There is a great deal of interest in attributing the high critical temperatures of the cuprates to either the proximity of the Fermi level to a van Hove singularity or to structure of the superconducting pairing potential in momentum space far from the Fermi surface, the latter being particularly important for spin-fluctuation-mediated pairing mechanisms. We examine these ideas by calculating the critical temperature $T_c$ for model Einstein-phonon- and spin-fluctuation-mediated superconductors within both the standard, Fermi-surface-restricted Eliashberg theory and the exact mean field theory, which accounts for the full momentum structure of the pairing potential and the energy dependence of the density of states. Our calculations employ band structures chosen to model both the $\text{La}_2\text{Sr}_{2-x}\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ families. By using two models of spin-fluctuation-mediated pairing in the cuprates, we demonstrate that our results are independent of the details of the dynamical susceptibility, which is taken to be the pairing potential. We also compare these two models against available magnetic neutron scattering data, since these data provide
the most direct constraints on the susceptibility. We conclude from our studies that the van Hove singularity does not drastically alter $T_c$ from its value when the density of states is constant and that the effect of momentum structure is significant but secondary in importance to that of the energy dependence in the density of states.

PACS numbers: 74.20.Mn, 74.20.Fg, 74.25.Jb, 74.25.Ha
I. INTRODUCTION

The discovery of the cuprate superconductors with critical temperates in excess of 90 K has motivated the theoretical community to look for ways in which the accepted BCS theory of superconductivity can yield such large transition temperatures. Accomplishing this task is particularly difficult because the energy scale of both phonons and spin fluctuations, which are prime candidates for the pairing interaction in the cuprates, are not so different from those in the low-temperature superconductors. Moreover, the coupling strength of these interactions to the electrons implied by transport measurements is small. We focus on two hypotheses regarding this dilemma which have attracted a great deal of attention in the literature. The first asserts that structure in the electronic density of states near the Fermi level on the scale of the pairing boson energy is mainly responsible for the enhanced critical temperature. The second postulates that structure of the pairing potential in momentum space far from the Fermi surface is the dominant effect.

Investigations into the influence of a strongly energy-dependent density of states on superconducting properties has a long history which begins with the A15 superconductors. In these materials, the density of states is thought to exhibit a square root singularity or Lorentzian peak near the Fermi level, and the analysis of the effect of this structure on the critical temperature $T_c$ has proceeded along both weak-coupling BCS and strong-coupling Eliashberg lines. Recently, these approaches have been applied to the copper oxide superconductors, where the density of states is thought to contain logarithmic van Hove singularities due to the quasi-two-dimensional nature of the CuO$_2$ planes. In the cuprates, however, studies have been carried out mainly in the BCS limit. These models result in s-wave pairing and have been used to explain the isotope effect in these materials.

Momentum structure in the superconducting pairing potential has not been investigated as systematically as has structure in the density of states. One reason for the scarcity of work in this area may be that the inclusion of momentum structure in the pairing potential far from the Fermi surface calls into question the validity of the usual Eliashberg theory.
and greatly complicates the calculation of transport properties such as the resistivity. For conventional, phonon-mediated superconductors, the difficulties associated with wavevector-dependence of the pairing potential do not arise, since Migdal’s theorem \( [10] \) holds and effectively restricts all quantities of interest to the Fermi surface. For superconductivity produced by an electronic pairing mechanism, in contrast, early studies have demonstrated that a simple RPA treatment of the interaction in Eliashberg theory including the full wavevector and frequency dependence of the pairing potential overestimates \( T_c \) \( [11] \). In effect, the RPA form of the electron-electron interaction is too strongly attractive due to the neglect of vertex corrections. In particular, these vertex corrections are found to be important when the characteristic pairing boson energy is larger than 5% of the Fermi energy \( [11] \), which is a criterion easily satisfied by most electronic pairing mechanisms. More recent studies have indicated that the opposite conclusion may hold in the two-dimensional Hubbard model: vertex corrections are significant and act to strengthen the electron-electron interaction \( [12] \).

In addition, since most transport calculations are based on an analogy with the electron-phonon interaction and therefore use a version of Migdal’s theorem, it is not clear whether or how these results can be used to describe systems in which direct electronic interactions dominate. The proper calculation of transport properties is important in the theory of superconductivity, since the measured resistivity and ac conductivity place constraints on the electron-pairing boson coupling strength and hence on \( T_c \) (see, for example, Ref. \( [13] \)).

Despite these difficulties, strongly wavevector-dependent pairing potentials have attracted a great deal of interest, especially within the context of spin-fluctuation-mediated interactions. Early work in this area was based on the Hubbard model treated in the random phase approximation \( [14] \). Current attention is centered around models of the cuprate superconductors, in which antiferromagnetic spin fluctuations have been shown to lead to d-wave pairing states \( [15,16,13] \). For the cuprates, calculations of \( T_c \) have been conducted in both weak- and strong-coupling Eliashberg formalisms and have used models fit to the dynamical susceptibility obtained from neutron scattering measurements \( [13] \), deduced from NMR data \( [15] \), or based on theoretical ideas regarding itinerant magnetism \( [16] \).
In all cases, the wavevector dependence of the pairing potential, which is assumed to be given by the dynamical susceptibility, is crucial to the existence of the superconducting phase; if the wavevector dependence is removed from these models, $T_c$ vanishes. The issues raised above regarding the applicability of Eliashberg theory to situations with strong momentum structure in the interaction are therefore extremely important here. For the case of antiferromagnetic spin-fluctuation-mediated interactions, work by Millis [17] has indicated that there may be a Migdal theorem which holds for this type of pairing mechanism, but this conclusion is controversial [18]. For the present purposes, we put aside reservations about Migdal’s theorem and transport constraints on the coupling constant in order to examine the effect of momentum structure on $T_c$ within the Eliashberg formalism. We do not directly answer the question of whether the $T_c$ computed in this formalism has anything to do with the physical transition temperatures.

To be specific, we will examine the ability of structure in the density of states and the pairing potential to enhance critical temperatures within Eliashberg theory. In order to accomplish this goal, we compute $T_c$ for pairing mediated by Einstein phonons and antiferromagnetic spin fluctuations using two approaches. The first employs the standard, Fermi-surface-restricted approximations to the Eliashberg theory, which assume a constant density of states and only include variation of the pairing potential around the Fermi surface [19,20]. The second solves the full Eliashberg equations at fixed band filling and therefore accounts for the energy-dependent density of states and the full wavevector dependence of the pairing potential. Since there is no wavevector dependence for the Einstein-phonon-mediated interaction, comparing the solution of the full Eliashberg equations to that of the Fermi-surface-restricted equations for these phonons illustrates the effect of an energy-dependent density of states on $T_c$. As noted above, the spin-fluctuation-mediated models have a strong wavevector dependence in addition to a variation in the density of states due to the band structure. Since we are unable to separate these two effects directly, we use the insights gained from the Einstein phonon calculation to extract the relative contribution of these structures to $T_c$ through a comparison of the solutions of the full and
Fermi-surface-restricted Eliashberg equations. For the models we consider, it is the density of states variation which provides the dominant influence on $T_c$.

**II. THEORY**

**A. The Eliashberg Equations**

We compute $T_c$ in the standard mean field formalism \[19,20\] in which the electron self-energy is solved self-consistently from the single-exchange graph. In light of the discussion in the Introduction regarding the validity of this approach for calculating $T_c$ in the cuprates, we reiterate that the critical temperatures obtained from this theory must not be taken too literally. Given this caveat, the equations for the electron self-energy in Matsubara space $\Sigma(k, i\omega_n)$ can be written in the Nambu matrix notation \[19\] as

$$\Sigma(k, i\omega_n) = -\frac{T}{N} \sum_{k' m} g^2 P(k - k', i\omega_n - i\omega_m) \tau_b G(k', i\omega_m) \tau_b$$

(1)

where $G(k, i\omega_n)$ is the electron Green’s function which satisfies the Dyson equation

$$G^{-1}(k, i\omega_n) = G_0^{-1}(k, i\omega_n) - \Sigma(k, i\omega_n)$$

(2)

and $G_0(k, i\omega_n)$ is the bare propagator. In these expressions, $N$ is the number of unit cells in the crystal, $T$ is the temperature, and $g^2 P$ is the pairing potential. $\tau_b$ is a Pauli matrix which corresponds to $\tau_3$ if the pairing interaction occurs through the density-density channel (e.g., Einstein phonons) and $\tau_0$ if the pairing occurs through the spin-spin channel (e.g., spin fluctuations). Throughout this paper, we set $\hbar = k_B = 1$. In solving these equations, we work at a fixed number of holes per site $n$, which is determined by

$$n = 1 + \frac{1}{N} \sum_{k n} e^{-i\omega_n 0^+} \text{Tr} [\tau_3 G(k, i\omega_n)].$$

(3)

We solve Eqs. (1) - (3) as a function of temperature to give $T_c$.

Recent work has shown that these equations can be solved directly on lattices of small size (32 x 32, 64 x 64) \[15,21\]. Alternatively, when momentum structure in the pairing potential...
can be ignored, as for Einstein phonons, these equations can be solved without discretizing the Brillouin zone \cite{4,5}. We have performed calculations for the Einstein phonons in the latter scheme and those for the spin fluctuations in the former; in the Einstein phonon case, the two schemes give the same critical temperatures.

Most of the calculations in this paper are done in the strong-coupling limit, where the effects of the modification of the normal-state propagator by the pairing interaction are included. For completeness, we also solve for $T_c$ in the weak-coupling limit, where the normal-state propagator is not renormalized; these solutions amount to solving the BCS equation with a retarded interaction.

In addition to employing the exact Eliashberg equations [Eqs. (1) - (3)] to compute $T_c$, we also use an approximate form of these equations in which all the wavevectors and energies are restricted to the Fermi surface. For the Einstein phonon case, these equations are the usual form of the strong-coupling Eliashberg equations \cite{19}; the equations used for the spin fluctuations have been described in an earlier publication \cite{13}. Throughout this paper, we will refer to the solution of Eqs. (1) - (3) as the exact Eliashberg solution, and we will refer to the solution of the approximate equations as the Fermi-surface-restricted solution.

**B. Model Interactions**

In order to solve Eqs. (1) - (3) in either the exact or Fermi-surface-restricted scheme, two ingredients are required: the pairing potential $g^2P$ and the band structure $\epsilon_k$. In this section we will discuss the model pairing potentials used in our calculations, paying particular attention to the spin-fluctuation-mediated interactions and comparing their spectral functions to the trends extracted from available neutron data. In the next section, we will describe the band structure.

In spin-fluctuation-mediated superconductors, the pairing potential is taken to be the magnetic susceptibility. We consider two models of this susceptibility taken from Ref. \cite{13} and Ref. \cite{15}, which will be referred to as the RULN and MMP models, respectively \cite{22,23}. 
The RULN model is a phenomenological fit to magnetic neutron scattering measurements on YBa$_2$Cu$_3$O$_{6.7}$ \[24\] and simultaneously provides a reasonable fit to the microscopic calculations of Ref. \[25\]. The de-oxygenated material is used in this model because there is, as yet, no consensus between different neutron scattering experiments regarding the behavior of the fully oxygenated system. Since the de-oxygenated material is nearer to the antiferromagnetic insulator than the fully oxygenated compound, we view the YBa$_2$Cu$_3$O$_{6.7}$ susceptibility, and hence the RULN model, as an overestimate of the strength of the spin fluctuations in YBa$_2$Cu$_3$O$_7$. As opposed to the RULN model, the MMP model for the dynamical susceptibility is inferred from NMR data in the YBa$_2$Cu$_3$O$_{7-\delta}$ family; details of this model may be found in Ref. \[26\].

The dependence of the spectral functions of these two model interactions on frequency, temperature, and wavevector are shown in Figs. 1 - 3. From Fig. 1(a), we see that the spectral function of the RULN pairing potential at the antiferromagnetic wavevector ($\pi, \pi$) has a peak in frequency around 30 meV at low temperatures which broadens and shifts to slightly larger frequencies at higher temperatures. For comparison, neutron scattering data \[27\] are shown in the inset to Fig. 1(b) and demonstrate that the experimentally measured spin fluctuation frequency is around 30 to 40 meV. This spin fluctuation frequency is found to be roughly constant or slightly decreasing with temperature. The corresponding plot for the MMP model is displayed in Fig. 1(b) and shows a similar temperature dependence of the peak frequency and peak width, but the magnitude of the peak frequency, roughly 5 to 10 meV, is smaller than that observed experimentally at ($\pi, \pi$). We note, however, that the spin fluctuation energy in the MMP model is strongly wavevector-dependent and can be as large at 1000 meV at the zone center at low temperatures \[28\].

The temperature dependence of these model interactions is compared in Fig. 2 and experimental data are presented in the inset to Fig. 2(b) \[29\]. We see that the spectral function of the RULN pairing potential shows a strong temperature dependence at high frequencies which disappears at lower frequencies, in agreement with the data. The MMP model has the opposite tendency. The low-temperature behavior of the two models is also
different: the MMP spectral function always exhibits a downward curvature for the parameters shown, but the low-temperature curvature of the RULN interaction changes sign at high frequencies.

Finally, we compare the wavevector-dependence of these models in Fig. 3 and include experimental data in the inset to Fig. 3(b) [29]. In both cases, the spectral function has maxima at the \((\pi, \pi)\) points of the first Brillouin zone. The RULN model displays a constant half-width of this maximum and an increasing peak height as a function of increasing frequency for the frequencies shown. The MMP model shows a weakly increasing half-width but a decreasing peak height as a function of increasing frequency. The measured full width at half-maximum \(\Delta q\) is approximately 0.2 r.l.u. for \(YBa_2Cu_3O_{6.7}\) and increases to roughly 0.3 r.l.u. in \(YBa_2Cu_3O_7\) [27]. In the MMP model at the latter stoichiometry, \(\Delta q\) is about a third of the experimental value; in the RULN model for \(YBa_2Cu_3O_{6.7}\), \(\Delta q\) is roughly 0.2 r.l.u.

Since the RULN model was constructed to describe the neutron scattering experiments, it is not at all surprising that it accounts for those measurements better than the MMP model, which evolved from fits to NMR data. If we now consider the results from NMR experiments, we see that the MMP model provides good fits to these results [30,26]. In contrast, the RULN model agrees with the Cu NMR relaxation rate but does not yield the form factor cancellations which are necessary to explain the observed Korringa behavior at the O sites in the fully oxygenated system. It may be inferred from the inset to Fig. 3(b) that there is considerable weight in the magnetic susceptibility away from \((\pi, \pi)\) in the de-oxygenated case, and this situation only intensifies as one moves towards \(YBa_2Cu_3O_7\). If one makes the standard assumption that the O nuclei relax via the same susceptibility as do the Cu, then it is difficult to reconcile this experimental fact with the perfect form factor cancellations used in interpreting NMR data. Thus, the inability of the RULN model to explain O site NMR measurements implies more about an inherent inconsistency between the neutron scattering and NMR results than about either model.

If these experiments are in conflict, then we must decide which experiment provides more
reliable constraints on the pairing potential. In order to extract the wavevector dependence of the magnetic susceptibility from NMR data, one must examine the form factors which are used to compute the relaxation rate. Neutron scattering, on the other hand, measures this structure directly. Additionally, the frequencies important for forming Cooper pairs are those probed by neutron scattering and not the low frequencies observed in NMR. Hence, it is reasonable to expect that any pairing mechanism involving spin fluctuations which purports to describe superconductivity in the cuprates must reproduce at least the qualitative features of the magnetic neutron scattering experiments.

Before proceeding, we note two commonalties in the two theoretical models. First, the order parameter arising from spin-fluctuation-mediated interactions with a spectral function peaked at the antiferromagnetic points of the Brillouin zone must have d-wave symmetry \[15,16,13\]. Second, we observe that the average frequency of the spin fluctuations is well within the range of phonon energies in the high-\(T_c\) cuprates (roughly 0 - 80 meV) near the \((\pi, \pi)\) point, where these pairing potentials are largest.

In addition to spin-fluctuation-mediated interactions, we also employ an Einstein-phonon-mediated interaction. The pairing potential in this case is simple; it has no wavevector dependence and the spectral function has a delta function peak at the phonon frequency \(\omega_0\). We choose \(\omega_0\) to be 35 meV in order to give the same energy scale as in neutron scattering experiments. Finally, we note that the resulting superconducting order parameter in this case is required to have s-wave symmetry.

When applying the model interactions discussed in this section, we should in principal use the measured transport properties to constrain the electron-pairing boson coupling constant as was done in Ref. \[13\]. We abandon this constraint here and use large coupling constants in order to obtain critical temperatures which are accessible to our numerical routines. Consequently, the computed critical temperatures are larger than what we view as realistic.
C. Band Structure

The electron energy dispersion we use is a two-dimensional, tight-binding band structure which is chosen to agree with local density approximation calculations and angle-resolved photoemission experiments where they are available. We work in the hole picture and write the dispersion as

$$\epsilon_k = -2t_1 [\cos k_x a + \cos k_y a + 2t \cos k_x a \cos k_y a] - \mu.$$ (4)

In this expression, we choose $t_1 = 80$ meV in order to agree with the measured plasma frequency in YBa$_2$Cu$_3$O$_{6.7}$ [13,31]. The parameter $t$ controls the Fermi surface rotation and is set to 0.45 to model the YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) family and to 0.00 in order to model the La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) family. In both cases, the chemical potential $\mu$ is determined from the constraint equation Eq. (3). We note that this band structure has a van Hove singularity in the bare density of states when $\mu = 4t_1 t$.

III. RESULTS AND DISCUSSION

A. Einstein Phonons

Having discussed the theoretical framework underlying our calculations, we now present our numerical results. In Fig. 4, we plot the $T_c$ of an Einstein-phonon-mediated superconductor as a function of the band filling. In this figure, we include the solutions to the strong-coupling Fermi-surface-restricted, strong-coupling exact, and weak-coupling exact equations for both the YBCO and LSCO band structures [32]. One sees immediately that the sharp peak in the Fermi-surface-restricted calculations caused by the van Hove singularity is completely removed when account is taken of the energy-dependent density of states by the exact solution of the Eliashberg equations. We emphasize that the Einstein phonon pairing potential has no wavevector dependence, so the difference between the Fermi-surface-restricted and exact critical temperatures is due entirely to the energy-dependent density of states.
Similar behavior has recently been observed by Penn and Cohen [33], who used an effective density of states smeared out by the inclusion of lifetime effects in a weak-coupling computation. Our results may be understood within the same context, but with $T_c$ playing the role of the lifetime; that is, the structure in the density of states is removed by thermal broadening. We also note that the weak-coupling exact calculation gives a stronger $T_c$ enhancement near the van Hove singularity than that produced from the strong-coupling calculation. Thus, the inelastic scattering due to the electron-pairing boson interaction acts with temperature to reduce the effect of sharp structure in the density of states on $T_c$.

Fig. 4 also illustrates that, for band fillings far from the van Hove singularity, the Fermi-surface-restricted and strong-coupling exact calculations give nearly the same $T_c$, indicating that the standard, Fermi-surface-restricted theory gives accurate results when there is no strong variation in the electronic density of states. Additionally, we observe that the critical temperature in the exact calculations goes to zero at the band edge (cf. Fig. 4(a)), as one expects when the number of charge carriers vanishes. The Fermi-surface-restricted $T_c$, however, produces an unphysical non-zero value at the band edge.

In attempting to evaluate the effect of the van Hove singularity on $T_c$, what one wishes to know is how the singularity affects $T_c$ compared to that of an energy-independent density of states. One can crudely estimate this flat density-of-states $T_c$ by looking for the average value of the Fermi-surface-restricted critical temperature in Fig. 4. This number can then be compared to the $T_c$ computed in the exact calculation at the band filling where the van Hove singularity is located. In this way, we estimate from Fig. 4(a) that an energy-independent density of states would give $T_c \approx 90$ K, whereas the exact calculation gives $T_c \approx 80$ K at the van Hove singularity. Similar numbers can be extracted from Fig. 4(b). On the basis of this analysis, we conclude that the van Hove singularity does not strongly enhance $T_c$ and may even suppress it, in disagreement with the work of Ref. [9]. This result supports a statement which appeared several years ago: $T_c$ alone does not provide a unique indicator of structure in the density of states, since it is determined only by a particular average of the density of states [5]. We also note that recent calculations of the interacting density of states above $T_c$
show that the van Hove singularity in the bare density of states is completely removed by interactions which are strong enough to yield critical temperatures greater than about 30 K [34]. These calculations are completely consistent with the featureless $T_c$ vs. band filling curves which we report here and strengthen our conclusion that van Hove singularities alone cannot explain the large critical temperatures of the cuprates.

B. Antiferromagnetic Spin Fluctuations

Turning now to spin-fluctuation-mediated pairing, we show in Fig. 5 the $T_c$ calculations using the RULN model [13] for both the YBCO and LSCO band structures [35]. As in the s-wave case, the sharp peak in $T_c$ due to the van Hove singularity in the Fermi-surface-restricted formalism is removed in the exact calculation. In contrast to the s-wave case, though, the Fermi-surface-restricted and exact $T_c$’s differ away from the van Hove singularity with the magnitude of the discrepancy depending on the band filling. In particular, we see that the exact Eliashberg $T_c$ is not necessarily larger than the Fermi-surface-restricted $T_c$. In interpreting this behavior, one must keep in mind that the spin fluctuation model has both wavevector dependence and energy variation in the density of states which influence the results. Comparing Fig. 5 to Fig. 4, where only density of states structure affects $T_c$, we see that the disappearance of the sharp van Hove feature in the exact calculation in Fig. 5 can be attributed to the inclusion of density of states variation in that scheme. On the other hand, the discrepancy between the exact and Fermi-surface-restricted Eliashberg $T_c$’s away from the van Hove singularity is most probably due to momentum structure in the pairing potential. Of the two effects, it is clear that the density of states plays the dominant role in causing the disagreement between the Fermi-surface-restricted and exact Eliashberg critical temperatures.

In Fig. 6, we plot $T_c$ vs. band filling for the MMP model [15] computed for the YBCO band structure [36]. We note that the qualitative features of the these curves are the same as those noted above for the RULN model. Hence, our results for spin-fluctuation-mediated
superconductors are not strongly model-dependent [37,38].

IV. CONCLUSIONS

To sum up, we have recovered the expected results that Fermi-surface-restricted calculations should be reliable when there is no sharp structure in the density of states, when momentum structure in the pairing potential is not critical, and when one is not near the band edge. More importantly, we can conclude that the proximity of the Fermi level to a van Hove singularity cannot substantially enhance $T_c$ in either s- or d-wave superconductors. When the energy dependence in the density of states and strong-coupling effects are properly taken into account, we find that the van Hove singularity produces a broad peak in $T_c$ as a function of band filling but does not increase $T_c$ markedly over the value computed from a structureless density of states. We also find that including the full wavevector dependence of the pairing potential over the entire Brillouin zone is important for computing d-wave transition temperatures in the Eliashberg formalism but that the influence of this structure off the Fermi surface on $T_c$ is less important than density-of-states effects. In other words, there is a discrepancy between the exact evaluation of the Eliashberg equations and the evaluation of the standard, Fermi-surface-restricted equations, but the discrepancy is not always large or positive and can be attributed mainly to the effects of a strongly energy-dependent density of states. Finally, we observe that these conclusions appear to be model-independent.

Our results for spin-fluctuations must be treated cautiously. As discussed in the Introduction, critical temperatures computed in the Eliashberg theory for strongly momentum-dependent interactions are not necessarily physical due to the neglect of vertex corrections. It is known in $^3$He that, although the ratio of the paramagnon energy to the Fermi energy is small, Migdal’s theorem still fails [39]. It is not clear whether a similar result holds for antiferromagnetic spin fluctuations (anti-paramagnons) in the cuprates; results have appeared in the literature which argue both points of view [L7, L8]. Additionally, BCS theory was built up from the supposition that only interactions near the Fermi surface are important.
for driving the superconducting instability. Whether or not this theoretical underpinning must be re-examined if the pairing potential is attractive over the entire zone has not been addressed. Therefore, we view the results of this paper pertaining to spin fluctuations and all related work in the literature thus far as preliminary.

ACKNOWLEDGMENTS

This work was supported by NSF-STC-9120000. HBS would also like to acknowledge financial support from NSF-DMR-8913878 and NSF-DMR-9215123 and computer support from the University of Georgia; MRN was supported by the U. S. Department of Energy, BES-Materials Sciences, under Contract #W-31-109-ENG-38.
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[32] For these calculations, the electron-phonon coupling constant $g^2$ is chosen to be 0.01 eV^2 for the strong-coupling calculations and 0.005 eV^2 for the weak-coupling calculation. Additionally, the Matsubara sum is cut-off at 500 meV, although the results are insensitive to the precise value of this cut-off.

[33] D. R. Penn and M. L. Cohen, Phys. Rev. B 46, 5466 (1992).

[34] J. Zhong and H.-B. Schüttler (to be published).

[35] The exact calculations are done on a 32 x 32 lattice with the Matsubara sum truncated after the lowest 254 Matsubara frequencies; the Fermi-surface-restricted $T_c$’s are computed with a Matsubara cut-off of 250 meV. The results presented are insensitive to the choice of these parameters.

[36] The exact calculations are done on a 32 x 32 lattice with the Matsubara sum truncated after the lowest 512 Matsubara frequencies; the Fermi-surface-restricted $T_c$’s are computed
with a Matsubara cut-off of 1000 meV. The results presented are insensitive to the choice of these parameters.

[37] We have also performed calculations of $T_c$ with this model when the imaginary part of the normal self-energy at a particular wavevector on the Fermi surface is fixed. This procedure is roughly equivalent to fixing the slope of the resistivity vs. temperature curve. At a band filling where the exact $T_c$ is larger than the Fermi-surface-restricted $T_c$ at fixed coupling constant, we find that the exact $T_c$ is lower than the Fermi-surface-restricted $T_c$ at fixed self-energy. This result suggests that the exact $T_c$ calculations may, when constraints from transport measurements are enforced, yield lower critical temperatures than the corresponding Fermi-surface-restricted calculations. Without a more systematic study, however, this conclusion remains speculative.

[38] By changing $Q$ in this model from $(\pi, \pi)$ to the incommensurate value $(\pi, 0.76\pi)$, we have found a suppression of the d-wave $T_c$ as was suggested in A. V. Chubukov, Phys. Rev. B 46, 5588 (1992), although the effect is only moderate (30 % for the one example we considered).

[39] J. A. Hertz et al., Solid State Commun. 18, 803 (1976).
FIGURES

FIG. 1. Spectral function \( \text{Im} \chi(Q, \omega) \) in arbitrary units as a function of frequency \( \omega \) in meV for (a) the RULN (Ref. [13]) and (b) the MMP (Ref. [15]) models of spin-fluctuation-mediated interactions \( \chi(q, \omega) \) in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\). The spectral functions are evaluated at the antiferromagnetic wavevector \( Q = (\pi, \pi) \) and temperatures \( T = 0 \) K (solid line), 100 K (long-dashed line), 200 K (short-dashed line), and 300 K (dot-dashed line). Inset to the second figure: experimental data from Ref. [27] of YBa\(_2\)Cu\(_3\)O\(_{6.6}\) at \( T = 100 \) K plotted as in the main figures.

FIG. 2. Spectral function \( \text{Im} \chi(Q, \omega) \) in arbitrary units as a function of temperature \( T \) in K for (a) the RULN (Ref. [13]) and (b) the MMP (Ref. [15]) models of spin-fluctuation-mediated interactions \( \chi(q, \omega) \) in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\). The spectral functions are evaluated at the antiferromagnetic wavevector \( Q = (\pi, \pi) \) and frequencies \( \omega = 10 \) meV (solid line), 20 meV (long-dashed line), and 30 meV (short-dashed line). Inset to the second figure: experimental data from Ref. [28] of YBa\(_2\)Cu\(_3\)O\(_{6.6}\) plotted as in the main figures for \( \omega = 5 \) meV (open circles), 8 meV (crossed boxes), 12 meV (solid circles), and 16 meV (open diamonds).

FIG. 3. Structure function \( S(q, \omega) = 2 \text{Im} \chi(q, \omega) / (1 - e^{-\omega/T}) \) in arbitrary units as a function of wavevector \( q = (k, k) \) in reciprocal lattice units for (a) the RULN (Ref. [13]) and (b) the MMP (Ref. [15]) models of spin-fluctuation-mediated interactions \( \chi(q, \omega) \) in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\). The spectral functions are evaluated at frequencies \( \omega = 10 \) meV (solid line), 20 meV (long-dashed line), and 30 meV (short-dashed line). Inset to the second figure: experimental data from Ref. [28] of YBa\(_2\)Cu\(_3\)O\(_{6.6}\) at \( T = 10 \) K and \( \omega = 8 \) meV plotted as in the main figures.
FIG. 4. Critical temperature $T_c$ in K vs. the number of holes per site $n$ in the two-dimensional, tight-binding band structure of Eq. (4) with $t_1 = 80$ meV and with (a) $t = 0.45$ to model the YBCO family and (b) $t = 0.00$ to model the LSCO family. The pairing boson is an Einstein phonon of frequency 35 meV. $T_c$ is computed in the strong-coupling exact (solid line), the weak-coupling exact (dot-dashed line), and the strong-coupling Fermi-surface-restricted Eliashberg schemes (dashed line). The sharp feature in the Fermi-surface-restricted calculation is the van Hove singularity. Note that the electron-phonon coupling constant in the weak-coupling calculation is half that used in the strong-coupling calculations and that the coupling constants, and hence the $T_c$’s, are not necessarily physical (see text).

FIG. 5. Critical temperature $T_c$ in K vs. the number of holes per site $n$ in the two-dimensional, tight-binding band structure of Eq. (4) with $t_1 = 80$ meV and with (a) $t = 0.45$ to model the YBCO family and (b) $t = 0.00$ to model the LSCO family. The pairing is mediated by spin-fluctuations as described in Ref. [13]. $T_c$ is computed both in the strong-coupling exact (solid line) and in the strong-coupling Fermi-surface-restricted schemes (dashed line). The sharp feature in the Fermi-surface-restricted calculations is the van Hove singularity. Note that the electron-spin fluctuation coupling constant, and hence the $T_c$’s, are not necessarily physical (see text).

FIG. 6. Critical temperature $T_c$ in K vs. the number of holes per site $n$ in the two-dimensional, tight-binding band structure of Eq. (4) with $t_1 = 250$ meV and with $t = 0.45$ to model the YBCO family. The pairing is mediated by spin-fluctuations as described in Ref. [15]. $T_c$ is computed both in the strong-coupling exact (solid line) and in the strong-coupling Fermi-surface-restricted schemes (dashed line). The sharp feature in the Fermi-surface-restricted calculations is the van Hove singularity.