also an example of an r=1 system. In this paper we show that these two problems can be mapped onto each other in spite of the fact that spin fluctuations do break Cooper pairs.

One aspect of the physics of magnetic impurities in a d-wave superconductor that we will not consider here are the effects of the depression (and/or actual vanishing) of the d-wave order parameter near the impurity site. This effect is independent of the spin and it actually static. In any event, the vanishing of the condensate at the impurity site leads to terms that do not conserve fermion number in the effective Hamiltonian and hence may lead to important (spin-independent) effects. This is a conceptually important problem and it will be addressed elsewhere.³⁰ A self-consistent calculation based on the BCS approximation can be found in Ref. 23.

In this paper we will make use of a very simple model of the quasiparticle dynamics in a $d_{x^2-y^2}$ superconductor.^{31,32} We will use the fact, strongly supported by the corner-junction interference experiments³³ as well as by angle-resolved photoemission spectroscopy^{34,35} (ARPES), that the high-temperature superconductors have a $d_{x^2-y^2}$ condensate with four symmetrically arranged nodes where the quasiparticle gap vanishes. The first evidence that the gap vanishes at the $d_{x^2-y^2}$ nodal line was reported by Shen *et al.*³⁴ Ding et al.35 reported measurements of the momentum dependence of the superconductor gap in Bi₂Sr₂CaCu₂O_{8+x} consistent with a gap function of the form $\cos(k_x) - \cos(k_y)$, as expected for a *d*-wave order parameter. Interestingly enough, in underdoped systems, photoemission supports the idea that the gap may survive through a large range of temperature into the normal state.^{34,35} It is also well established that the high-temperature superconductors are not conventional BCS systems in the sense that their normal states deviate strongly from the predictions of Fermi-liquid theory and that the interactions are strong. Thus, a straightforward BCS selfconsistent approach should not work, particularly in view of the fact that there is not a well-established mechanism for superconductivity in these materials. Nevertheless, whatever actual the mechanism is, it should describe a system with nodes and with gapless quasiparticle branches. The actual coefficients of this effective Hamiltonian cannot be derived in a simpleminded way from a microscopic system but its form will be determined by the requirements of $d_{x^2-y^2}$ symmetry. Thus we will use a phenomenologically motivated BCS-like model for the quasiparticles with nodes consistent with $d_{x^2-y^2}$ symmetry but without a self-consitent derivation of its coefficients. We will consider the case of a very clean system and at very low temperatures so as to neglect fluctuations of the amplitude of the superconducting order parameter.

In Sec. III we derive an effective Kondo-like Hamiltonian for the problem of a single magnetic impurity in an otherwise perfect $d_{x^2-y^2}$ superconductor. In this model we focus on the effects of the quasiparticles close to the nodes of the $d_{x^2-y^2}$ state within an energy range Δ_0 , the gap of the superconductor away from the nodes. We also include, albeit in rather crude fashion, the effects of the states above the superconducting gap since they affect the value of the critical exchange constant. By expanding the electron operator in the exact quasiparticle states of the $d_{x^2-y^2}$ superconductor, we map this problem of two-dimensional physics into an effective one-dimensional system of chiral fermions coupled to the impurity. The effective Hamiltonian is almost identical to the problem of a magnetic impurity in a flux phase that we discussed in Ref. 29. The only difference here is that the symmetry is SU(2) (spin) but there are four species (or flavors) of chiral fermions, one per node. The mapping of the *electron* operator into the effective one-dimensional fermion contains all the information about the coherence factors of the $d_{x^2-y^2}$ state and, hence, it includes the pair-breaking effects caused by the spin fluctuations of the impurity. As a bonus, we get explicit (although qualitative) relations between the effective coupling constants, the relative importance of intranode and internode scattering processes, and important parameters such as the location of the impurity (relative to the CuO plane) and the superconducting gap Δ_0 . We will find that, in fact, there is always one effective channel that matters.

A considerable number of theoretical tools have been developed to study Kondo systems. For magnetic impurities in a metallic host, which have an essentially constant density of states near the Fermi energy, the different methods complement each other in a manner such that we now have a rather complete understanding of this phenomenon at a nonperturbative level. However, with the exception of large-N methods or Wilson's numerical renormalization group, all the other methods (including the powerful mapping to onedimensional logarithmic gases, the exact solution via the Bethe ansatz and the conformal field theory approach) cannot be appiled to systems with a vanishing density of states. For these reasons in this work we use the large- N_c approach, even though $N_c = 2$ for the *d*-wave superconductor. In conventional Kondo systems $N_c = 2$ and $N_c = \infty$ are known to be smoothly connected and, although it is likely that this will also hold for a *d*-wave system, there is still no evidence that it is also true for this problem. In any case, given the lack of alternative approaches, we will present here a large- N_c theory of our problem.

Our large- N_c theory predicts that magnetic impurities in *clean* cuprate superconductors should undergo a quantum phase transition at a critical exchange constant whose typical value is crudely estimated to be below the superconducting gap Δ_0 (details are given in the next and in the last two sections). Our estimates indicate that, for an exchange coupling J with strength about 10% larger than the critical coupling, the anomalous behaviors that we predict should be accessible to measurements of the low-temperature heat capacity and magnetic susceptibility [such as in nuclear quadrupole resonance (NQR)] with magnetic fields $H \sim 1-10$ T and at temperatures $T \sim 1-10$ K. The magnetic fields should be *in plane* so as not to disturb the kinematic properties of

the quasiparticles on the CuO planes. At temperatures higher than T_K (but still below T_c) the system behaves as if it were at its quantum critical point at J_c .

In Ref. 29 we discussed the solution of the problem of a magnetic impurity in a flux phase problem which, as we indicated above, is closely related the problem of a *d*-wave superconductor. In that work we used the large- N_c limit to investigate a similar phase transition. However, the results that we present here for the scaling behavior of the physical observables near this transition disagree with our previous work of Ref. 29. The reason for the discrepancy is that in the process of carrying out the large- N_c limit divergent series need to be handled and in Ref. 29 these series were regulated in in a manner that is incompatible with an integer filling Q_f of the impurity in the slave fermion representation. This inconsistency is removed in this paper and the results that we present here supersede those of Ref. 29.

This paper is organized as follows. In Sec. II we present a summary of the main results of this paper including experimentally accessible predictions for magnetic impurities in high-temperature superconductors. In Sec. III we describe the mapping of the model of a single magnetic impurity coupled to a $d_{x^2-y^2}$ superconductor to an effective theory of chiral fermions in one dimension with a non marginal coupling. In Sec. IV we discuss the large- N_c approximation and in Sec. V we discuss the solution of the saddle point equations, valid in the $N_c \rightarrow \infty$ limit, and use it to investigate the phase diagram of this problem at zero temperature and zero magnetic field. In Sec. VI we calculate the low- and zerotemperature magnetic susceptibility of the impurity at zero and finite (but small) fields in the $N_c \rightarrow \infty$ limit. Similarly, the impurity entropy and specific heat (at low temperatures and fields) are calculated in Sec. VII again in the $N_c \rightarrow \infty$ limit. In Sec. VIII we conclude with a discussion of the implications of our results and their relation with other work, particularly the RG work of Ingersent. Relevant details of the computation of various integrals are given in the Appendix.

II. SUMMARY OF RESULTS

In this section we give a brief summary of our main results and discuss their implications for magnetic impurities in high-temperature superconductors.

(1) We introduce a model for a single magnetic impurity in a $d_{x^2-y^2}$ condensate (see Sec. III) with Hamiltonian *H*

$$H = \sum_{\vec{k},\sigma} \epsilon(\vec{k}) c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} - \sum_{\vec{k}} \Delta(\vec{k}) c_{\vec{k}\uparrow}^{\dagger} c_{-\vec{k}\downarrow}^{\dagger} + \text{H.c.}$$
$$+ \vec{S} \cdot \int d^2 x J(\vec{x}) c_{\sigma}^{\dagger}(\vec{x}) \vec{\tau}_{\sigma\sigma'} c_{\sigma'}(\vec{x}). \qquad (2.1)$$

This is accurate at energies and temperatures low with respect to the gap Δ_0 of the $d_{x^2-y^2}$ condensate away form the nodes. We use a simple lattice model for the $d_{x^2-y^2}$ quasiparticles (see Ref. 1), which yields a qualitative description of the superconductor, but it has the correct nodal structure and that is all that we actually need to know. Next we construct an effective model of one-dimensional chiral fermions coupled to the impurity:

$$H_{\rm eff} = \sum_{a=1}^{4} \sum_{\sigma=\uparrow,\downarrow} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \sqrt{vv'} p d^{\dagger}_{a\sigma}(p) d_{a\sigma}(p) + \sum_{a=1}^{4} \sum_{\sigma,\nu=\uparrow,\downarrow} (J_a/2) \bigg[\int_{-\infty}^{\infty} \frac{dp}{2\pi} \sqrt{|p|} d^{\dagger}_{a\sigma}(p) \bigg] \times \vec{\tau}_{\sigma\nu} \cdot \vec{S}_{\rm imp} \bigg[\int_{-\infty}^{\infty} \frac{dp'}{2\pi} \sqrt{|p'|} d_{a\nu}(p') \bigg], \qquad (2.2)$$

where v and v' are the velocities of the quasiparticles of the *d*-wave state along the two lattice directions. This is the model that we actually investigate. The nature of the $d_{x^2-y^2}$ state is present: (a) in the momentum dependence of the interaction between the chiral fermions and the impurity [see Eq. (3.32)] and (b) in the number and angular momenta of the channels that are coupled to the impurity [see Eqs. (3.23) and (3.24)]. We truncate the momentum dependence of the interaction beyond a momentum scale $\sim \Delta_0/(2\pi\sqrt{vv'})$ where it saturates, indicating that the effective density of states is nearly constant for states above the gap Δ_0 and up to an upper cuttoff scale *D*, the bandwidth of the normal quasiparticles $\epsilon(\vec{k})$. A typical value of Δ_0 for a CuO superconductor is 100 K and $D/\Delta_0 \ge 10$.

(2) In Secs. IV and V we solve this effective model in the large- N_c limit. The physical properties of the system in the $N_c \rightarrow \infty$ limit are determined by the behavior of the *phase shift* $\delta(\epsilon)$ of Eq. (4.8). This is the phase shift acquired by the quasiparticles of the superconductor as they scatter off the magnetic impurity. We find that, in contrast with the conventional Kondo problem, the phase shift $\delta(\epsilon)$ has a strong energy dependence. $\delta(\epsilon)$ is parametrized by the singlet amplitude Δ and the impurity Fermi level ϵ_f (which plays the role of the Kondo scale). These are determined by solving the saddle point equations [Eqs. (5.1) and (5.2)] which yield Δ and ϵ_f as functions of the impurity filling Q_f , the exchange constant J, the temperature T, and the magnetic field H.

(3) Phase transition: We find that, at T = H = 0, the system has a quantum phase transition at a critical coupling constant $J_c \approx (2vv'/\Delta_0)/[1 + \ln(D/\Delta_0)]$. This transition separates a weak-coupling free phase in which the impurity is nearly free with a Curie-like susceptibility, from a strong-coupling phase where the impurity is screened. We find that the impurity is actually *overscreened* since the impurity magnetic susceptibility vanishes for $J \ge J_c$ at T = H = 0. A naïve use of the BCS estimates yields $J_c \approx D \sin^2(k_0)/[1 + \ln(D/\Delta_0)]$ which is larger than Δ_0 unless $k_0 \leq 1$ (which is not unreasonable). However, strong-coupling corrections in the superconductor (which, at best, can only be estimated and depend strongly on the details of the mechanism of superconductivity) in general will invalidate the simple relation between the velocities k_0 and Δ_0 . However, we expect that $J_c \leq \Delta_0$, typically being of order of $\Delta_0/2$ or so. However, a precise estimate requires a more sophisticated calculation than the one we do here. For the puroposes of this work it will be sufficient to know that $J_c < \Delta_0$.

(4) Kondo scale: We find that, close to and above J_c , the Kondo scale $T_K = \epsilon_f$ is related to the singlet amplitude Δ by [Eq. (5.9)]

$$\epsilon_f(x,\Delta) = \Delta_0 \sqrt{e} \exp\left(-\frac{1}{\Delta} \frac{2x}{1-2x+\Delta} + \frac{1}{1-2x+\Delta}\right) \\ \times [1+O(\Delta,\Delta \ln \Delta)], \qquad (2.3)$$

where e = 2.7172... and $x = Q_f/N_c$. This singular relation between ϵ_f and Δ results from a logarithmic singularity in the saddle point equation for the impurity occupancy. This singularity is absent for r < 1. In this sense, r = 1 is like an "upper critical dimension" for impurity problems. The actual dependence on the coupling constant is determined by solving the equation of state, Eq. (5.15),

$$\frac{1}{J_c} - \frac{1}{J} \approx \left(\frac{\Delta_0}{\pi v v'}\right) \Delta + O(\Delta^3).$$
(2.4)

A rough estimate of T_K can be obtained by setting $Q_f = 1$ and $N_c = 2$. We find that, for $(J/J_c) - 1 \approx 0.2$ and $\Delta_0 \approx 100$ K, $T_K = \epsilon_f \approx 9$ K, while, for $(J/J_c) - 1 \approx 0.1$, $T_K \approx 1$ K.

(5) We have calculated the impurity susceptibility and specific heat in the overscreened phase $J > J_c$ for magnetic fields and temperatures $H, T < T_K$ which can be realized unless *J* is too close to J_c . For $T \ll H \ll T_K$ we find [Eq. (6.15)] the susceptibility

$$\chi_{\rm imp} \sim N_c \left(\frac{\Delta}{\epsilon_f}\right)^2 H \ln \frac{\Delta_0}{H},$$

while, in the opposite regime $H \ll T \ll T_K$ [Eq. (6.16)],

$$\chi_{\rm imp} \sim 2N_c \ln 2 \left(\frac{\Delta}{\epsilon_f}\right) T \ln \left(\frac{\Delta_0}{T}\right).$$

Similarly, the specific heat in the regime $H \ll T \ll T_K$ is [Eq. (7.5)]

$$C_{\rm imp}(0,T) \approx 9\zeta(3)N_c \frac{\Delta^2}{\epsilon_f^2}T^2 \ln\left(\frac{\Delta_0}{T}\right)$$

while for $T \ll H \ll T_K$ we find instead the result [Eq. (7.7)]

$$C_{\rm imp}(H,T) \approx N_c \frac{\pi^2}{3} \left(\frac{\Delta}{\epsilon_f}\right) T H \ln\left(\frac{\Delta_0}{H}\right)$$

The low-field regime is clearly very different from a Fermi liquid although a Wilson ratio can still be defined and it is finite [Eq. (7.6)]

$$\frac{C_{\rm imp}(H,T)}{T\chi_{\rm imp}(H,T)} \approx \frac{9\zeta(3)}{2\ln 2}.$$

The behavior in the high field regime is more like a Fermi liquid. These behaviors should be accessible to experiments in clean samples of cuprate superconductors at magnetic fields of 1-10 Tesla.

We have not investigated yet the quantum critical regime $H,T>T_K$, which we will discuss in a separate publication.³⁰

III. THE MODEL

In this section we construct the model that describes the coupling of the quasi-particles of a d-wave superconductor to a localized magnetic impurity. We will show explicitly

that this model maps exactly onto a model of a magnetic impurity coupled to the spinons of a flux phase that we discussed in Ref. 29. The strategy that we will follow in this section consists of first writing down a simple model for the quasiparticles of the *d*-wave superconductor with a physically reasonable coupling to a local magnetic moment. Next we will carry a dimensional reduction of this problem down to a model of effective one-dimensional (chiral) fermions which has all the symmetries of the *d*-wave superconductor. The effective one-dimensional model coincides exactly with the nonmarginal Kondo problem that was discussed in Ref. 29. In the next section we will use the results of Ref. 29 to draw conclusions on the effects of magnetic impurities in *d*-wave superconductors.

A. Free Hamiltonian

We begin by choosing a model of a *d*-wave superconductor with the form of a BCS-type Hamiltonian. It has a kinetic energy term (which we choose to be of the form of a tight-binding Hamiltonian) and a pairing term with *d*-wave symmetry. In Sec. III B we will describe the way magnetic impurities couple to the quasiparticles. Here we will make the phenomenological assumption that there is *d*-wave pairing regardless of the mechanism that gives rise to that pairing. BCS-type models which exhibit *d*-wave pairing (driven by antiferromagnetic fluctuations) have been proposed by Bickers, Scalapino, and White³⁶ and by Monthoux and Pines.¹ Here we will use a BCS model of this type to describe the dynamics of the quasiparticles.

What will be important for the dynamics is that the model exhibits four nodes where the gap vanishes and that the gap is fairly large away from the nodes. Thus, we will concentrate on the behavior of the quasiparticles close to the nodes. Instead of using the full detailed form of the gap, we will replace it by a linearized spectrum with a wave vector cutoff Λ (relative to the location of the node) such that the energy of the quasiparticles with wavevector Λ is approximately equal to the value Δ_0 of the superconductor gap away from the nodes. The actual structure of the quasiparticle spectrum away from the nodes will play a very small role and such states will be neglected. This view is supported by recent photoemmission experiments by Shen et al.³⁴ and Ding et al.³⁵ in YBaCuO superconductors where a Fermi surface is seen at optimal doping and it disappears progressively away from the nodes (where the gap vanishes) for underdoped systems. Hence, the important features of the quasiparticle spectrum that we will keep are the four nodes where the excitations are gapless, the correct behavior under lattice symmetries (and parity), and the Fermi velocities at the nodes.

The Hamiltonian for the quasiparticles of a BCS-type superconductor in the absence of impurities is

$$H_0 = \sum_{\vec{k},\sigma} \epsilon(\vec{k}) c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} - \sum_{\vec{k}} \Delta(\vec{k}) c_{\vec{k}\uparrow}^{\dagger} c_{-\vec{k}\downarrow}^{\dagger} + \text{H.c.} \quad (3.1)$$

To make the model concrete we use a lattice model for the quasiparticles with a bare energy $\epsilon(\vec{k})$ of the form

$$\boldsymbol{\epsilon}(\vec{k}) = \boldsymbol{\epsilon}(-\vec{k}) = -2t[\cos(k_1) + \cos(k_2)] + \boldsymbol{\mu}. \quad (3.2)$$

The Fermi operators $c_{\vec{k}\sigma}^{\dagger}$ create quasiparticles with momentum \vec{k} , spin σ , and energy $\epsilon(\vec{k})$. Here μ is the chemical potential for the quasiparticles. The gap function $\Delta(\vec{k})$ for a $d_{x^2-y^2}$ superconductor given by

$$\Delta(k) = \Delta_0 [\cos(k_1) - \cos(k_2)].$$
(3.3)

Here Δ_0 set the scale for the gap away from the nodes. The one-particle spectrum of this simple Hamiltonian agrees qualitatively with the observed photoemission spectrum.

Next we write the quasiparticle operators in the Nambu-Gorkov form^{32}

$$\Phi(\vec{k}) = \begin{pmatrix} c_{\vec{k}\uparrow} \\ c_{-\vec{k}\downarrow}^{\dagger} \end{pmatrix}.$$
(3.4)

In terms of the Nambu-Gorkov (NG) spinors, the free part of the Hamiltonian H_0 can now be written as

$$H_0 = \sum_{\vec{k}} \Phi^{\dagger}(\vec{k}) \{ [\epsilon(\vec{k}) - \mu] \tau_3 - \Delta(\vec{k}) \tau_1 \} \Phi(\vec{k}), \quad (3.5)$$

where τ_1 and τ_3 are two Pauli matrices. This model has four nodes² at the points in the Brillouin zone given by $(\pm k_0, \pm k_0)$, with $k_0 \equiv \arccos(\mu/4t)$. The spectrum of the quasiparticles crosses the Fermi surface at those points and the gap closes. As a consequence, the quasiparticles have a linear dispersion relation in the vicinity of these *nodes*. This can be shown² by expanding for small momentum departures around the $(\pm k_0, \pm k_0)$ points.

The next step in the construction of an effective lowenergy model is to describe the dynamics of the quasiparticles close to the nodes. To this end we assign a label for each one of the four nodes. Let a=1,2,3,4 be this label and we assign the label a=1 to the node (k_0,k_0) , a=2 to the node $(-k_0,-k_0)$, a=3 to the node $(-k_0,k_0)$, and a=4 to the node $(k_0,-k_0)$. Let \vec{q} be the momentum relative to the node. It is useful to work in the rotated basis $p_1 \equiv (1/\sqrt{2})(q_1+q_2)$ and $p_2 \equiv (1/\sqrt{2})(q_1-q_2)$, with velocities $v \equiv 2\sqrt{2}t \sin(k_0)$, $v' \equiv \sqrt{2}\Delta_0 \sin(k_0)$, where Δ_0 is the size of the superconductor gap at its maximum value. Let $\Phi_a^{\dagger}(\vec{p})$ denote the (Nambu-Gorkov spinor) operator which creates a quasiparticle with (rotated) momentum \vec{p} relative to the wave vector of node a. The free Hamiltonian now takes the form

$$H_{0} = \int \frac{d^{2}p}{(2\pi)^{2}} \{ \Phi_{1}^{\dagger}(\vec{p})(vp_{1}\tau_{3} + v'p_{2}\tau_{1})\Phi_{1}(\vec{p}) - \Phi_{2}^{\dagger}(\vec{p})(vp_{1}\tau_{3} + v'p_{2}\tau_{1})\Phi_{2}(\vec{p}) \} - \int \frac{d^{2}p}{(2\pi)^{2}} \{ \Phi_{3}^{\dagger}(\vec{p})(vp_{2}\tau_{3} + v'p_{1}\tau_{1})\Phi_{3}(\vec{p}) - \Phi_{4}^{\dagger}(\vec{p})(vp_{1}\tau_{3} + v'p_{2}\tau_{1})\Phi_{4}(\vec{p}) \}.$$
(3.6)

In the long-wavelength limit the Hamiltonian splits into four (anisotropic) Dirac-like Hamiltonians. In what follows we will refer to these four sets of excitations (which represent the four nodes of the *d*-wave superconductor) as to the four *flavors* (or channels).

$$\Phi_a(\vec{k}) = \frac{1}{\sqrt{2}} (1 - i\tau_1) \psi_a(\vec{k}), \qquad (3.7)$$

and to write H_0 in terms of ψ_a ,

$$H_{0} = \int \frac{d^{2}p}{(2\pi)^{2}} \begin{pmatrix} 0 & \epsilon_{+}e^{-i\theta_{+}} \\ \epsilon_{+}e^{i\theta_{+}} & 0 \end{pmatrix} [\psi_{1}^{\dagger}(\vec{p})\psi_{1}(\vec{p}) \\ -\psi_{2}^{\dagger}(\vec{p})\psi_{2}(\vec{p})] - \int \frac{dp^{2}}{(2\pi)^{2}} \begin{pmatrix} 0 & \epsilon_{-}e^{-i\theta_{-}} \\ \epsilon_{-}e^{i\theta_{-}} & 0 \end{pmatrix} \\ \times [\psi_{3}^{\dagger}(\vec{p})\psi_{3}(\vec{p}) - \psi_{4}^{\dagger}(\vec{p})\psi_{4}(\vec{p})].$$
(3.8)

In Eq. (3.8) the following definitions have been used:

$$\epsilon_{+} \equiv \sqrt{(vp_{1})^{2} + (v'p_{2})^{2}} \equiv \sqrt{vv'}p_{+},$$

$$\theta_{+} \equiv \tan^{-1}(vp_{1}/v'p_{2}),$$

$$\epsilon_{-} \equiv \sqrt{(v'p_{1})^{2} + (vp_{2})^{2}} \equiv \sqrt{vv'}p_{-},$$

$$\theta_{-} \equiv \tan^{-1}(vp_{2}/v'p_{1}),$$

where $v \equiv 2\sqrt{2}t \sin(k_0)$ and $v \equiv \sqrt{2}\Delta_0 \sin(k_0)$.

Next we notice the fact that, as far as the kinetic energy is concerned, p_+ , p_- , θ_+ , and θ_- are just dummy variables and that the measure in the integrals is invariant under the change p_1, p_2 into p_+, p_- . It turns out—and we show this below—that the integration term is also invariant under a redefinition of the integration variables. Naturally, the quasiparticle operators themselves are not invariant under these redefinitions of variables. Hence, although all explicit reference to the anisotropy can be removed from the Hamiltonian, it remains quite explicit in the relation between the quasiparticle (fermion) operators and the fields that will describe the effective Hamiltonian, i.e., in generalized coherence factors.

Taking these observations into consideration, H_0 can be put in a much simpler form

$$H_{0} = \int_{0}^{\infty} \frac{p dp}{2\pi} \int_{0}^{2\pi} \frac{d\theta}{2\pi} \begin{pmatrix} 0 & \sqrt{vv'} p e^{-i\theta} \\ \sqrt{vv'} p e^{i\theta} & 0 \end{pmatrix}$$
$$\times \sum_{a=1}^{4} \psi_{a}^{\dagger}(\vec{p}) T_{ab} \psi_{b}(\vec{p}), \qquad (3.9)$$

where T_{ab} is the 4×4 diagonal matrix in flavor indices diag(1,-1,-1,1). The signs in the matrix T_{ab} account for the *parity* of each node. Here we have only kept explicitly the flavor (node) indices.

We now diagonalize the kinetic energy and expand the fields in energy eigenmodes,

$$\psi(\vec{p}) = \psi_{+}(\vec{p})u_{+}(\theta) + \psi_{-}(\vec{p})u_{-}(\theta), \qquad (3.10)$$

where

$$u_{\pm}(\theta) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ \pm e^{i\theta} \end{pmatrix}$$
(3.11)

are the spinors that diagonalize the *d*-wave BCS Hamiltonian near the nodes. The effective rotational invariance around each node (in terms of the redefined momenta) enables us to expand in angular momentum eigenmodes around each node,

$$\psi_{\pm}(\vec{p}) = \sum_{m=-\infty}^{\infty} e^{im\theta} \psi_{\pm m}(|p|).$$
 (3.12)

This is effectively an angular momentum expansion in elliptic coordinates around each node.

 H_0 is now diagonal and takes the simpler form

$$H_{0} = \sum_{a=1}^{4} \int_{0}^{\infty} \frac{p \, dp}{2 \, \pi} \, \sqrt{v v' p}$$

$$\times \sum_{m=-\infty}^{\infty} T_{ab} [\psi_{a,+,m}^{\dagger}(|p|)\psi_{b,+,m}(|p|)$$

$$-\psi_{a,-,m}^{\dagger}(|p|)\psi_{b,-,m}(|p|)]. \tag{3.13}$$

B. Impurity interaction

Now we consider the interaction term for spin impurities given by

$$H_{\rm imp} \equiv \vec{S} \cdot \int d^2 x J(\vec{x}) c^{\dagger}_{\sigma}(\vec{x}) \vec{\tau}_{\sigma\sigma'} c_{\sigma'}(\vec{x}). \qquad (3.14)$$

In practice we will be interested in well localized impurities. This means that $J(\vec{x})$ is sharply peaked at some point \vec{x}_0 where the impurity is located. Realistic magnetic impurities in YBaCuO and other high-temperature superconductors¹ almost always involve magnetic atoms which either substitute a Cu atom or hybridize strongly with it. This is the case for Ni which, due to its hybridization with oxygen, it is believed to behave like a S = 1/2 impurity spin.¹ Similarly, Zn substitutes Cu, which now behaves like a missing S = 1/2 magnetic moment and in this sense is a magnetic impurity. In all cases of Cu substitution we will model the impurity as a localized S = 1/2 moment residing at a site of the square lattice which we will consider as the origin. Notice, however, that O can also behave like a magnetic impurity in the cuprates. An O magnetic impurity sits in the middle of the bond instead of a corner Cu site. This case leads to more complicated form of the effective interaction which we will not discuss in this thesis.

The effects of magnetic impurities on Cu sites can be modeled qualitatively in terms of an exchange coupling constant $J(\vec{x})$ which couples most strongly to the quasiparticles at $\vec{x}=0$ and decays rapidly and symmetrically around $\vec{x}=0$. For simplicity we will use a model in which $J(\vec{x})$ is a narrow Gaussian. We can see clearly from the discussion that led to the effective free Hamiltonian that the only properties of $J(\vec{x})$ that are important are the amplitudes of its Fourier transform at the relative wave vector of the nodes. These amplitudes play the role of the effective coupling constants. Physically, the strength of the exchange coupling is determined by an overlap integral which decays very quickly. Thus, impurities which substitute Cu atoms *in the plane* are more strongly coupled than those that substitute Cu *out of* We now proceed to find the contribution of the impurity interaction to the effective Hamiltonian. In momentum space Eq. (3.14) becomes

$$H_{\rm imp} \equiv \int \frac{d^2k}{(2\pi)^2} \int \frac{d^2k'}{(2\pi)^2} J(\vec{k} - \vec{k'}) \vec{S} \cdot c^{\dagger}_{\sigma}(\vec{k}) \vec{\tau}_{\sigma\sigma'} c_{\sigma'}(\vec{k'}).$$
(3.15)

In terms of the NG spinors it reads

$$H_{\rm imp} = \int_{\vec{k}, \vec{k}' i, j=1}^{2} \{ J(\vec{k} - \vec{k}') [S_3 \Phi_i^{\dagger}(\vec{k}) \Phi_i(\vec{k}') + S_- \epsilon_{ij} \Phi_i^{\dagger}(\vec{k}) \Phi_j^{\dagger}(-\vec{k}') + \text{H.c.}] \}, \quad (3.16)$$

where S_j represents the impurity spin, $S_{-} \equiv \frac{1}{2}(S_x - iS_y)$ and ϵ_{ij} is a 2×2 skew symmetric tensor.

As before, we expand the NG spinors in their components centered around the nodes. Since we have four nodes, the impurity Hamiltonian has terms which describe spin-flip scattering processes involving, in addition, eventual internode scattering processes. The strength of these scattering processes is determined by $J(\vec{Q})$ where \vec{Q} is the relative wave vector of a pair of nodes. There are four cases of interest.

(1) $Q \sim 0$, corresponding to scattering processes that do not mix nodes ("forward scattering"). The corresponding coupling constant is $J(0) \equiv J_0$.

(2) $Q \sim 2k_0 \hat{e}_1$, which mixes nodes 1 with 3 and 2 with 4. This coupling constant is J_1 .

(3) $\hat{Q} \sim 2k_0 \hat{e}_2$, which mixes nodes 1 with 4 and 2 with 3. This coupling constant is J_2 . For systems with exact tetragonal (square) symmetry $J_1 = J_2$.

(4) $Q \sim 2k_0(\hat{e}_1 \pm \hat{e}_2)$, which mixes nodes 1 with 2 and 3 with 4. These coupling constants are J_d^{\pm} . For tetragonal systems they reduce to just one (diagonal) coupling J_d .

For example, consider an impurity seated at the Cu site at x=0. As a crude approximation we may assume $J(\vec{x}) \approx \vec{J}\delta(\vec{x})$. The Fourier transform tells us that all the couplings will be the same, and equal to \vec{J} . A more realistic shape for $J(\vec{x})$ would be a Gaussian centered at the impurity site $\vec{x}=0$ and decaying rapidly within a distance of the order of a lattice constant λ . Thus we take that $J(x) \approx \vec{J}/(2\pi\lambda^2)e^{-(1/2\lambda^2)\vec{x}^2}$ will generate, for a generic k vector [which in our case will be $2k_0\hat{e}_1$, $2k_0\hat{e}_2$, $2k_0(\hat{e}_1+\hat{e}_2)$, and $2k_0(\hat{e}_1-\hat{e}_2)$],

$$J(\vec{k}) = \overline{J}e^{-\lambda^2 k^2/2}.$$
 (3.17)

For the impurity at the origin in a tetragonal (square) lattice, all the coupling constants are real, with $J_0 > J_1 = J_2 > J_d$. In the language of the fields introduced in Eq. (3.7) the impurity Hamiltonian now becomes

$$H_{\rm imp} = S_{3} \sum_{a,b=1}^{4} \mathbf{K}_{ab}^{3} \sum_{i=1}^{2} \int \frac{d^{2}p}{(2\pi)^{2}} \psi_{a,i}^{\dagger}(\vec{p}) \int \frac{d^{2}p'}{(2\pi)^{2}} \psi_{b,i}(\vec{p}') \\ + S_{-} \sum_{a,b=1}^{4} \mathbf{K}_{ab}^{+} \sum_{i=1}^{2} \int \frac{d^{2}p}{(2\pi)^{2}} \psi_{a,i}^{\dagger}(\vec{p}) \\ \times (i\tau_{2})_{i,j} \int \frac{d^{2}p'}{(2\pi)^{2}} \psi_{b,j}^{\dagger}(-p') + \text{H.c.}$$
(3.18)

In Eq. (3.18) the indices a, b are the flavor indices which label the effective Dirac fermions species associated with each node. The indices i, j run through the spinor components (two per each NG spinor, i.e., per node) and label linear combinations of quasiparticles with spin up with holes with spin down. Also notice that p and p' now label small departures from the appropriate node. Using the fact that $i\tau_2$ is an antisymmetric matrix, we can rewrite Eq. (3.18) in the form

$$H_{\rm imp} = S_{3} \sum_{a,b=1}^{4} \mathbf{K}_{ab}^{3} \sum_{i=1}^{2} \int_{0}^{\infty} p \frac{dp}{2\pi} \int_{0}^{2\pi} \frac{d\theta}{2\pi} \psi_{a,i}^{\dagger}(\vec{p}) \\ \times \int_{0}^{\infty} p' \frac{dp'}{2\pi} \int_{0}^{2\pi} \frac{d\theta'}{2\pi} \psi_{b,i}(\vec{p'}) \\ + S_{-a,b=1} \sum_{a,b=1}^{4} \mathbf{K}_{ab}^{+} \sum_{i=1}^{2} \int_{0}^{\infty} p \frac{dp}{2\pi} \int_{0}^{2\pi} \frac{d\theta}{2\pi} \psi_{a,1}^{\dagger}(\vec{p}) \\ \times \int_{0}^{\infty} p' \frac{dp'}{2\pi} \int_{0}^{2\pi} \frac{d\theta'}{2\pi} \psi_{b,2}^{\dagger}(-p') + \text{H.c.} \quad (3.19)$$

The 4×4 matrices \mathbf{K}_{ab}^3 and \mathbf{K}_{ab}^+ used in Eqs. (3.18) and (3.19) are given by

$$\mathbf{K}_{ab}^{3} = \begin{pmatrix} J_{0} & J_{d} & J_{1} & J_{2} \\ J_{d} & J_{0} & J_{2} & J_{1} \\ J_{1} & J_{2} & J_{0} & J_{d} \\ J_{2} & J_{1} & J_{d} & J_{0} \end{pmatrix}, \quad \mathbf{K}_{ab}^{+} = \begin{pmatrix} J_{d} & J_{0} & J_{2} & J_{1} \\ J_{0} & J_{d} & J_{1} & J_{2} \\ J_{2} & J_{1} & J_{d} & J_{0} \\ J_{1} & J_{2} & J_{0} & J_{d} \end{pmatrix}.$$
(3.20)

The form of Eq. (3.19) strongly suggests the following change of variables (particle-hole transformations) performed on the second component of all four flavors:

$$\begin{split} \psi_{1,2}(p) &\to \psi_{1,2}^{\dagger}(-p), \quad \psi_{2,2}(p) \to \psi_{2,2}^{\dagger}(-p), \\ \psi_{3,2}(p) &\to \psi_{3,2}^{\dagger}(-p), \quad \psi_{4,2}(p) \to \psi_{4,2}^{\dagger}(-p) \quad (3.21) \end{split}$$

to express the interaction term as a scalar product of two spin- $\frac{1}{2}$ operators.

We can now separate the modes and find an effective one-dimensional model. After integration over the angle variable θ , the fields involved in Eq. (3.19) become

$$\int_{0}^{2\pi} \frac{d\theta}{2\pi} \psi_{1a} = \frac{1}{\sqrt{2}} [\psi_{0+}(|p|) + \psi_{0-}(|p|)]_{a},$$
$$\int_{0}^{2\pi} \frac{d\theta}{2\pi} \psi_{2a} = \frac{1}{\sqrt{2}} [\psi_{-1+}(|p|) - \psi_{-1-}(|p|)]_{a}. \quad (3.22)$$

Now we define, for each flavor *a*, an effective onedimensional *chiral* (right-moving) Fermi field

$$d_{1a}(p) = \begin{cases} \sqrt{|p|} \psi_{0,+,a}(|p|) & \text{for } p > 0, \\ \sqrt{|p|} \psi_{0,-,a}(|p|) & \text{for } p < 0, \end{cases}$$
(3.23)

$$d_{2a}(p) \equiv \begin{cases} \sqrt{|p|} \psi_{-1,+,a}(|p|) & \text{for } p > 0, \\ -\sqrt{|p|} \psi_{-1,-,a}(|p|) & \text{for } p < 0, \end{cases}$$
(3.24)

and Eq. (3.19) can be recast as

$$H_{\rm imp} = S_3 \frac{1}{2} \sum_{ab,i} \mathbf{K}_{ab}^3 \int_{-\infty}^{\infty} \frac{dp}{2\pi} \sqrt{|p|} d_{ai}^{\dagger}(p)$$

$$\times \int_{-\infty}^{\infty} \frac{dp'}{2\pi} \sqrt{|p'|} d_{bi}(p')$$

$$+ S_{-} \sum_{ab} \mathbf{K}_{ab}^{+} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \sqrt{|p|} d_{a1}^{\dagger}(p)$$

$$\times \int_{-\infty}^{\infty} \frac{dp'}{2\pi} \sqrt{|p'|} d_{b2}^{\dagger}(p') + \text{H.c.} \qquad (3.25)$$

Here we perform the change of variables suggested above by setting

$$d_{a2}(p) \rightarrow d_{a2}^{\dagger}(-p)$$
 for $a = 1, \dots, 4,$ (3.26)

and thus, in the definition given by Eq. (3.24) we rename $d_{1a}(p)$ as the $d_{\uparrow a}(p)$ component of an effective spin- $\frac{1}{2}$ onedimensional chiral fermion, and $d_{2a}^{\dagger}(-p)$ as the $d_{\downarrow a}(p)$ component. Please notice that this label is *not* equivalent to the spin of the original quasiparticles. In fact, the relation between these effective one-dimensional chiral fermions and the original quasiparticles is actually quite complicated. The (flavor) coupling matrices commute with each other [as required by the SU(2) spin rotation invariance] and can be diagonalized simultaneously by means of the unitary transformation

$$d'_{ai} = \mathbf{U}_{ab} d_{bi}, \qquad (3.27)$$

where $i = \uparrow$ or \downarrow , the flavor indices *a* and *b* run from 1 to 4, and

This rotation brings the coupling matrices \mathbf{K}_{ab}^3 and \mathbf{K}_{ab}^+ to the diagonal form

$$\mathbf{K}_{ab}^{3} = \begin{pmatrix} J_{1}^{\prime} & 0 & 0 & 0 \\ 0 & J_{2}^{\prime} & 0 & 0 \\ 0 & 0 & J_{3}^{\prime} & 0 \\ 0 & 0 & 0 & J_{4}^{\prime} \end{pmatrix}$$

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$$\mathbf{K}_{ab}^{+} = \begin{pmatrix} J_{1}^{\prime} & 0 & 0 & 0\\ 0 & -J_{2}^{\prime} & 0 & 0\\ 0 & 0 & J_{3}^{\prime} & 0\\ 0 & 0 & 0 & -J_{4}^{\prime} \end{pmatrix}, \qquad (3.29)$$

with

$$J'_{1} = J_{0} + J_{d} + J_{1} + J_{2},$$

$$J'_{2} = J_{0} - J_{d} + J_{1} - J_{2},$$

$$J'_{3} = J_{0} + J_{d} - J_{1} - J_{2},$$

$$J'_{4} = J_{0} - J_{d} - J_{1} + J_{2}.$$
(3.30)

As one can see in Eq. (3.29) flavors 2 and 4 appear to have S_x and S_y with the sign reversed. However, this can be compensated by the following additional rotation in the spin components:

$$d_{2\uparrow}(p) \rightarrow i d_{2\uparrow}(p), \quad d_{2\downarrow}(p) \rightarrow -i d_{2\downarrow}(p),$$

$$d_{4\uparrow}(p) \rightarrow i d_{4\uparrow}(p), \quad d_{4\downarrow}(p) \rightarrow -i d_{4\downarrow}(p). \quad (3.31)$$

After all of these manipulations we find that the effective one-dimensional theory for this model is

$$H_{\rm eff} = \sum_{a=1}^{4} \sum_{\sigma=\uparrow,\downarrow} \int_{-\infty}^{\infty} \frac{dp}{2\pi} E(p) d^{\dagger}_{a\sigma}(p) d_{a\sigma}(p) + \sum_{a=1}^{4} \sum_{\sigma,\nu=\uparrow,\downarrow} (J_a/2) \left[\int_{-\infty}^{\infty} \frac{dp}{2\pi} \sqrt{|p|} d^{\dagger}_{a\sigma}(p) \right] \times \vec{\tau}_{\sigma\nu} \cdot \vec{S}_{\rm imp} \left[\int_{-\infty}^{\infty} \frac{dp'}{2\pi} \sqrt{|p'|} d_{a\nu}(p') \right].$$
(3.32)

In Eq. (3.32) we dropped the primes in Eq. (3.27) and in the effective coupling constants. The kinetic energy of the chiral fermions is $E(p) = \sqrt{vv'}p$.

Equation (3.32) can be recognized to be *exactly* the nonmarginal Kondo Hamiltonian that was discussed in Ref. 29. Hence, the effective Hamiltonian for a *d*-wave superconductor coupled to a magnetic impurity is essentially equivalent to a (multichannel) generalization of a nonmarginal Kondo problem. There are four channels, one for each node. The channel degeneracy is generally lifted by the internode scattering. In fact, Eq. (3.30) shows that in the absence of internode scattering (i.e., $J_1 = J_2 = J_d = 0$) the four flavors couple to the impurity with exactly the same exchange interaction strength $J'_a = J_0$ (a = 1,...,4). For a strictly tetragonal system the couplings are ordered in the sequence $J'_1 > J'_2 = J'_4 > J'_3$. Intuitively one expects the channel with the largest coupling to dominate the low-energy limit. In the extreme limit in which all internode and intranode amplitudes are exactly equal one finds that channels 2, 3, and 4 decouple and that only the remaining channel 1 couples to the impurity. Thus, in this limit, the physics of the system is that of a single-channel nonmarginal Kondo problem.

Given that these two seemingly different systems are actually equivalent, most of the results found in Ref. 29 carry over to this problem almost without change but with a new physical meaning and processes, in particular including pairbreaking effects. In Ref. 29 we found that there is a critical value of the exchange coupling constant J_c , above which the impurity spin is screened. We also found there that the critical value J_c was of the same order as the energy cutoff, which here is the superconducting gap Δ_0 . The reason behind the existence of a finite J_c is that the effective interaction between the impurity and the normal excitations is momentum dependent and that it vanishes at small momenta [see Eq. (3.32)]. However, the same momentum dependence makes the effective coupling grow arbitrarily large at large momenta. This last behavior is unphysical and it results from the approximations, which are accurate at small momenta only. This observation motivates a simple redefinition of the model with a finite, momentum-independent, coupling at momenta larger than a scale of the order of $\Delta_0/(2\pi\sqrt{vv'})$.

In Ref. 29 we showed that a momentum-dependent coupling is equivalent to a change in the density of states (DOS) for a theory with a momentum-independent coupling constant. The model of Ref. 29 and the model discussed above have a DOS vanishing linearly with the energy. We consider a modified model with the DOS

$$\rho(\boldsymbol{\epsilon}) = \begin{cases}
\frac{|\boldsymbol{\epsilon}|}{2\pi v v'} & \text{for } |\boldsymbol{\epsilon}| \leq \Delta_0, \\
\frac{\Delta_0}{2\pi v v'} & \text{for } \Delta_0 < |\boldsymbol{\epsilon}| < D,
\end{cases}$$
(3.33)

where Δ_0 is the size of the superconductor gap away from the nodes. This change in the DOS is equivalent to a saturation of the coupling constant at the momentum scale $\Delta_0/(2\pi\sqrt{vv'})$.

In other words, we are assuming a linear dependence of the DOS with the energy around the gap nodes, up to the energy scale of the superconductor gap. For energies higher than the superconducting gap Δ_0 , the normal quasiparticles are, for all practical purposes, identical to normal electrons. In a realistic cuprate superconductor, the band structure is actually rather complicated. Nevetheless, we can take into account the contribution of these states to the physics by considering a flat fermion band characteristic of a continuum spectrum from Δ_0 up to a bandwidth *D*, which works as a high-energy cutoff. As we will see below, the contribution of these states can almost always be ignored but they will enter in our results in two important places: (a) by shifting (downwards) the critical value of the coupling constant J_c and (b) in the scaling behavior for "half-filled" impurities. The shift in J_c is quantitatively important and it results in a downwards shift of J_c from the nominal value of the superconducting gap Δ_0 . Hence, we will assume that $J_c \leq \Delta_0$. This happens if the scales of Δ_0 and D are reasonably well separated.

IV. LARGE-N_c THEORY

In the previous section we constructed a model for a magnetic impurity embedded in a *d*-wave superconductor and showed that it is equivalent to a special nonmarginal Kondo problem. In this section we solve this model in the large- N_c approximation, where N_c is the rank of the symmetry group of the impurity spin. In the physically relevant situation N_c =2 (i.e., spin one-half). Clearly, in this situation N_c is not large. Nevertheless, we expect the large- N_c theory to give a qualitatively correct description. We now proceed with a brief summary of the large- N_c theory¹⁴ as adapted²⁹ to the physical situation described by the Hamiltonians of the previous section.

In order explore the physics of this system we extend the symmetry from SU(2) (spin) to SU(N_c) and look at it within the large- N_c approximation. Notice that, unlike the Coqblin-Schrieffer model, N_c is not related to a magnetic impurity in a higher-spin representation. Similarly, the four flavors of fermions originate from the nodal structure of the superconductor and are not related to an orbital degeneracy as in the multichannel Kondo problem in metals. Thus the problem we want to study has $N_c = 2$ "colors." The number of "flavors" is $N_f=1$ if there is node mixing and $N_f=4$ in the absence of internode scattering. However, there is a subtlety in the treatment of the impurity once symmetry is extended from SU(2) to SU(N_c). For the group SU(2), the lowest representation for an impurity is S = 1/2. For SU(N_c) many more representations are allowed. For example, the fundamental representation, which has dimension N_c , is constructed by occupying an N_c -fold degenerate multiplet with a single "slave" fermion.¹⁴ For general N_c , with the exception of $N_c = 2$, this representation is not self-conjugate or, in other terms, it is not particle-hole symmetric. Other representations can be constructed²⁶ by occupying the multiplet with Q_f slave fermions. For $Q_f = N_c/2$, which is available for N_c even, particle-hole symmetry is exact. We will see below that particle-hole symmetry (self-conjugation) is a case of special interest. Notice that all choices of representation are, in principle, valid extensions from the physical SU(2)invariant system. Similar caveats have to be made about the choice of a particular generator in the algebra of $SU(N_c)$ that will represent the Zeeman term for $N_c > 2$. In fact, in Ref. 26 it was shown that some care has to be taken in this choice in order to describe a smooth weak-to-strong field crossover. In any event, we are only interested in the extrapolation of the results at $N_c > 2$ down to $N_c = 2$ where there is no ambiguities but they are present for all $N_c > 2$.

In Ref. 29 it was shown that, after integrating out the fermion and impurity degrees of freedom, the impurity contribution to the effective action, $S_{\text{eff}} \equiv \beta F_{\text{imp}}$, takes the form

$$F_{\rm imp} = -\frac{1}{\beta} \sum_{\sigma=1}^{N_c} \operatorname{Tr} \ln \left[\partial_{\tau} + \epsilon_f + \sum_{l=1}^{N_f} |\phi_l|^2 G_0(z) \right] \\ + \int d\tau \left[\frac{N_c}{J_0} \left(\sum_{l=1}^{N_f} |\phi|^2 \right) - Q_f \epsilon_f \right] \\ \equiv \overline{F}_{\rm imp} + \int d\tau \left[\frac{N_c}{J_0} \left(\sum_{l=1}^{N_f} |\phi|^2 \right) - Q_f \epsilon_f \right], \quad (4.1)$$

where ϕ_l are the Hubbard-Stratonovich fields introduced to decouple the impurity in the large-*N* formalism. The properties of the normal excitations is encoded in the function $G_0(z)$ (where the complex number $z = \epsilon + i\lambda$ is the analytic extension of the energy). With the new definition of the DOS of Eq. (3.33), the function $G_0(z)$, defined by

$$G_0(z) \equiv -\int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi v v'} \frac{\rho(\epsilon)}{\epsilon - z},$$
(4.2)

now takes the form

$$\operatorname{Re} G_{0}(\epsilon + i\lambda) \equiv \begin{cases} -\frac{\epsilon}{\pi v v'} \ln \left| \frac{\Delta_{0}}{\epsilon} \right| & \text{for} \quad |\epsilon| < \Delta_{0}, \\ 0 & \text{for} \quad |\epsilon| > \Delta_{0}, \end{cases}$$

$$(4.3)$$

$$\operatorname{Im} G_{0}(\epsilon + i\lambda) = \begin{cases} -\frac{|\epsilon|}{2vv'} \operatorname{sgn}(\lambda) & \text{for} \quad |\epsilon| < \Delta_{0}, \\ -\frac{\Delta_{0}}{2vv'} \operatorname{sgn}(\lambda) & \text{for} \quad |\epsilon| > \Delta_{0}. \end{cases}$$

$$(4.4)$$

We define

$$\Delta \equiv \frac{\sum_{l=1}^{N_f} |\phi_l|^2}{\pi v v'},\tag{4.5}$$

where N_f is the number of "flavors." For the problem of the *d*-wave superconductor, N_f in principle is the number of nodes and N_f =4. However, we showed above that the *internode* couplings are always different (and smaller) than the *intranode* coupling. This coupling anisotropy reduces to *one* the number of effective flavors. Hence, from now on, we will set N_f =1.

At finite temperature T, the effective action of Eq. (4.1) becomes an (infinite) series running over (imaginary) Matsubara frequencies. Using this approach³⁷ the effective free energy becomes

$$\overline{F}_{\rm imp} = \frac{N_c}{2\pi i} \int_{-\infty}^{\infty} d\epsilon \, \frac{e^{\,\eta\epsilon}}{e^{\beta\epsilon} + 1} \ln \left[\frac{-(\epsilon + i\lambda) + \epsilon_f + (\Sigma_c |\phi|^2) G_0(\epsilon + i\lambda)}{-(\epsilon - i\lambda) + \epsilon_f + (\Sigma_c |\phi|^2) G_0(\epsilon - i\lambda)} \right] = \frac{N_c}{\pi} \int_{-\infty}^{\infty} d\epsilon n(\epsilon) \,\delta(\epsilon), \tag{4.6}$$

where $\delta(\epsilon)$ is the *phase shift*³⁹ and $n(\epsilon)$ is the Fermi function,

$$n(\epsilon) = \frac{1}{e^{\beta\epsilon} + 1}.$$
(4.7)

Explicitly we find

$$\delta(\boldsymbol{\epsilon}) \equiv \tan^{-1} \left(\frac{\lambda + \pi |\boldsymbol{\epsilon}| \Delta/2}{\boldsymbol{\epsilon} + \boldsymbol{\epsilon} \Delta \ln |\Delta_0/\boldsymbol{\epsilon}| - \boldsymbol{\epsilon}_f} \right) \quad (\lambda \to 0^+).$$
(4.8)

 $G_0(z)$ has a branch cut and the jump of the function across this cut is energy dependent. This is an important difference with the usual Kondo effect in which the jump across the cut for the function $G_0(z)$ (see, for example, Ref. 14) is energy independent and gives essentially the (constant) width of the resonance. This will not be the case any longer as the width of the resonance now becomes energy dependent. This marks an important departure from the "local Fermi-liquid" (or the resonant level model) behavior^{10,38} characteristic of the usual marginal Kondo systems.

The large- N_c analysis of this problem proceeds in the usual manner. Given the impurity free energy F_{imp} , a set of values of ϵ_f and Δ that minimize this free energy is sought. The extremal values of ϵ_f and Δ satisfy the saddle point equations (SPE's)

$$\frac{\partial F_{\rm imp}}{\partial \Delta} = 0$$
 and $\frac{\partial F_{\rm imp}}{\partial \epsilon_f} = 0.$ (4.9)

In the next subsection we will write explicit expressions for the SPE's and solve them. Thermodynamic magnitudes such as the impurity entropy S_{imp} , the impurity contribution to the specific heat C_{imp} , and the impurity contribution to the susceptibility χ_{imp} as functions of temperature (and magnetic field) can be computed from the thermodynamic formulas

$$S_{\rm imp} = -\frac{\partial F_{\rm imp}}{\partial T}, \quad \overline{C}_{\rm imp} = -T\frac{\partial^2 \overline{F}_{\rm imp}}{\partial T^2}, \quad \chi_{\rm imp} = -\frac{\partial^2 \overline{F}_{\rm imp}}{\partial H^2}, \quad (4.10)$$

where the total impurity contribution to the free energy $F_{\rm imp}$ is given by

$$F_{\rm imp} = \overline{F}_{\rm imp}(\Delta, \epsilon_f, H, T) + \pi \frac{v_F^2 N_c}{J_0} \Delta - Q_f \epsilon_f. \quad (4.11)$$

Since both Δ and ϵ_f are also functions of *T* and *H*, care must be taken to account for their contribution. However, since Δ and ϵ_f satisfy the SPE's, we get

$$\frac{\partial F_{\rm imp}}{\partial T} = \frac{\partial \overline{F}_{\rm imp}}{\partial T} \bigg|_{\Delta, \epsilon_f} \quad \text{and} \quad \frac{\partial F_{\rm imp}}{\partial H} = \frac{\partial \overline{F}_{\rm imp}}{\partial H} \bigg|_{\Delta, \epsilon_f}. \quad (4.12)$$

Thus, only the explicit dependence on T and H matters.

V. SADDLE POINT EQUATIONS

Using the formalism of the previous section, the saddle point equations (SPE's) take the form

$$Q_f = \frac{1}{\pi} \int_{-D}^{+D} d\epsilon n(\epsilon) \frac{\partial \delta}{\partial \epsilon_f}(\epsilon)$$
(5.1)

and

$$N_c \frac{\pi v_F^2}{J_0} = -\frac{1}{\pi} \int_{-D}^{+D} d\epsilon n(\epsilon) \frac{\partial \delta}{\partial \Delta}(\epsilon), \qquad (5.2)$$

where *D* is the bandwidth cutoff. In general we will be interested in the regime $T, H \ll \Delta_0 < D$. In this regime, the contributions to the SPE's from energies higher than Δ_0 can be well approximated by setting T=H=0. This amounts to setting the Fermi function to be $n(\epsilon)\approx 0$, for $\Delta_0 \leq \epsilon \leq D$, and

 $n(\epsilon) \approx N_c$, for $-D \leq \epsilon \leq -\Delta_0$. The SPE's thus are a sum of two terms, one coming from energies $|\epsilon| \leq \Delta_0$ and one from $D \geq |\epsilon| \geq \Delta_0$.

A. Impurity occupation

The saddle point equation (5.1) reduces to

$$Q_{f} = \int_{-\Delta_{0}}^{\Delta_{0}} \frac{d\epsilon}{\pi} n(\epsilon) \frac{(\pi/2) |\epsilon| \Delta}{[(\pi/2) |\epsilon| \Delta]^{2} + (\epsilon + \epsilon \Delta \ln|\Delta_{0}/\epsilon| - \epsilon_{f})^{2}} + \frac{N_{c}}{2} \left[1 - \frac{2}{\pi} \arctan\left(\frac{\Delta_{0} + \epsilon_{f}}{(\pi/2) \Delta_{0} \Delta}\right) \right].$$
(5.3)

For the reminder of this paper, we will be interested in the physics of this system close to the critical coupling constant. In that regime, the singlet amplitude Δ becomes very small and the asymptotic behavior of the SPE's in this domain can be evaluated explicitly.

Thus, close enough to the phase transition, where Δ is very small, the contribution from the last term in Eq. (5.3) becomes

$$\lim_{\Delta \to 0} \left[1 - \frac{2}{\pi} \arctan\left(\frac{\Delta_0 + \epsilon_f}{(\pi/2) \Delta_0 \Delta}\right) \right] \\ \sim \left(\frac{\Delta_0}{\Delta_0 + \epsilon_f}\right) \Delta - \frac{2}{3\pi} \left(\frac{(\pi/2) \Delta_0 \Delta}{\Delta_0 + \epsilon_f}\right)^3 + \cdots, \quad (5.4)$$

provided $\epsilon_f + \Delta_0 > 0$.

For the remainder of this section we will consider the saddle point equation in the case T=H=0. In this case, the SPE takes the form

$$I = \frac{N_c}{\pi} \int_{e^{1/\Delta}}^{\infty} \frac{dz}{z} \frac{\pi \Delta/2}{(\pi \Delta/2)^2 + (\Delta \ln z + \nu e^{-1/\Delta} z)^2}, \quad (5.5)$$

where $z \equiv e^{1/\Delta} \Delta_0 / \epsilon$ and $\nu \equiv \epsilon_f / \Delta_0$. It is clear that the integrand in Eq. (5.5) shows a crossover behavior at

$$\Delta \ln z_0 = \nu e^{-1/\Delta} z_0.$$

In the regime $\nu \ll \Delta \ll 1$, this equation has a root at large z, given by

$$z_0 \approx \left(\frac{\Delta}{\nu} e^{1/\Delta}\right) \ln \left(\frac{\Delta}{\nu} e^{1/\Delta}\right) > e^{1/\Delta}.$$

Taking into account the change in the behavior of its denominator, Eq. (5.5) can be re-written in two pieces with the asymptotic form

$$I^{<} \approx \frac{N_c}{2} \left[1 - \frac{1}{1 + \Delta \ln(\Delta/\nu)} + \frac{\Delta \ln(1/\Delta)}{\left[1 + \Delta \ln(\Delta/\nu)\right]^2} \right] + \cdots$$
(5.6)

and

$$I^{>} \approx \frac{N_c}{\pi^2 \Delta} \ln \left[1 + \frac{(\pi \Delta/2)^2}{\left[1 + \Delta \ln(\Delta/\nu) \right]^2} \right] + \cdots$$
 (5.7)

Getting everything together, Eq. (5.1) reduces to the expression

$$Q_{f} \approx \frac{N_{c}}{2} \frac{\Delta}{1+\nu} + \frac{N_{c}}{2} \frac{\Delta \ln(\Delta/\nu)}{1+\Delta \ln(\Delta/\nu)} + \frac{N_{c}}{2} \frac{\Delta \ln(1/\Delta)}{[1+\Delta \ln(\Delta/\nu)]^{2}} + \frac{N_{c}}{\pi^{2}\Delta} \ln \left[1 + \frac{(\pi \Delta/2)^{2}}{[1+\Delta \ln(\Delta/\nu)]^{2}} \right] + \cdots$$
(5.8)

It is important to stress that, regardless of the approximations made in evaluating the integrals, the first SPE, Eq. (5.1), is a relation between Δ (the amplitude of the singlet) and the impurity Fermi level (in units of the gap Δ_0) ν at fixed occupation Q_f . This relation is independent of the coupling constant and it must be solved first. For the problem that we are discussing here, the relation between ν and Δ is *singular*, as implied by the logarithmic singularities in Eq. (5.8). We will see below that, due to the presence of this singularity, the impurity Fermi level ϵ_f is no longer simply related to the singlet amplitude Δ . This phenomenon does not occur in the conventional Kondo problem in metals, where the DOS is constant. It occurs for systems with a DOS vanishing *faster* than linear with the energy. In this sense, the case of a linear DOS is a *marginal* system.

Let x be the impurity filling fraction $x = Q_f / N_c$. The solution of Eq. (5.8) takes the form

$$\nu(x,\Delta) = \sqrt{e} \exp\left(-\frac{1}{\Delta} \frac{2x}{1-2x+\Delta} + \frac{1}{1-2x+\Delta}\right)$$
$$\times [1+O(\Delta,\Delta \ln \Delta)], \tag{5.9}$$

where e = 2.7172....

Hence, for generic values of $x = Q_f/N_c$, the impurity Fermi level ν depends on the singlet amplitude Δ through an essential singularity of the form $\exp(-\operatorname{const}/\Delta)$. As $Q_f \rightarrow N_c/2(x \rightarrow \frac{1}{2})$, there is a crossover in the functional form of ν which now behaves like $\exp(-\operatorname{const}/\Delta^2)$, which vanishes much faster as Δ approaches zero. It is interesting to note that if the contributions from the states with energies between -D to $-\Delta_0$ had been neglected altogether, ν would have vanished identically at $Q_f = N_c/2$, for all finite values of Δ . Since at $Q_f = N_c/2$ the Hamiltonian has an exact particlehole symmetry, it may appear that $\nu = \epsilon_f/\Delta_0$ should have to vanish exactly at this point. In fact, it does not vanish due to states whose DOS violate the strict linear behavior of the DOS at low energies.

B. Equation of state

Let us consider now the second SPE, Eq. (5.2). This equation relates Δ (the amplitude of the singlet) to the coupling constant (once the relation between ϵ_f and Δ is known). We will regard this equation as an *equation of state*.

At T=0 and H=0 the second SPE, Eq. (5.2), can be written as

$$\frac{\pi^2 v_F^2}{J_0} = \int_0^{\Delta_0} d\epsilon \frac{\pi}{2} \frac{\epsilon(\epsilon + \epsilon_f)}{(\pi \epsilon \Delta/2)^2 + [\epsilon + \epsilon_f + \epsilon \Delta \ln(\Delta_0/\epsilon)]^2} + \int_{\Delta_0}^D d\epsilon \frac{\pi}{2} \Delta_0 \frac{\epsilon(\epsilon + \epsilon_f)}{(\pi \Delta_0 \Delta/2)^2 + (\epsilon + \epsilon_f)^2}.$$
 (5.10)

In the second integral of the right-hand side (RHS) of Eq. (5.10) it is useful to perform the change of variables $u = \epsilon_f / \epsilon$

$$\frac{1}{g_0} = \frac{\pi}{2} e^{1/\Delta} \int_{e^{1/\Delta}}^{\infty} \frac{dz}{z^2} \frac{(1 + \nu z e^{-1/\Delta})}{(\Delta \pi/2)^2 + (\nu z e^{-1/\Delta} + \Delta \ln z)^2} + \frac{\pi}{2} \int_{\nu_D}^{\nu} \frac{du}{u} \frac{1 + u}{(\Delta \pi/2)^2 + (1 + u)^2}, \quad (5.11)$$

where we have defined the dimensionless coupling constant g_0 by

$$\frac{1}{g_0} = \frac{1}{\Delta_0} \frac{\pi^2 v_F^2}{J_0}.$$

The second integral on the RHS of Eq. (5.11) can be shown to give the leading contributions

$$\frac{\pi}{2} \int_{\nu_D}^{\nu} \frac{du}{u} \frac{1+u}{(\Delta \pi/2)^2 + (1+u)^2} \sim \frac{\pi}{2} \ln \frac{D}{\Delta_0} \frac{1}{1+a^2} - \frac{\pi}{2} \nu \left(1 - \frac{\Delta_0}{D}\right) \times (1 - 7a^2) + \cdots, \qquad (5.12)$$

where $a^2 \equiv (\pi \Delta/2)^2 \ll 1$ in accordance with the hypothesis that Δ is small in the regimes in which we are interested. The first integral of the RHS of Eq. (5.11) is treated in the Appendix as an example of the approximations used. Retrieving here the results of Eq. (A8) we write Eq. (5.11) in the form

$$\frac{1}{g_0} = \frac{\pi}{2} \ln \left(\frac{D}{\Delta_0} \right) + \frac{\pi}{2} \frac{1}{1 + (\pi \Delta/2)^2} - \pi \frac{\Delta}{\left[1 + (\pi \Delta/2)^2 \right]^2} + O(\Delta^2) + \cdots$$
(5.13)

Now we define the *critical coupling constant* as the limit for $\Delta \rightarrow 0$ of Eq. (5.13),

$$\frac{1}{g_c} = \frac{\pi}{2} \ln\left(\frac{D}{\Delta_0}\right) + \frac{\pi}{2}.$$
 (5.14)

For small Δ we obtain the scaling equation

$$\frac{1}{g_c} - \frac{1}{g_0} = \pi \Delta + \frac{\pi}{4} \left(\frac{\pi \Delta}{2}\right)^2 \left[3 - \left(\frac{\Delta_0}{D}\right)^2\right] + \cdots \quad (5.15)$$

VI. IMPURITY MAGNETIC SUSCEPTIBILITY

In order to consider the effect of a magnetic field in our model it is necessary to proceed with some care. In principle we need to go back to the original model to look into the effects of a finite H. In terms of the Nambu-Gorkov spinors the "free Hamiltonian" H_0 now becomes

$$H_{0} = \sum_{\vec{k}} \Phi^{\dagger}(\vec{k}) \{ [\epsilon(\vec{k}) + \mu] \tau_{3} - \Delta(\vec{k}) \tau_{1} - H \} \Phi(\vec{k}).$$
(6.1)

Here the magnetic field H is multiplied by the 2×2 identity matrix. The consequence of the introduction of a finite magnetic field is thus, the generation of a finite relative shift in

the zero point for the energy, but not necessarily a finite density of quasiparticle states within the nodes of the gap (however, see below). The eigenfunctions remain unchanged but the eigenenergies are shifted by H,

$$E = -H \pm \sqrt{\epsilon^2(\vec{k}) + \Delta^2(\vec{k})}.$$
 (6.2)

Thus, after the expansion in small momentum around the *nodes* of the gap, the two-dimensional spinors will disperse with

$$E = -H \pm \sqrt{vv'}p, \qquad (6.3)$$

where p has been defined before, in the model without field.

It is not difficult to convince oneself, by going through the (several) transformations involved in the reduction to the effective one-dimensional model, that, at the level of the one-dimensional Hamiltonian, the magnetic field enters as a *true* magnetic field coupled now to the one-dimensional chiral fermions. Thus,

$$H_{\rm eff} = \sum_{\ell=1}^{4} \sum_{\sigma=\uparrow,\downarrow} \int_{-\infty}^{\infty} \frac{dp}{2\pi} (\sqrt{vv'}p - H\tau_3) d_{\ell\sigma}^{\dagger}(p) d_{\ell\sigma}(p) + \sum_{\ell=1}^{4} \sum_{\sigma,\nu=\uparrow,\downarrow} J_{\ell} \left[\int_{-\infty}^{\infty} \frac{dp}{2\pi} \sqrt{|p|} d_{\ell\sigma}^{\dagger}(p) \right] \times \vec{\tau}_{\sigma\nu} \cdot \vec{S}_{\rm imp} \left[\int_{-\infty}^{\infty} \frac{dp'}{2\pi} \sqrt{|p'|} d_{\ell\nu}(p') \right].$$
(6.4)

The change in the kinetic energy, depending on the spin polarization, changes the form of the function $G_0(\omega, H)$,

$$G_{0}(\omega,H) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{|p|}{\omega - \sqrt{vv'}p + H\tau^{3}}$$

$$= \frac{1}{2\pi vv'} \int_{-\infty}^{\infty} \frac{|\epsilon|d\epsilon}{(\omega+H) - \epsilon} \frac{1}{2}(1+\tau_{3})$$

$$+ \frac{1}{2\pi vv'} \int_{-\infty}^{\infty} \frac{|\epsilon|d\epsilon}{(\omega-H) - \epsilon} \frac{1}{2}(1-\tau_{3}),$$

(6.5)

where τ_3 represents an SU(N_c) diagonal generator having r elements with eigenvalue +1 and $N_c - r$ elements with eigenvalue -1. In what follows we will take $r = N_c/2$ which respects the $H \rightarrow -H$ symmetry of the SU(2) theory. For general r, a particle-hole transformation is not equivalent to $H \rightarrow -H$. But for $r = N_c/2$ these symmetry transformations are equivalent. In other terms, for general r this magnetic field breaks both the $H \rightarrow -H$ and particle-hole symmetries. Notice, however, that the representation of the impurity is determined solely by the charge Q_f and it is unrelated to r. In the presence of the field, the impurity level has an effective filling factor $2Q_f/N_c$. We will see below that $Q_f = N_c/2$ is a special case. For the physical case $N_c = 2$ there is only one possible representation (i.e., spin S = 1/2) which corresponds to $Q_f = 1 = N_c/2$. For general N_c these two situations do not necessarily coincide.

11 258

<u>56</u>

These changes will be reflected in the phase shift defined in Sec. IV. In presence of a finite field the impurity free energy \overline{F}_{imp} can be written as

$$\overline{F}_{\rm imp} \equiv \frac{N_c}{2\pi} \int_{-\infty}^{\infty} d\epsilon n(\epsilon) [\delta(\epsilon + H) + \delta(\epsilon - H)], \quad (6.6)$$

where $\delta(\epsilon)$ is given by Eq. (4.8) and $n(\epsilon)$ is the Fermi function. Equation (6.6) is manifestly invariant under the transformation $H \rightarrow -H$.

The magnetization and the susceptibility are given, respectively, by

$$M_{\rm imp} = -\frac{\partial \overline{F}_{\rm imp}}{\partial H}, \quad \chi_{\rm imp} = -\frac{\partial^2 \overline{F}_{\rm imp}}{\partial H^2}, \quad (6.7)$$

which take the form

$$M_{\rm imp} = \frac{N_c}{2\pi} \int_{-\infty}^{+\infty} d\epsilon \left(\frac{\partial n}{\partial \epsilon} (\epsilon - H) - \frac{\partial n}{\partial \epsilon} (\epsilon + H) \right) \delta(\epsilon).$$
(6.8)

In the limit $T \rightarrow 0$, the function $\partial n(\epsilon) / \partial \epsilon$ approaches a negative Dirac δ function localized at $\epsilon = 0$. In this limit we find

$$M_{\rm imp}(0,H) = -\frac{N_c}{2\pi} [\delta(H) - \delta(-H)].$$
(6.9)

Now we can use Eq. (4.8) to write an explicit expression for the magnetization

$$M(0,H) = -\frac{N_c}{2\pi} \tan^{-1} \left(\frac{(\pi/2) H\Delta}{H + H\Delta \ln(\Delta_0/H) - \epsilon_f} \right) -\frac{N_c}{2\pi} \tan^{-1} \left(\frac{(\pi/2) H\Delta}{H + H\Delta \ln(\Delta_0/H) + \epsilon_f} \right).$$
(6.10)

It is easy to see that in the limit $H \leq \epsilon_f(0)$, one has

$$M_{\rm imp} \sim \frac{N_c}{2} \frac{\Delta(0)}{\epsilon_f^2(0)} H^2 \left(1 + \Delta(0) \ln \frac{\Delta_0}{H} \right). \tag{6.11}$$

This expression shows that the impurity contribution to the magnetization vanishes as $H^2 \ln H$ with $H \rightarrow 0$. As expected, the impurity magnetization vanishes as the field goes to zero, thus showing that the magnetic impurity has been screenined. However, in a conventional *marginal* Kondo system, the magnetization vanishes *linearly* with the field. Here instead we find a faster field dependence.

It can be shown, using similar arguments, that a general expression for the impurity contribution to the magnetic susceptibility is given by

$$\chi_{\rm imp}(T,H) = \frac{N_c}{2\pi} \int_{-\infty}^{+\infty} \frac{\partial n}{\partial \epsilon} \left[\frac{\partial \delta}{\partial \epsilon} (\epsilon + H) + \frac{\partial \delta}{\partial \epsilon} (\epsilon - H) \right]$$
$$= -\frac{N_c}{2\pi} \int_{-\infty}^{+\infty} dx \frac{e^x}{(e^x + 1)^2}$$
$$\times \left[\frac{\partial \delta}{\partial \epsilon} \Big|_{xT+H} + \frac{\partial \delta}{\partial \epsilon} \Big|_{xT-H} \right]. \tag{6.12}$$

At zero temperature the susceptibility becomes

$$\chi_{\rm imp}(0,H) = -\frac{N_c}{2\pi} \left[\frac{\partial \delta}{\partial \epsilon} \right|_{-H} + \frac{\partial \delta}{\partial \epsilon} \right|_{H} \right]. \tag{6.13}$$

Thus, we find that the susceptibility at zero temperature and at low fields $[H \leq \epsilon_f(0)]$ is

$$\chi_{\rm imp}(0,H) = \frac{N_c \Delta(\epsilon_f^2 [H + H\Delta \ln(\Delta_0/H)] - \frac{1}{2} H\Delta\{(\pi H\Delta/2)^2 + [H + H\Delta \ln(\Delta_0/H)]^2 + \epsilon_f^2\})}{\{(\pi H\Delta/2)^2 + [H + H\Delta \ln(\Delta_0/H)]^2 + \epsilon_f^2\}^2 - 4\epsilon_f^2 [H + H\Delta \ln(\Delta_0/H)]^2}.$$
(6.14)

It should be noticed that in all of these expressions, the quantities ϵ_f and Δ are functions of the field H, with a limiting value $\epsilon_f(0)$ and $\Delta(0)$ for T=H=0 found in Sec. V. The quantity $\Delta(0)$ should not be confused with Δ_0 . Hereafter we will set $\Delta = \Delta(0)$ and $\epsilon_f = \epsilon_f(0)$. The magnetic susceptibility obtained from Eq. (6.11) agrees with the limit $\epsilon_f \gg H$ of Eq. (6.14) and gives

$$\chi_{\rm imp} \sim N_c \left(\frac{\Delta}{\epsilon_f}\right)^2 H \ln \frac{\Delta_0}{H} + N_c \frac{\Delta}{\epsilon_f^2} H \left(1 - \frac{\Delta}{2}\right) + \cdots$$
(6.15)

In the opposite regime $H \ll T \ll \epsilon_f$, the susceptibility is

$$\chi_{\rm imp}(T,0) \approx 2N_c \ln 2 \left(\frac{\Delta}{\epsilon_f}\right) T \ln\left(\frac{\Delta_0}{T}\right).$$
 (6.16)

To summarize, we find that in the low-field limit the zerotemperature magnetization vanishes like $H^2 \ln(\Delta_0/H)$. However, in contrast with the conventional "Fermi-liquid" behavior of the Kondo effect in metals, the magnetic susceptibility is *also* found to vanish in the low-field limit as $H \ln(\Delta/H)$ and at zero temperature. Hence, in this nonmarginal Kondo system, the magnetic impurity is *overscreened* even for a single channel of fermions. In the lowtemperature, zero-field regime, the impurity susceptibility has a $T \ln(\Delta_0/T)$ behavior which again shows that the impurity is overscreened.

VII. IMPURITY ENTROPY AND SPECIFIC HEAT

We can estimate the impurity contribution to the specific heat in the limit $T \ll H$, in the screening regime. Using the

SPE and some straightforward algebra, the impurity contribution to the entropy is

$$S_{\rm imp} = -\left.\frac{\partial F}{\partial T}\right|_{\epsilon_f, \Delta} = \frac{N_c}{2\pi} \int_{-\infty}^{\infty} d\epsilon \frac{\epsilon}{T} \frac{\partial n}{\partial \epsilon} \left[\delta(\epsilon + H) + \delta(\epsilon - H)\right].$$
(7.1)

Using the scaling $\epsilon = xT$ this is

$$S_{\rm imp} = -\frac{N_c}{2\pi} \int_{-\infty}^{\infty} dx x \frac{e^x}{(e^x + 1)^2} [\delta(xT + H) + \delta(xT - H)].$$
(7.2)

In the limit $T \ll H$, we may expand the phase shift around the point x = 0 to get

$$S_{\rm imp} = \chi_{\rm imp}(0,H) T \int_{-\infty}^{\infty} dx x^2 \frac{e^x}{(e^x + 1)^2}, \qquad (7.3)$$

where $\chi_{imp}(0,H)$ has been obtained in the previous section. The impurity contribution to the specific heat is then equal to the impurity contribution to the entropy in this limit. Our result shows that the impurity entropy vanishes at $T \rightarrow 0$ and finite field, for $T \ll H$.

The general form of the specific heat is

$$C_{\rm imp} = \frac{N_c}{2\pi T} \int_{-\infty}^{+\infty} d\epsilon \epsilon^2 \frac{\partial n}{\partial \epsilon} \left[\frac{\partial \delta}{\partial \epsilon} (\epsilon + H) + \frac{\partial \delta}{\partial \epsilon} (\epsilon - H) \right]$$
$$= -\frac{N_c T}{2\pi} \int_{-\infty}^{+\infty} dx x^2 \frac{e^x}{(e^x + 1)^2} \left[\frac{\partial \delta}{\partial \epsilon} \Big|_{xT+H} + \frac{\partial \delta}{\partial \epsilon} \Big|_{xT-H} \right].$$
(7.4)

In the regime $H \ll T \ll \epsilon_f$ we find

$$C_{\rm imp}(0,T) \approx 9\zeta(3) N_c \; \frac{\Delta^2}{\epsilon_f^2} T^2 \; \ln\left(\frac{\Delta_0}{T}\right), \tag{7.5}$$

where $\zeta(3)$ is the Riemann zeta function at 3 and it is a number of the order of unity.

Using the results of Eq. (6.16) and Eq. (7.5), we can compute the Wilson ratio for the regime $H \ll T \ll \epsilon_f$ and find

$$\frac{C_{\rm imp}(H,T)}{T\chi_{\rm imp}(H,T)} \approx \frac{9\zeta(3)}{2\ln 2}.$$
(7.6)

It is interesting that the ratio is still finite in spite of the fact the both the specific heat and the susceptibility behave very differently than in a Fermi liquid.

In the high-field limit $T \ll H \ll \epsilon_f$ the impurity specific heat is

$$C_{\rm imp}(H,T) \approx N_c \frac{\pi^2}{3} \left(\frac{\Delta}{\epsilon_f}\right) T H \ln\left(\frac{\Delta_0}{H}\right),$$
 (7.7)

which obeys the relation

$$C_{\rm imp}(H,T) \approx \frac{\pi^2}{3} T \chi_{\rm imp}(0,H).$$
 (7.8)

This result leads to a new Wilson ratio

$$W = \frac{C_{\rm imp}(H,T)}{T\chi_{\rm imp}(H,0)} = \frac{\pi^2}{3},$$
(7.9)

which is essentially identical to the Wilson ratio for the Kondo effect in Fermi liquids.

Hence we found that in the strong-coupling Kondo phase, the impurity specific heat at low temperature and low fields behaves like $T^2 \ln(\Delta_0/T)$ and $TH \ln(\Delta_0/H)$ depending on whether $H \ll T$ or $T \ll H$. Only for $T \ll H$ do we find the conventional linear T behavior of the (zero-field) specific heat of the (marginal) Kondo effect in Fermi liquids. Notice, however, that the slope γ of the specific heat in this regime is field dependent and behaves like $H \ln(\Delta_0/H)$. However, in spite of these differences, we found that the conventionally defined Wilson ratio is still finite but it is different in both regimes.

VIII. DISCUSSION

In this paper we constructed a model for the problem of a magnetic impurity in a $d_{x^2-y^2}$ superconductor. We solved this problem using the large- N_c approximation and found that there is a quantum phase transition from a phase in which the impurity is nearly free to a phase in which it is overscreened. We estimated the value of the critical coupling constant J_c . We found that J_c could be both smaller or larger than Δ_0 , the gap of the *d*-wave superconductor, but it is certainly smaller than the bandwidth D of the electrons that participate in the superconductivity.

This result agrees with recent work by Ingersent²⁸ on a related system. Ingersent used a Wilsonian numerical RG approach and found that the critical coupling runs off to the cutoff (strong coupling) unless either particle-hole symmetry is broken (for the band fermions) or additional high-energy states with a flat DOS were added. In the problem of the *d*-wave superconductor the former possibility is excluded by the superconductivity itself but the latter is required since such states are always there. In any event there is no reason to require that J_c should be smaller than Δ_0 . In fact, even if $J_c \ge \Delta_0$, the Kondo scale T_K does not track J_c and it is almost always smaller than Δ_0 (in fact, quite a bit smaller). The value of the critical coupling constant is nonuniversal and it depends on details of the high-energy physics of the system. Thus, our approximations have emphasized the role of the nodes and replaced the states above Δ_0 by a "flat band." Clearly, the solution of the saddle point equations with the full band structure of the Hamiltonian of Eq. 2.1 will yield a different (possibly smaller) value of J_c . The same caveats apply to the numerical RG calculation of Ingeresent, in which a specific discretization of the effective model is used. In fact, in most of his work, Ingeresent uses Wilson's logarithmic discretization which is very accurate for the Kondo problem in metals since it is tailored to reproduce the logarithmic singularities at high energies of the conventional (marginal) Kondo problem. In the case that we examine here, the system is very far away for its "lower critical dimension." This approach should overestimate J_c , probably by quite a bit. In any event, the actual value of Jitself depends on microscopic physics of the cuprates and there is no reason to believe that it should be tied to Δ_0 .

We investigated in detail the thermodynamic behavior

(impurity susceptibility and specific heat) in the overscreened phase where we found that the impurity susceptibility vanishes like $H \ln(\Delta_0/H)$ (for $T \ll H \ll T_K$) or $T \ln(\Delta_0/T)$ (for $H \ll T \ll T_K$) with a crossover at $T \approx H$. For a Fermi liquid, the impurity susceptibility approaches a constant value at $T \rightarrow 0$. The specific heat, on the other hand, was found to vanish like $TH \ln(\Delta_0/H)$ (for $T \ll H \ll T_K$) or $T^2 \ln(\Delta_0/T)$ (for $H \ll T \ll T_K$). In a Fermi liquid it vanishes linearly with T. The change in the power law behavior is an extension of the earlier work by Withoff and Fradkin.²⁶ The additional logarithmic singularity is an indication that r = 1is like an upper critical dimension for the Kondo problem.²⁹ The interesting quantum critical behavior, accessible for $T, H \gg T_K$, was not discussed here and will be the subject of a separate publication.³⁰

There are several important effects that we have not included here. One is the effect of *random* potential scattering which, naively may induce a nonzero DOS at the Fermi energy $E_F = 0$. Even if this effect is there, the effective DOS N(E) is very small. In Refs. 17 and 18 it was shown that $N(E) \approx \exp(-\operatorname{const}/w)$ (where w is the width of the distribution) and that the elastic mean free path is exponentially long, $\ell \sim \exp(+\operatorname{const}/w)$. Since at J_c we have a transition from a state with a *divergent* zero-temperature susceptibility (Curie like) to an overscreened state with vanishing susceptibility, the rounding effects of a finite (but very small) DOS should be a very small correction if the material is clean. A more interesting, and perhaps more important, effect that was not included here is the presence of explicit pair breaking by the vanishing of the amplitude of the *d*-wave order parameter at the impurity site. This effect should give rise to interesting Andreev-like processes which may well alter the physics of this problem. We will discuss this problem elsewhere.³⁰ Finally, corrections to the $N_c \rightarrow \infty$ limit remain to be estimated.

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APPENDIX: ESTIMATION OF INTEGRALS

The integral of Eq. (5.10) is a good representative for the approximations made in treating the integrals of Sec. V. The expression given in Eq. (5.12) is easy to obtain. As for the first integral of the RHS of Eq. (5.11) we have

$$\frac{\pi}{2}e^{1/\Delta}\int_{e^{1/\Delta}}^{\infty}\frac{dz}{z^2}\frac{(1+\nu z e^{-1/\Delta})}{(\Delta \pi/2)^2 + (\nu z e^{-1/\Delta} + \Delta \ln z)^2} \equiv K + I,$$
(A1)

where the splitting of the integral corresponds to the + sign in the numerator. At the value $z_0 = [(\Delta/\nu) e^{1/\Delta}] \ln z_0$ there is a crossover in the behavior of the denominator of the integrand. For $z < z_0$ the leading term is $\Delta \ln z$; for $z > z_0$ we can keep the term $\nu z e^{-1/\Delta}$. Also z_0 can be approximated by

$$z_0 \approx \left(\frac{\Delta}{\nu} e^{1/\Delta}\right) \ln\left(\frac{\Delta}{\nu} e^{1/\Delta}\right) > e^{1/\Delta}.$$

Then we can split the integrals as

$$I^{<} = \frac{\pi}{2} \frac{\nu}{\Delta^{2}} \int_{e^{1/\Delta}}^{z_{0}} \frac{dz}{z} \frac{1}{\ln^{2} z + (\pi/2)^{2}}.$$
 (A2)

The change of variables $t = (2/\pi) \ln z$ makes the integration straightforward to give

$$I^{<} = \frac{\nu}{\Delta^{2}} \left[\arctan\left(\frac{2}{\pi} \ln z_{0}\right) - \arctan\left(\frac{2}{\pi\Delta}\right) \right]$$
$$\sim \nu \frac{\pi}{2} \frac{\ln\{(\Delta/\nu)\ln[(\Delta/\nu) e^{1/\Delta}]\}}{1 + \Delta \ln\{(\Delta/\nu)\ln[(\Delta/\nu) e^{1/\Delta}]\}}.$$
 (A3)

On the other hand,

$$I^{>} = \nu \frac{\pi}{2} \frac{1}{\nu^{2} e^{-2/\Delta}} \int_{z_{0}}^{\infty} \frac{dz}{z} \frac{1}{z^{2} + (e^{1/\Delta} \pi \Delta/2\nu)^{2}}, \quad (A4)$$

which can be integrated by partial fractions to give

$$I^{>} = \nu \frac{\pi}{2} \frac{1}{\left[1 + \Delta \ln(\Delta/\nu)\right]^{2}}.$$
 (A5)

Similarly we have

$$K^{<} = \frac{\pi}{2} e^{1/\Delta} \frac{1}{\Delta^{2}} \int_{1/\Delta}^{\ln z_{0}} e^{-t} \frac{dt}{(\pi/2)^{2} + t^{2}}$$
(A6)

and

$$K^{>} = \frac{\pi}{2} \frac{e^{3/\Delta}}{\nu^{2}} \int_{z_{0}}^{\infty} \frac{dz}{z^{2}} \frac{1}{z^{2} + [e^{1/\Delta}(\pi\Delta/2\nu)]^{2}} < \frac{e^{1/\Delta}}{\nu} \frac{1}{z_{0}} I^{>} \sim \frac{\pi}{2} \nu \frac{1}{[1 + \Delta \ln(\Delta/\nu)]^{3}}.$$
 (A7)

Hence, again $K^>$, as was the case with $I^>$, can be neglected since its contribution is at least of the $o(\nu) \sim o(e^{-1/\Delta}) \ll \Delta$. The leading contribution comes from Eq. (A6) which can be

recast in terms of an exponential integral function and produces a constant contribution and a linear term in Δ . The leading contribution for small Δ gives

$$K^{<} \sim \frac{\pi}{2} \left[\frac{1}{1 + (\pi \Delta/2)^2} - \frac{2\Delta}{[1 + (\pi \Delta/2)^2]^2} + O(\nu) + \cdots \right].$$
(A8)

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With these results, the equation of state, keeping only the leading order contributions is

$$\frac{1}{g_0} = \frac{\pi}{2} \ln\left(\frac{D}{\Delta_0}\right) + \frac{\pi}{2} \frac{1}{1 + (\pi \Delta/2)^2} - \pi \frac{\Delta}{\left[1 + (\pi \Delta/2)^2\right]^2} + O(\Delta^2) + \cdots$$
(A9)

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