Weak-coupling theory of photoemission and inelastic neutron scattering and the mechanism of superconductivity in the cuprates

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ARPES and low-energy inelastic neutron-scattering studies of cuprate superconductors are described using a weak-coupling theory in which quasiparticles on a square lattice interact via scalar and spin-dependent effective interactions. In this paper we point out that in underdoped Bi2212 both probes are consistent with dominant near-neighbor Heisenberg interactions. We discuss the implications of this finding for the mechanism of high- T_c superconductivity.

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I. INTRODUCTION

It is evident from many experiments^{$1-3$} that the superconductivity of the high- T_c cuprates can be described at low energies and temperatures by a BCS theory with effective interactions between square-lattice quasiparticles that lead to short-coherence-length *d*-wave superconductivity. After many years of study, the source of this effective interaction has still not been established with certainty. The *d*-wave property is naturally associated with near-neighbor interactions, but these could be spin independent and attractive *V* or Heisenberg-type and antiferromagnetic (J) . The effective interactions could be mediated by a lattice or electronicfluctuation boson, as in conventional superconductivity, or fall outside of the familiar Eliashberg scenario. The resonance feature in inelastic neutron scattering, 2 which appears to be generic in cuprates but absent in conventional superconductors, can be explained $4-7$ if interaction parameters are chosen so that the system is close to an antiferromagnetic instability, possibly one driven by strong on-site repulsion *U*.

In this paper we describe an attempt to draw conclusions about the relative importance of *U*, *V*, and *J* low-energy effective interactions from the numerical arcana of cuprate superconductivity by requiring quantitative consistency between weak-coupling descriptions of inelastic neutronscattering resonance (INSR) and angle-resolved photoemission spectroscopy (ARPES) data in $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_8/Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212). To describe the INSR we derive weak-coupling expressions for the (π, π) dynamic spin susceptibility which are exact for any *U*-*V*-*J* model. The spin susceptibility appears as a member of a quartet of coupled response functions; we find that a fourchannel response-function theory is required for any nonzero value of *U*, *V*, or *J*.

We view the use of a weak-coupling theory, in which the fermionic excitations are BCS theory Bogoliubov quasiparticles, as something which is justified at low temperatures by experiment. This work is motivated by the expectation that a clearer understanding of the character of the low-energy effective interactions might hint at its microscopic origin. Starting from the assumption that only the *U*, *V*, and *J* effective interactions are important and using ARPES experimental values for the square-lattice energy band which crosses the Fermi energy, we conclude from ARPES antinodal gap values that in the moderately underdoped regime 3*J*/2−2*V* \sim 250 meV. Similarly from the occurrence of the INSR phenomenon we conclude that $2J+U \sim 350$ meV. The proximity of these two energy scales strongly suggests that the Heisenberg effective interaction *J* is dominant. We argue that this finding suggests that superconductivity is mediated by short-range antiferromagnetic superexchange interactions between low-energy quasiparticles which are a remnant of the parent antiferromagnetic Mott insulator and discuss some of the challenges which stand in the way of a completely satisfactory microscopic theory of superconductivity in doped Mott insulators.

II. PHENOMENOLOGICAL MODEL FOR THE SUPERCONDUCTING STATE AT *T***= 0**

A. Effective Hamiltonian

We consider a low-energy effective Hamiltonian for underdoped Bi2212,

$$
H = \sum_{\vec{k}} \epsilon(\vec{k}) - \mu + H_U + H_V + H_J,\tag{1}
$$

where $\epsilon(\vec{k})$ is the band energy and the interaction terms are

$$
H_U = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad H_V = V \sum_{\langle i,j\rangle \sigma \sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'},
$$

$$
H_J = J \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j.
$$
(2)

The angle bracket notation $\langle i, j \rangle$ is used to specify that the *V* and *J* interactions in our model are restricted to near neighbors. We do not view this phenomenological Hamiltonian as microscopic but as what remains after incoherent higherenergy electronic fluctuations are integrated out. In view of the Luttinger theorem, the chemical potential μ is nevertheless fixed by the doping concentration $x=1-\sum_{\vec{k},\sigma} \langle c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} \rangle$. The effective interaction parameters *U*, *V*, and *J* are assumed to be at least weakly doping dependent.

B. Antinodal Gap

The order parameter for the *d*-wave superconducting state is $\langle c_{i\uparrow} c_{i+\hat{\tau}\downarrow} \rangle = (-)^{\tau} \Delta$, where $(-)^{\tau} = +1$ for $\hat{\tau} = \pm \hat{x}$ and -1 for

TABLE I. Singlet-pairing potential V_p for several underdoped Bi2212 samples. The doping *x* is extracted from experimental T_c data, assuming the parabolic relation proposed by Presland *et al.* $(Ref. 11).$ $(Ref. 11).$ $(Ref. 11).$

\mathcal{X}	T_c (K)	V_p (meV)	μ (meV)
0.144	92	250	-116.467
0.126	85	256	-111.358
0.11	75	278	-105.584
0.099	65	284	-102.369

 $\hat{\tau} = \pm \hat{y}$, accounting for the *d*-wave character. Applying BCS mean-field theory to Eq. ([1](#page-0-0)) leads to a gap function $\Delta(\vec{k})$ $=V_p\Delta(\cos k_x - \cos k_y)$ and to band energies $\epsilon \rightarrow \epsilon'$ which are modified by interactions. Here

$$
V_p = 3J/2 - 2V\tag{3}
$$

has contributions from both of the interactions which can induce *d*-wave superconductivity. Mean-field ground-state properties are completely determined by $\epsilon'(\vec{k})$ and V_p . The BCS Hamiltonian yields quasiparticles energies $\pm E(\vec{k})$ $= \pm [\epsilon'^2(\vec{k}) + \Delta^2(\vec{k})]^{1/2}$ which are measured in ARPES experiments. For $\epsilon'(\vec{k})$ we use the experimental Bi2212 normalstate quasiparticle band structure.⁸ The pairing potential V_p of the *d*-wave superconductor is fixed by setting the meanfield maximum gap $\Delta_0 = 2|V_p|\Delta$ equal to the ARPES anti-nodal gap.^{9[,10](#page-7-7)} Table [I](#page-1-0) summarizes V_p values obtained in this way for several underdoped Bi2212 samples. For concreteness we focus our discussion of numerical consistency between ARPES and INSR in the case of doping $x=0.144$, reserving a discussion of doping dependence to the end of the paper. For $x=0.144$, $V_p \sim 250$ meV. One of the central question of cuprate superconductivity theory is whether this pairing is due primarily to an attractive spin-independent effective interaction $(V < 0)$ or primarily due to an antiferromagnetic spin-dependent effective interactions $(J>0)$.

C. Competing orders

The conclusions reached in this paper depend critically on using the same weak-coupling Hamiltonian to consistently describe ARPES quasiparticle data and the INSR feature in neutron-scattering experiments. As we explain in more detail below, the emergence of a spin resonance well below¹² the particle-hole continuum signals an incipient instability in cuprates, almost certainly the instability toward the antiferromagnetic state. In a weak-coupling generalized randomphase approximation (GRPA) theory the energy cost of static antiferromagnetic fluctuations K^s is the sum of quasiparticle and interaction energy contributions. The quasiparticle contribution K_{qp}^s is a property of the mean-field state, and based on ARPES data we can conclude that its value is \sim 400 meV. We find below that $K^s = K_{qp}^s - 2J - U$ and conclude from qualitative and quantitative aspects of the INSR phenomenon that $K^s \ll K_{\text{qp}}^s$; more quantitatively a value close \sim 50 meV seems likely. It follows that $2J+U$

 \sim 350 meV. This conclusion is consistent with many experiments which hint at a close competition¹³ between spin and superconducting order in cuprates. To explain this assessment more completely, it is necessary to describe the weakcoupling theory of spin and superconducting fluctuations in *d*-wave superconductors in greater detail.

III. WEAK-COUPLING INSR THEORY

Because the interactions in our model Hamiltonian are either on site or nearest neighbor, fluctuations at the highsymmetry wave vector $\vec{q} = \vec{Q}$, where \vec{Q} is the ordering wave vector of the parent antiferromagnetic Mott insulator, can be expressed in terms of a small number of coupled channels.^{4[,6](#page-7-10)} To demonstrate this, we specialize to the $S_z=+1$ projection of the triplet fluctuation spectrum which is the one relevant to the INS measurements. Expanding the Hamiltonian to quadratic order around the mean-field state leads to the fluctuation Hamiltonian:⁷

$$
H^{f}(t) = \frac{1}{A} \sum_{\vec{p}, \vec{k}, \vec{q}, \sigma} I(\vec{k} - \vec{p}) \left[\delta \langle c^{\dagger}_{\vec{p}\sigma} c_{\vec{p} - \vec{q}\bar{\sigma}} \rangle c^{\dagger}_{\vec{k} - \vec{q}\sigma} c_{\vec{k}\sigma} \right] + J(\vec{k} - \vec{p})
$$

$$
\times \left[\delta \langle c^{\dagger}_{\vec{q} - \vec{p}\sigma} c^{\dagger}_{\vec{p}\sigma} \rangle c_{\vec{k}\sigma} c_{\vec{q} - \vec{k}\sigma} + \text{H.c.} \right], \tag{4}
$$

where

$$
I(\vec{k} - \vec{p}) = \{- U + 2V[\cos(k_x - p_x) + \cos(k_y - p_y)]\},\tag{5}
$$

and

$$
J(\vec{k} - \vec{p}) = -V[\cos(k_x - p_x) + \cos(k_y - p_y)].
$$
 (6)

The momentum-dependent term which appears in both interaction form factors, $I(\vec{k} - \vec{p})$ and $J(\vec{k} - \vec{p})$, can be rewritten as a sum of separable contributions using

$$
\cos(k_x - p_x) + \cos(k_y - p_y) = (s_{\vec{k}}s_{\vec{p}} + d_{\vec{k}}d_{\vec{p}} + ss_{\vec{k}}ss_{\vec{p}} + sd_{\vec{k}}sd_{\vec{p}})/2,
$$

(7)

where

$$
s_{\vec{k}} = (\cos k_x + \cos k_y), \quad d_{\vec{k}} = (\cos k_x - \cos k_y),
$$

$$
ss_{\vec{k}} = (\sin k_x + \sin k_y), \quad sd_{\vec{k}} = (\sin k_x - \sin k_y).
$$
 (8)

At wave vector $\vec{q} = \vec{Q}$, the channels involving sine functions all vanish and we then can identify seven operators, some with *s*- or *d*-wave form factors $(s_k \text{ or } d_k)$, whose fluctuations are influenced by the following interactions:

$$
\hat{A}_1 = \frac{1}{\sqrt{N}} \sum_{\vec{p}} S_{\vec{p}}^+, \quad \hat{A}_2 = \frac{1}{\sqrt{2N}} \sum_{\vec{p}} s_{\vec{p}} S_{\vec{p}}^+, \n\hat{A}_3 = \frac{1}{2\sqrt{N}} \sum_{\vec{p}} d_{\vec{p}} (D_{\vec{p}} + \bar{D}_{\vec{p}}), \quad \hat{A}_4 = \frac{1}{2\sqrt{N}} \sum_{\vec{p}} d_{\vec{p}} (D_{\vec{p}} - \bar{D}_{\vec{p}}), \n\hat{A}_5 = \frac{1}{\sqrt{2N}} \sum_{\vec{p}} d_{\vec{p}} S_{\vec{p}}^+, \quad \hat{A}_6 = \frac{1}{2\sqrt{N}} \sum_{\vec{p}} s_{\vec{p}} (D_{\vec{p}} + \bar{D}_{\vec{p}}),
$$

WEAK-COUPLING THEORY OF PHOTOEMISSION AND... PHYSICAL REVIEW B 78, 174506 (2008)

$$
\hat{A}_{7} = \frac{1}{2\sqrt{N}} \sum_{\vec{p}} s_{\vec{p}} (D_{\vec{p}} - \bar{D}_{\vec{p}}),
$$
\n(9)

where $S_{\vec{p}}^+ = c_{\vec{p}}^+ c_{\vec{p}+\vec{Q}\downarrow}$ is a spin-flip operator and $D_{\vec{p}} = c_{\vec{Q}-\vec{p}\downarrow} c_{\vec{p}\downarrow}$ and $\overline{D}_{\vec{p}} = c_{\vec{Q}-\vec{p}\uparrow}^{\dagger}$ [†]_{*Q*- \vec{p}}[†] \vec{p} [†] are the pair annihilation and creation operators. It follows that \hat{A}_3 induces *d*-wave-pair amplitude and \hat{A}_4 *d*-wave-pair-phase applications. The two-particle Green's functions which capture the fluctuations of these operators are

$$
\hat{\chi}_{ab}(\vec{Q}, \omega) = -i \int dt e^{i\omega t} \theta(t) \langle [\hat{A}_a(t), \hat{A}_b^{\dagger}(0)] \rangle.
$$
 (10)

We focus¹⁴ on the *s*-wave spin and *d*-wave-pair fields (\hat{A}_{1-4}) , which decouple from the *d*-wave spin and *s*-wave-pair fields (\hat{A}_{5-7}) and are responsible for the INSR. We emphasize that none of the earlier theoretical interpretations of the INSR feature at $\vec{q} = \vec{Q}$ have accounted properly for four-channel coupling which appears when the weak-coupling calculation is executed correctly.

The GRPA Green's functions can be obtained by solving the equation of motion for $\hat{\chi}_{ab}(\vec{Q}, \omega)$ with the quadratic Hamiltonian given in Eq. ([4](#page-1-1)). Since the BCS mean-field theory with effective interactions describes the low-energy charged excitations probed by ARPES, the same theory should also describe the low-energy particle-hole excitations probed by inelastic neutron scattering. We find that

$$
\hat{\chi}^{-1}(\vec{Q},\omega) = \hat{\chi}_{qp}^{-1}(\vec{Q},\omega) - \hat{V},\tag{11}
$$

where $\hat{V} = \text{diag}(-U - 2J, J/2 - 2V, V + J/4, V + J/4)$ is the interaction kernel and

$$
\hat{\chi}_{\text{qp},ab}(\vec{Q},\omega) = \frac{1}{N} \sum_{\vec{k}} \left(\frac{f_a f_b}{\omega - E(\vec{k}) - E(\vec{k}')} - \frac{(-1)^{a+b} f_a f_b}{\omega + E(\vec{k}) + E(\vec{k}')} \right)
$$
\n(12)

is the bare mean-field-quasiparticle response function. In Eq. ([12](#page-2-0)), $\vec{k}' = \vec{Q} - \vec{k}$, the factor $(-1)^{a+b}$ specifies the simple relationship between quasiparticle pair-creation and pairannihilation matrix elements⁶ at $\vec{q} = \vec{Q}$, and the form factors f_a are ⁶

$$
f = \left(p^-(\vec{k}, \vec{k}'), \frac{s_{\vec{k}}}{\sqrt{2}} p^+(\vec{k}, \vec{k}'), d_{\vec{k}} l^+(\vec{k}, \vec{k}'), d_{\vec{k}} l^-(\vec{k}, \vec{k}') \right),
$$

$$
p^{\pm}(\vec{k}, \vec{k}') = \frac{(u_{\vec{k}} v_{\vec{k}'} \pm v_{\vec{k}} u_{\vec{k}'})}{\sqrt{2}},
$$

$$
l^{\pm}(\vec{k}, \vec{k}') = \frac{(u_{\vec{k}} u_{\vec{k}'} \pm v_{\vec{k}} v_{\vec{k}'})}{\sqrt{2}},
$$
 (13)

 $l^{\pm}(\vec{k}, \vec{k}') = \frac{(u_{\vec{k}} u_{\vec{k}'} \pm v_{\vec{k}} v_{\vec{k}'})}{\sqrt{2}}$. (13) (13) In the GRPA the ω dependence of $\hat{\chi}^{-1}$ comes entirely from the ω dependence of $\tilde{\chi}_{qp}^{-1}$, which depends only on the band

structure, on the doping x , and on V_p . Typical numerical

results for $\hat{\chi}_{qp}^{-1}(\vec{Q})$ are summarized in Fig. [1.](#page-3-0)

Since the INSR frequency is well below the lower edge of the $\vec{q} = \vec{Q}$ particle-hole continuum, it is useful to expand $\hat{\chi}_{\text{qp},ab}(\mathcal{Q},\omega)$ to leading order in ω

$$
\hat{\chi}_{qp,ab}(\vec{Q},\omega) \approx R_0(a,b) - R_1(a,b)\omega + O(\omega^2),
$$

$$
R_0(a,b) = \sum_{\vec{k}} \frac{-f_a f_b [1 + (-1)^{a+b}]}{E(\vec{k}) + E(\vec{k}')} ,
$$

$$
R_1(a,b) = \sum_{\vec{k}} \frac{f_a f_b [1 - (-1)^{a+b}]}{[E(\vec{k}) + E(\vec{k}')]^2} .
$$
 (14)

The leading coupling between even and odd *a* operators is the Berry-phase coupling which appears at first order in ω ; the most important $4,6,7$ $4,6,7$ $4,6,7$ of these is the coupling between spin $(a=1)$ and *d*-wave-pair phase $(a=4)$. Even-even and oddodd fluctuations have no Berry-phase coupling but are coupled in the static limit. χ_{qp}^{-1} has a similar low-frequency expansion in which even-even and odd-odd fluctuations have relatively little frequency dependence until ω approaches the particle-hole continuum closely as seen in Fig. [1.](#page-3-0) The eveneven and odd-odd elements of $-\chi^{-1} \equiv K$ specify the energy cost of the corresponding particle-hole channel fluctuations while the even-odd elements, approximately linear in frequency, specify how the collective fluctuation energy is quantized. The even-odd elements satisfy $\chi_{\text{qp},ab}^{-1} \approx \omega C_{ab}$.

IV. MAGNETIC PLASMON

The INSR energy *E*res solves

$$
det|\hat{\chi}^{-1}| = det|\hat{\chi}_{qp}^{-1} - \hat{V}| = 0.
$$
 (15)

The results for E^{res} which are implied by Eq. (15) (15) (15) when it is assumed that the antiferromagnetic *J* interaction is dominant are summarized in Fig. [2;](#page-3-1) the same values of *E*res can be obtained by the time-dependent mean-field theory described in our ealier work⁷ which did not specialize to and take advantage of the simplifications possible at $\vec{q} = \vec{Q}$. The agreement of these results with INSR data is remarkable. If one interaction is assumed to be dominant the model parameters are completely determined by ARPES data. *The Heisenberg effective interaction model predicts accurate INSR position values over a broad range of doping.*

To achieve a qualitative understanding of this finding we neglect the $(a=2)$ extended-*s* spin-density fluctuations which are much stiffer than other fluctuation modes, as shown in Fig. [1](#page-3-0)(b), and the weak frequency dependence of the fluctuation energy contributions. With these approximations, 15

$$
E^{\rm res} \approx \sqrt{\frac{K^s K^{\phi} K^{\rm am} - K^{\phi} (K_{13}^{\rm qp})^2}{K^{\rm am} C_{14}^2 + K^s C_{34}^2 - 2K_{13}^{\rm qp} C_{14} C_{34}}} \sim \frac{\sqrt{K^s K^{\phi}}}{C_{14}},\tag{16}
$$

where $K^s = K_{11}^{qp} - U - 2J$, $K^{am} = K_{33}^{qp} + V + J/4$, and $K^{φ} = K_{44}^{qp} + V$ $+J/4$ are spin, π amplitude mode, and π phase mode stiffnesses, respectively. Since $C_{14} \sim 2$ and the experimental value of $E^{\text{res}} \sim 40 \text{ meV}$ is small compared to K_{11}^{qp}

FIG. 1. $\hat{\chi}_{\text{qp,ab}}^{-1}(\vec{Q}, \omega)$ for $\omega < \Omega_0$ where Ω_0 is the gap in the quasiparticle-pair excitation spectrum at $\vec{q} = \vec{Q}$ established by *d*-wave order. For each channel *a*, the solid, dotted, dashed, and dash-dotted lines represent, respectively, $\hat{\chi}_{qp,a1}^{-1}$, $\hat{\chi}_{qp,a2}^{-1}$, $\hat{\chi}_{qp,a2}^{-1}$, $\hat{\chi}_{qp,a4}^{-1}$. $(\Omega_0 \approx 70 \text{ meV}$ for $x=0.144$ using the V_p value listed in Table [I.](#page-1-0)) In a weak-coupling theory these results depend only on the normal-state band dispersion and on *Vp*= 3*J*/2−2*V*. Channel *a*= 1 corresponds to spin, *a*= 2 to spin with an extended *s*-wave form factor, *a*= 3 to *d*-wave-pair amplitude, and $a = 4$ to d -wave-pair phase.

 \approx 400 meV and $K_{44}^{\text{qp}} \approx$ 200 meV, it is clear that interactions must substantially reduce the values of either K^s or K^{ϕ} , or both. In the Heisenberg only model the interaction *J* reduces K^s to values which are \sim 50 meV and decrease as expected as the antiferromagnetic state is approached.

The lines in our three-dimensional interaction parameter space which are consistent with both ARPES and INSR data are illustrated for several doping values in Fig. [3.](#page-4-0) We note that the intersection of all lines with $U=0$ also yields $V=0$ to an excellent approximation. If we imagine that the *U*, *V*, and *J* effective interactions have independent origins, it is natural to expect that one of the three is likely to be dominant. Our analysis is consistent with this expectation and selects the Heisenberg interaction among the three possibilities. This argument suggests a remarkably simple single-interaction lowenergy effective model with strength *J* ranging from \approx 166 meV for *x*=0.144 to \approx 190 meV for *x*=0.099.

The INSR position could of course also be accounted for by fine tuning both *U* and *V* at fixed V_p , ^{[16](#page-7-14)} although we have argued that this is less likely. For example, if we first assume that *d*-wave pairing is due entirely to attractive spinindependent effective interactions, $V=-V_p/2$ ≈ -130 meV. This value of *V* results in a small phase stiffness, K^{ϕ} \sim 70 meV, and would require that $U \sim 300$ meV in order to reduce *E*res into the experimental range. As we explain later, this parameter set would correspond to a weaker correlation

FIG. 2. INSR energy E^{res} calculated from Eq. (15) (15) (15) (solid dots) assuming that with $U=V=0$. When only *J* is nonzero, its value $(J$ $=\frac{2}{3}V_p$) is fixed by the ARPES antinodal gap. As shown in this figure this assumption predicts the correct value for the INSR position. The long-dashed line plots in this figure plot the empirical rule $E^{res} = 5.4k_BT_c$. The triangles, white dots, and the black squares show the doping dependencies of Ω_0 , and $2\Delta_0$ calculated from V_p and the band structure and the value of K^s obtained when these are combined with the ARPES determined value J in the $U=V=0$ model.

FIG. 3. Lines in (U, J) parameter space which reproduce both the experimental antinodal gaps Δ_0 and the INSR energy E^{res} for a series of doping values. Note that $V=3J/4-V_p/2$ where the V_p values are listed in Table [I.](#page-1-0) For all doping values the intersection of these lines with $U=0$ also yields $V=0$. We argue in the text that this is strongly suggestive that the Heisenberg *J* interaction is dominant. This figure was constructed using the 4×4 expression given in Eq. (15) (15) (15) for the resonance frequency.

scenario in which the effective value of *U* is still fairly large. The INSR *magnetic plasmon* in this case has approximately equal pair phase and spin character; in the large *J* scenario on the other hand the INSR mode has dominant spin character because $K^s \ll K^\phi$. None of these arguments are sufficiently quantitative to favor the *V*= 0 model choice over the *V* =−*J*/4 choice, commonly used in the *t*-*J* model calculations and motivated by the theory of the superexchange mechanism. Compared to the *J*-only model, this choice shifts *J* slightly from $J = 2V_p/3$ to $V_p/2$, resulting in slightly larger K^s and smaller K^{ϕ} without shifting the INSR position significantly.

We close this section by commenting briefly on the role of interchannel Berry-phase coupling, which has often been neglected in theoretical analyses in determining the INSR position and character. When only the spin channel is included the equation for the resonance frequency is $K^s(E^{res}) = 0$. Because of the weak-energy dependence of K_{qp}^s below the particle-hole continuum we see that when coupling is ignored, $U+2J$ has to be adjusted to more than 90% of K_{qp}^s to explain the resonance position, placing the system even closer to the antiferromagnetic state instability point. For a given value of the interaction strength, mode coupling substantially lowers the resonance frequency. Mode coupling is therefore important in explaining the experimental relationship between the value of the resonance frequency and the proximity of the antiferromagnetic state.

V. DISCUSSION

This work starts from the observation that in the lowtemperature limit cuprates act like ordinary superconductors with elementary quasiparticle excitations that are describable by BCS theory. ARPES experiments find a Fermi surface

with area proportional to electron doping 1−*x*, rather than hole-doping x and a Fermi velocity which shows no sign¹⁷ of declining with *x*. The most remarkable feature of cuprate superconductors at low temperatures is the sharp collective excitation which appears at wave vectors near $\tilde{Q} = (\pi, \pi)$ in neutron studies of quantum spin fluctuations. The apparently banal character of the low-energy excitations suggests that the ground state of these superconductors can be described using a weak-coupling theory in which the quasiparticles seen in ARPES experiments interact in a way which leads to both *d*-wave superconductivity and the inelastic neutronscattering mode. Given this starting point, it is natural to ask if quantitative comparison with experiments gives any indication as to the character of the presumably renormalized interactions which appear in this low-energy effective theory. In making this assessment, it is important to acknowledge that the properties of cuprate superconductors are not entirely universal, and not all experimental data are available on any one material. Nevertheless we judge that well established broad trends allow generic conclusions. The numbers mentioned below are intended to apply most closely to the Bi2212 cuprate family.

In order to make progress toward identifying the renormalized interactions it seems to be necessary to start by limiting the forms which can reasonably be considered. The fact of singlet *d*-wave superconductivity on the cuprate square lattice appears to require either spin-independent attractive interactions (possibly due to phonons) or spin-dependent antiferromagnetic Heisenberg interactions (possibly due to short-range antiferromagnetic order) between electrons on neighboring sites. The proximity of a Mott insulator state for hole doping $x=0$ would seem to require allowing for the possibility of a strongly repulsive on-site Hubbard-type interaction *U*. We have therefore considered how the properties of the system depend on all three parameters *U*, *V*, and *J*. The simplest experimental constraint on this parameter set is imposed by the magnitude of the *d*-wave antinodal gap which, when combined with the band structure known from ARPES, constrains $V_p = 3J/2 - 2V$ to a value ~250 meV which increases moderately with decreasing *x* as summarized in Table [I.](#page-1-0)

An understanding of the implications of the strong INSR at $\vec{Q} = (\pi, \pi)$ requires a more subtle analysis. In a weakcoupling theory we can determine collective excitation properties by examining the influence of interactions on single particle-hole excitations. As explained in Sec. III, for the case $\vec{Q} = (\pi, \pi)$ excitations of a *d*-wave superconductor on a square lattice the spin-response function probed by neutrons is coupled to pair-magnitude, pair-phase, and extended-*s* spin-response functions. A correct analysis of weak-coupling collective fluctuations therefore requires that all four modes be treated simultaneously, rather than singling out spin respons[e5](#page-7-16)[,18](#page-7-17)[–24](#page-7-18) as has been common in RPA theories or including only first few modes. $4,6,25,26$ $4,6,25,26$ $4,6,25,26$ $4,6,25,26$ We emphasize that a theory of the spin-response function requires consideration of the four-coupled modes whenever *any* of the three interactions we consider is nonzero. In this theory the energy cost of antiferromagnetic spin fluctuations is reduced from K_{11}^{qp} \sim 400 meV to $K^s = K_{11}^{qp} - U - 2J$ by interactions. $(K_{11}^{qp}$ is

purely a property of the BCS mean-field theory and is therefore specified by the ARPES bands and V_p .) In order for the INSR to appear, as it does in experiment, below the particlehole continuum K^s must be reduced to a small value by interactions, i.e., the system must be close to an antiferromagnetic instability. A theory which did not account for coupling between spin and other modes would require that *K^s* be reduced to an even smaller value in order to account for the INSR data.) On this basis we conclude that $U+2J$ \sim 350 meV.

Both ARPES and INSR experiments are therefore consistent with a *J*-dominated renormalized interaction model. The strength for *J* is comparable to the strength of the superexchange interactions in the undoped antiferromagnetic insulator state of the cuprates. The effective interactions that are consistent with experiment are therefore similar to the effective interactions which appear²⁷ in t -*J* models, intended to describe quasiparticles which live nearly entirely in the Gutzwiller projected $28-32$ no-double-occupancy Hubbardmodel subspace. The absence of a large Hubbard replusion *U* in the effective interaction is also expected for quasiparticles which avoid this strong interaction by residing dominantly in the no-double-occupancy subspace. Any other choice of interaction model requires improbable fine tuning to achieve consistency with the main experimental facts.

The consistency of the *J*-only interaction model with ARPES and INSR data partially affirms one of the main pictures²⁷ of cuprate superconductivity, namely, that it emerges from the antiferromagnetic interactions in the parent $x=0$ Mott insulator state when holes in the lower Hubbard band become itinerant at sufficiently large doping. There are, however, at this point major challenges which still stand in the way of a fully consistent theoretical picture to accompany this scenario. Mean-field-theory slave boson and other related formulations^{27,[33](#page-7-24)} of the t - J model, for example, tend to lead to quasiparticle band widths which decreases with hole doping and to superfluid density which is strictly proportional to hole doping *x*. These predictions are, however, clearly at odds with $ARPES$ $(Ref. 17)$ $(Ref. 17)$ $(Ref. 17)$ and penetration-dept[h34](#page-7-25)[–36](#page-7-26) temperature-dependence observations, both of which indicate that the Fermi velocity has a weak doping dependence and that the penetration depth vanishes at a rather large value of hole doping. A second theoretical approach motivated by the *t*-*J* model proceeds from the *ansatz* that the superconducting state can be described by Gutzwiller-projected BCS paired states[.28](#page-7-22)[–31,](#page-7-27)[37,](#page-7-28)[38](#page-7-29) Variational Monte Carlo calculations 37 have demonstrated that the Gutswiller-projected BCS wave function reproduces a variety of quantities observed in experiments. Furthermore, using the Gutzwiller approximation,³² the effect of the Gutzwiller projector can be replaced approximately by doping-dependent band energy and interaction renormalization factors, leading to mean-field equations similar to those of slave-boson mean-field theories and of the same form as those of the weak-coupling BCS theory. This simple approximation can reproduce the results of the variational Monte Carlo studies to a remarkable degree. As a result, the *plain vanilla* theory helps provide a theoretical explanation for weak-coupling low-energy behavior in the superconducting state with effective interaction parameters that arise in a complex way from the correlated fluctuations of higherenergy degrees of freedom. From this point of view, our main finding in this paper is that the same interactions are also quantitatively consistent with the INSR feature. In addition, as we have shown⁷ previously, the pairing wave-vector dependence of these low-energy antiferromagnetic fluctuations provides a natural explanation for the fact that the superfluid density goes to zero at a finite value of hole doping.

One very interesting property of cuprate superconductivities is that the Fermi velocity remains nearly constant throughout the underdoped regime, even as^{39} the superfluid density and the low-frequency infrared spectral-weight weight decline, presumably reflecting in part a decrease in the quasiparticle renormalization factor *Z*. Although this property is reproduced by Gutswiller-projected variational Monte Carlo calculations, 37 it seems surprising from a perturbation-theory point of view that *Z* should decline to a small value without a corresponding decrease in Fermi velocity; large values for the energy dependence of the selfenergy can easily arise from small energy denominators associated with resonances near the Fermi energy, but it is not so obvious how correspondingly large values for the wavevector dependence of the self-energy could arise. We suspect that the quasiparticle renormalization factor in the cuprates is not as small as suggested by the Gutzwiller-projected BCS state *ansatz*.

Another very interesting property of cuprate superconductores is the *marginal Fermi-liquid* behavior which often occurs when superconductivity is suppressed by temperature (in the overdoped regime) or by a magnetic field. Marginal Fermi-liquid behavior suggests that quasiparticles are strongly coupled to very-low-energy bosonic excitations or that the system would be very close to a quantum phase transition if superconductivity was suppressed. It seems likely to be more than a coincidence that in the low-energy effective model we have extracted from experiment, the cuprates would be very close to antiferromagnetism throughout much of the superconducting dome if they did not form a superconducting state. This statement is quantified in the Appendix in which we discuss quantitative aspects of the competition between superconductivity and antiferromagnetism. Decreasing the gap $\Delta_0 \rightarrow 0$ decreases K_{11}^{qp} by approximately 50 meV, just the amount required to reach the antiferromagnetic instability. Because superconductivity suppresses antiferromagnetism, pair-condensation must raise a part of the electron-electron interaction energy. This property may be part of the explanation for the apparent increase $39,40$ $39,40$ in kinetic energy in the superconducting state.

In conclusion, we have performed a weak-coupling analysis of ARPES and INSR experiments in Bi2212 in an effort to indentify an effective interaction model which is consistent with both experiments. We find that the doping dependences of the superconducting gap, and the INSR energy *E*res can be consistently explained by a model with near-neighbor Heisenberg interactions with a strength that is consistent with superexchange interactions. This result suggests that strong short-range repulsion and incoherent remnants of the antiferromagnetic insulating parent compound are key to hightemperature superconductivity.

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APPENDIX: COMPETITION BETWEEN *d***-WAVE SUPERCONDUCTIVITY AND ANTIFERROMAGNETISM**

In this appendix we explain in more detail how *d*-wave superconductivity and antiferromagnetism compete in a weak-coupling GRPA theory. As pointed out in an earlier paper, $\frac{7}{1}$ this competition is responsible for a correlation induced suppression of the superfluid density as antiferromagnetism is approached.

The quantum zero-point energy associated with the collective fluctuations probed in INSR experiments is given approximately by

$$
E^{zp} = \frac{1}{2} \sum_{k}^{\prime} E_{\vec{k}}^{res} = \frac{1}{2} \sum_{k}^{\prime} \frac{\sqrt{K_{\vec{k}, \text{adia}}^{s} K_{\vec{k}, \text{adia}}^{\phi}}}{C_{14, \vec{k}}}, \tag{A1}
$$

where the prime refers to the sum over wave vectors near $\vec{k} = \vec{Q}$ for which the Berry curvature C_{14} is large. $K_{\vec{k}, \text{adia}}^s$ and $K^{\phi}_{\vec{k}, \text{adia}}$ are the adiabatic limit stiffnesses which equal $-\chi_{\text{qp},11}^{-1}(\vec{k}, \omega=0) - U - 2J$ and $-\chi_{\text{qp},44}^{-1}(\vec{k}, \omega=0) + V + J/4$, respectively. The correlation contribution to the superfluid density is then given by $⁷$ $⁷$ $⁷$ </sup>

$$
\rho^{\text{cor}} = \frac{1}{A} \frac{\partial E^{\text{zp}}}{\partial P^2} \approx \frac{1}{4A} \sum_{k}^{\prime} \frac{E_{\vec{k}}^{\text{res}}}{K_{\vec{k}, \text{adia}}^s} \frac{\partial K_{\vec{k}, \text{adia}}^s}{\partial P^2}, \tag{A2}
$$

where P is the norm of the pairing wave vector of the BCS wave function. We explain below why the *P* dependence of K^s is much stronger than the *P* dependence of K^{ϕ} .) Since both $E_{\vec{k}}^{\text{res}}$ and $K_{\vec{k}, \text{adia}}^{\text{s}}$ are positive quantities, $\partial K_{\vec{k}, \text{adia}}^{\text{s}} / \partial P^2$ determines the sign of ρ^{cor} . Using the chain rule leads to

$$
\frac{\partial K_{\vec{k},\text{adia}}^s}{\partial P^2} = \frac{\partial \Delta_0}{\partial P^2} \frac{\partial K_{\vec{k},\text{adia}}^s}{\partial \Delta_0}.
$$
 (A3)

Because we know that *d*-wave superconductivity is weakened by pair-breaking effect of finite *P* Doppler shifts on nodal quasiparticles we can conclude that $\partial \Delta_0 / \partial P^2 < 0$.

A positive value for $\partial K_{\vec{k},\text{adia}}^s / \partial \Delta_0$ characterizes competition between antiferromagnetism and superconductivity. When the two orders compete, the energy cost of antiferromagnetic fluctuations is increased when superconductivity strengthens. In other words, K^s will increase as Δ_0 increases,

FIG. 4. Numerical evaluation of $-\chi_{\text{qp},11}^{-1}(\vec{k} = \vec{Q}, \omega = 0)$ as a function of Δ_0 for the doping $x=0.144$ using Eq. ([12](#page-2-0)).

giving $\partial K_{\vec{k},\text{adia}}^s / \partial \Delta_0 > 0$ in this case. To confirm the competing nature of these interactions, we have performed a numerical calculation of Δ_0 dependence of K^s . Since K^s $=-\chi_{\text{qp},11}^{-1}(\vec{k}, \omega=0) - U - 2J$, the Δ_0 dependence of *K^s* comes entirely from $-\chi_{\text{qp},11}^{-1}(\vec{k}, \omega=0)$. Figure [4](#page-6-0) plots $-\chi_{\text{qp},11}^{-1}(\vec{k})$ $=\vec{Q}$, ω =0) as a function of Δ_0 for doping *x*=0.144 as an example. $-\chi_{\text{qp},11}^{-1}(\vec{k}=\vec{Q},\omega=0)$ clearly increases monotonically with Δ_0 , consistent with the competing order picture discussed above. It is important to realize that the relative change in K^s is larger than the relative change in K^{ϕ} by approximately a factor of 10 because of the interaction contributions to the inverse response functions. We have shown separately⁷ that the size of this effect combined with the reduction in Δ_0 at finite *P* can explain the large reduction in superfluid densities compared with mean-field theory values in underdoped cuprates.

Our demonstration that superconductivity and antiferromagnetism compete in the effective weak-coupling picture of cuprate superconductors contradicts the conclusion of Zhang *et al.*, [41](#page-7-32) who stated that weak-coupling theory predicts an enhancement of antiferromagnetism due to *d*-wave superconductivity. Our calculation shows that their conclusion is not valid when the normal-state Fermi surface is similar to what is observed in Bi2212 systems. As pointed out by Tchernyshyov *et al.*,^{[6](#page-7-10)} the response functions $\hat{\chi}_{qp}$ at $\vec{q} = \vec{Q}$ are dominated by the *hot spots* located near $(\pi, 0)$. If this is true, $-\chi_{\text{qp},11}^{-1}(\vec{k}, \omega=0) \sim 2\Delta_{\text{antinodal}} = 2\Delta_0$. This crude argument is consistent with $\partial K^s_{\vec{k},\text{adia}}/\partial \Delta_0 > 0$ and very crudely consistent with Fig. [4.](#page-6-0) The character of the competition between superconductivity and antiferromagnetism is dependent on the normal-state band structure. This dependence is likely responsible for some of the differences between hole-doped and electron-doped cuprates.

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