Spin-phonon coupling and q-dependence of spin excitations and high-Tc superconductivity from band models

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Abstract

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Reference


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Spin-phonon coupling and $q$-dependence of spin excitations and high-$T_c$ superconductivity from band models

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Spin-phonon coupling (SPC) has been shown to be compatible with many unusual properties of the high-$T_c$ copper oxides. Parameters from ab initio band calculations for unit cells of La$_2$CuO$_4$ are used in a free-electron-like model in order to study the variation in coupling between spin waves and different phonons. Different SPC for different phonons can explain the "hour-glass" shape of the spin excitations. The model predicts larger $q$ vectors at less doping and rather complex isotope shifts. A link between the SPC parameters and the parameters for superconductivity is proposed. Also the pseudogap depends on the efficiency of SPC, and it will interfere with superconductivity at low doping. Different contributions to the coupling parameters are discussed. It is argued that $\lambda_{SPC}$ coming from the interaction between spin waves and O phonons can be strong enough to explain high $T_c$.

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I. INTRODUCTION

Several different families of high-$T_c$ copper oxides exist with varying $T_c$ but they have many things in common. They are layered structures, where one or several rather flat CuO planes are separated by heavier elements, with two-dimensional (2D) electronic properties and very little interaction perpendicular to the layers. Angular resolved photoemission confirms that the band structure agrees well with calculations, where each CuO layer gives rise to a dispersive band along the planes with a barrel-like Fermi surface (FS) (or a FS "arc" when displayed in 1/4 of the Brillouin zone). The Cu $d$ states are the dominant electron states at the Fermi energy, $E_F$. The FS arc is not complete at low temperature, $T$, when it can only be observed in the diagonal direction ($k_x=k_y$). Many measurements have revealed the existence of complex superstructures and pseudogaps surrounding $E_F$ up to a temperature $T^*$, which is higher than $T_c$ in underdoped systems. Phonons are closely interacting with the electronic states, as shown by the softening of some phonon branches at certain dopings, by isotope effects on $T^*$, and on the width of the gap. Stripe-like regions with excitations of charge and spin modulations are seen in neutron-scattering experiments. Noncommensurate $q$-dependent spin excitations deviate from the (0.5,0.5) point and move linearly with doping up to a saturation at $x \approx 0.12$. Recent measurements on several cuprates reveal local-moment fluctuations and the underlying spin excitations have a characteristic "hour-glass-shaped" $(q, \omega)$ dispersion even at nonsuperconducting compositions.

Coupling between phonons and charge transfers as well as between phonon and spin waves has been proposed in relation to phonon softening and the mechanism for superconductivity. $Ab$ initio band calculations for supercells containing one-dimensional (1D) phonon and spin-wave modulations in the CuO bond direction ([1,0,0]) show large spin-phonon coupling (SPC) within the CuO plane. This means that an antiferromagnetic (AFM) wave of the correct wavelength and phase is stronger when it coexists with the phonon. These results, in combination with 2D nearly-free-electron (NFE)-like bands, have been used for modeling of many normal-state properties of the high-$T_c$ materials. Phonon softening, dynamical stripes, correlation between $q$ and $x$, smearing of the nondiagonal part of the FS, and abrupt disappearance of the spin fluctuations at a certain $T^*$ are possible consequences of SPC within a rather conventional band.

Here, it is suggested that the characteristic spin dispersion can be understood in terms of SPC and that phonons promote a large $\lambda_S$ for spin fluctuations, and therefore SPC is important for the mechanism of superconductivity. The calculations consider SPC between spin waves and four different types of phonon distortions.

Section II describes the band calculations and how the resulting parameters for SPC are used in the NFE model. In Sec. III there is a discussion of the results for the spin excitations with comparisons to experiments. Section IV presents a connection between the parameters for SPC and the mechanisms for superconductivity.

II. BAND CALCULATIONS

$Ab$ initio band calculations are made for long supercells of La$_{2-x}$Ba$_x$CuO$_4$ (LBCO), oriented along the CuO bond direction, where the virtual-crystal approximation (VCA) is applied to La sites to account for the doping. The calculations use the linear muffin-tin orbital (LMTO) method in the local spin-density approximation (LSDA), as has been described previously. It is necessary to know the distortion amplitudes for the atoms ($\mu$, the distance from the equilibrium position) and the size of Cu moments ($m$) when calculations are made for phonons and spin waves, respectively. They can in principle be calculated in LSDA, but it is convenient to derive these quantities from experimental data. Measured and calculated phonon frequencies for zone-boundary phonons for YBa$_2$Cu$_3$O$_7$ (YBCO) agree well. Such values are also indicative for typical $h\omega$ for each atomic character of the phonon density of states (DOS) in other copper oxides. Phonon energies and partial phonon DOS for each site $i$, calculated by Chen and Callaway for

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Nd$_2$CuO$_4$ (NBCO), can be assumed to be representative for LBCO. From those results and measurements it can be deduced that the main La modes are at 10–20 meV, Cu at 20–30 meV, planar O near 50 ± 20 meV, and apical O at 60 ± 15 meV. The reduction in the partial phonon DOS into single constants $C_i$ from the figures in Ref. 29, shown in the last part of Table I, might seem to be subjective, but the qualitative results of the spin excitations will not depend on fine details of the phonon DOS. The force constants $K_{ij}$ are accessible in calculations as $K_{ij} = d^2E/du_i^2$, where $E$ is the total energy, or experimentally from the vibration frequency of a mass $M_i$, $K_{ii} = M_i\omega_i^2$. Here they are defined from the site-dependent phonon energies, $\hbar\omega_i$, calculated for NBCO through the relations between $\omega$ and $K_{ii}$ for not too low $T$,

$$K_{ii} = M_{eff}i\omega_i^2$$

and

$$u_i^2 = 3\kappa_i T / K_{ii},$$

where the effective mass is given by $1/M_{eff} = \sum_i C_i / M_i$. The resulting $u/a_0$, where $a_0$ is the lattice constant, shown in Table I for $T \approx 120 \text{ K}$ (near $T_c$ and $T'$), compare well with experiment.\textsuperscript{30} The force constants for other high-$T_c$ cuprates, such as YBa$_2$Cu$_3$O$_7$, are not very different.\textsuperscript{25,26}

An analogous description of the magnetic counterparts gives $K_{m} = d^2E/ dm^2$ and $m^2 = k_B T / K_{m}$. Calculations for a short wave in HgBa$_2$CuO$_4$ (HBCO) resulted in magnetic moments on Cu of about $\sim 0.1 \mu_B$.\textsuperscript{22} Moments of about 0.1–0.15 $\mu_B$/Cu are obtained for LBCO if an AFM field of $\pm5$ mRy is applied on Cu sites in calculations for a cell of length $8a_0$, see Table I. The moments are larger for longer cells, in agreement with moments found within CuO layers in recent NMR measurements.\textsuperscript{31} The \textit{ab initio} calculations in HBCO show that $K_m$ is sensitive to structural modifications, doping, and details of the LSDA scheme.\textsuperscript{32} The exact values of $K_m$ are not used in calculations here, but later it is assumed that they are small compared to the value of phonon force constant.

The calculated results for the maximal potential shifts ($V_q^p$ on Cu) caused by phonons and by spin waves ($V_q^m$ in the spin-polarized potential) for the four types of movements in the cell are shown in Table I, together with the result for $V_q^m$ without phonons. These calculations consider distortions (and coexisting AFM spin waves) in cells extending $8d_0$ along $\bar{x}$, with displacements of La and apical O along $\bar{z}$, and Cu and planar O along $\bar{x}$. For the latter phonon there is a positive SPC when the nodes of the AFM waves are located at the “compressed” Cu sites (between the O atoms moving toward the Cu). Optimal SPC for displacements of out-of-plane atoms (La and apical O) occurs when these atoms move toward the CuO plane near the region of the AFM node. A modulation of apical O with the opposite phase will reduce $V_q^m$ from 10 to below 8 mRy.

The LMTO results for a wave of length $8a_0$ are made for $k_BT \sim 10$ meV. Longer waves (for $x$ closer to optimal doping) will have larger $m$ at this temperature and correspond to about 0.2 $\mu_B$/Cu when the spins are coupled to plane-O modes. A Cu mode or involvement of no phonon would stir up about half as large moments at this temperature. Note that the matrix elements in $\lambda$’s (see later) are made in the harmonic approximation, where the ratios between energy shifts and the amplitudes of the perturbations are constant.

The LMTO results calculated for waves of length $8a_0$ are rescaled to be valid for the longer waves at doping $x = 0.17$ (12–13 $d_0$ in the model calculation) when $V_q^p$ and $V_q^m$ are larger by factors of $\sim 1.1$ and $\sim 1.5$, respectively, see Ref. 24. The total $V_q$ can be summarized as

$$V_q = \sum_i \left( 1.1V_q^p + 1.5V_q^m \right) C_i,$$

where $i$ is the site index. The resulting $V_q^p$ are 17, 18, 23, and 22 mRy at the energies centered around 17 (La), 27 (Cu), 48 (plane O), and 58 mRy (apical O), respectively.

A calculation is also made for lower doping $x = 0.11$ when the wavelengths are longer and $V_q$ are larger. Precise \textit{ab initio} values are difficult to obtain because the requirement of long unit cells ($16a_0$ or more) makes the self-consistent convergence very tedious. By simple extrapolation and the use

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**Table I.** The four first lines: phonon distortion amplitudes, $u/a_0$, maximum $m(\mu_B)$, induced potential shifts, $V_q^p$ (mRy), and exchange splitting, $V_q^m$ (mRy) caused by spin waves ($\mu_B H = \pm 5$ mRy). All shifts/splittings refer to the maximal value on a Cu site, and they are determined in self-consistent LMTO calculations for supercells of length $8a_0$. Remaining lines: the partial characters of the phonon DOS, $N_i$, for different sites, $i$, as estimated from Ref. 29.

| Wave | No phonon | pl-O$_x$ | La$_x$ | ap-O$_z$ | Cu$_z$
<table>
<thead>
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<td>0.021</td>
<td>0.013</td>
<td>0.020</td>
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<tr>
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<td>0.12</td>
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<td>5</td>
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<tr>
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<td>12.5</td>
<td>12</td>
<td>10</td>
<td>8.5</td>
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<td>0.0</td>
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<td>$N_{ap-O}$</td>
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<tr>
<td>$N_{Cu}$</td>
<td>0.2</td>
<td>0.2</td>
<td>0.0</td>
<td>0.6</td>
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</table>

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of the NFE model one can estimate that $V^p_q$ are typically 40\% larger at $x=0.11$. The spin part ($V^\alpha_q$) is likely to grow faster as AFM stability approaches as $x \to 0$ and even more so for the waves which already have a large spin contribution such as the plane-O modes. The simple estimate with an overall increase of 40\% makes $V^p_q$ about 32, 31, 25, 23, and 12 mRy for ap-O, pl-O, Cu, La/Ba, and no phonon, respectively. As discussed later, spin waves at higher energy are not much dependent on phonons, and here it is assumed that $V^\alpha_q=0$.

In a second step we use the parameters $V^p_q$ in a 2D-NFE model.\textsuperscript{24} The AFM spin arrangement on neighboring Cu along $[1,0,0]$ in undoped LBCO corresponds to a potential perturbation, $V(\vec{x})=V^p_q \exp(-i\vec{Q} \cdot \vec{x})$ (and equivalently with $\vec{y}$ along $[0,1,0]$). The periodicity in real space is defined through the Cu-Cu distance, and a gap of size $2V^p_q$ appears at the zone boundary, at $\vec{Q}/2$. A further modulation ($\vec{q}$) of this order into 1D stripes perpendicular to $\vec{x}$ (or “checkerboards” in two dimensions along $\vec{x}$ and $\vec{y}$) is achieved by a multiplication of the potential by $\exp(i\vec{q} \cdot \vec{x})$, where $\vec{q} < \vec{Q}$. Totally, this makes $V(\vec{x})=V^p_q \exp(-i\vec{Q} \cdot \vec{x})$, where $\vec{Q}=\vec{Q}-\vec{q}$. The periodicity of this potential is now larger, and the gap moves away from $\vec{Q}/2$ to $(\vec{Q}-\vec{q})/2$. Magnetic side spots from the modulations would appear at $\vec{q}/2$ surrounding $\vec{Q}/2$. The main spots are caused by the underlying near-neighbor AFM correlation. A $3 \times 3$ eigenvalue problem with matrix elements $H_{11}=E-k_{\perp}^2-k_{\parallel}^2$, $H_{22}=E-(k_{x}-Q_{x})^2-k_{\parallel}^2$, $H_{33}=E-k_{\perp}^2-(k_{y}-Q_{y})^2$, $H_{12}=H_{13}=V^p_q$, and $H_{23}=0$ is solved. The effective mass of the NFE band is chosen so that the bandwidth from $\Gamma$ to the $M$ point is 0.3 Ry (when $V^\alpha_q=0$). This makes the band dispersion near $E_F$ quite close to the real band, and the NFE band is sufficient to demonstrate the effects of SPC. The model is entirely 2D (the DOS is constructed from a sum over all states in the plane), which is reasonable in view of the very small band dispersion along $k_{\parallel}$ of real band structures for the cuprates.\textsuperscript{18}

III. SPIN EXCITATIONS

An important result of the 2D-NFE model is that it leads to a correlation between doping and the amplitude of $V^p_q$.\textsuperscript{24} The reason is that the gap opens along $(k_{x},0)$ and $(0,k_{y})$ but not in the diagonal direction. Therefore, the dip in the total DOS (at which $E_F$ should fall for optimal doping) will not appear at the same energy for small and large $V_q$ even if the $q$ vector is the same. But it could reappear at $\vec{E}_F$ if the $q$ vector is allowed to change. This is why $\vec{q}$ will be different for different modes. The parameters in the calculations at 0.17 holes per Cu (which is close to $x$ in Ref. 14) are summarized in Table I. The total $V^p_q$ are obtained from Eq. (1). The calculations at $x=0.11$ (closer to the doping in Ref. 14) are based on larger $V^p_q$’s, as explained above.

The results are shown in Fig. 1 together with experimental data from Refs. 14 and 15. The spectra are shaped like an hour glass with a “waist” at intermediate energy, which in the SPC model is because the strength of $V^p_q$ differs with energy (no SPC would make $\vec{q}$ equal for all energies). The points below 70 meV are for the coupling to the four types of phonons. The general shape of the $q-\omega$ dependence and the amplitudes of $q$ are similar as in the measurements, with the smallest $q$ at about 0.05 for SPC dominated by O $p$ phonons around 50 meV. The weaker SPC for La at low energy makes

![Diagram](image-url)
TABLE II. Magnetic moments (m, μj/Cu) for two AFM spin waves along the [1,1,0] direction calculated for two unit-cell lengths with and without phonon distortions. Distortion amplitudes and magnetic fields as in Table I.

<table>
<thead>
<tr>
<th>Wavelength</th>
<th>No phonon</th>
<th>pl-Ox</th>
<th>La,</th>
<th>ap-Ox</th>
<th>Cu,</th>
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<td>8√2a0</td>
<td>0.09</td>
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<td>0.18</td>
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<tr>
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<td>0.09</td>
<td>0.08</td>
<td>0.08</td>
<td>0.07</td>
</tr>
</tbody>
</table>

$q$ larger. The calculated results depend on the different parameters in the NFE model, so that a larger band mass leads to smaller amplitudes of $q$. If no mixing of the phonon modes (through the $C_i$ coefficients) was made, it would increase the variations in $q$, even though the general hour-glass shape would remain.

Spin waves and phonons of the same frequency and $q$ vector are closely connected for an optimal mechanism of SPC. Spin waves with higher frequency than the phonons cannot profit from this mechanism. Here it is assumed that spin waves with frequencies higher than the phonon frequencies are independent of lattice vibrations, whereby $V_{q}=0$. This “phonon-independent” result is put rather arbitrarily at a $q$ vanishing spin wave. The two vectors, 0.13, is comparable to the wavelength in the presence of La/Ba along $z$ of $\La_{2−x}\Sr_{x}\CuO_{4}$, the energy spin excitations. As has been shown, slow movements of LaBa along $z$ lead to stronger spin waves. It can be imagined that rapid spin fluctuations, with different $q$ vectors than that of the phonon, can be enhanced during the slow movement of the atoms. The details of such a mechanism are complicated and will not be investigated here. But it is not excluded that phonons will have some effects on spin waves also at high energy through a mechanism of indirect coupling.

Less doping will make the waves longer and the waist in the $\vec{q}−\hbar\omega$ diagram becomes narrower. The results for $x$ =0.11 are shown by the open circles in Fig. 1. The band mass and the phonon energies are assumed to be the same as for $x=0.17$. The narrowing is relatively prominent for the O modes where the $V_q$ are largest. But some narrowings are noticed for all points even at the highest $E$ where spin waves are excited without direct coupling to phonons. Smaller $q$ vectors at less doping are in agreement with observations in LBCO for $x=1/8$, although the shifts are smaller than what is measured, see Fig. 1. Very small $q$ vectors have been observed recently in lightly doped La$_{1.96}$Sr$_{0.04}$CuO$_4$, but the spin modulation has turned from the parallel (the Cu-O bond) to the diagonal direction at this very low doping. Calculations for waves with $q$ vectors along [1,1,0] cannot consider sufficiently long wavelengths to correspond to the low doping, but the results for short waves show that $V_q$ for movements of oxygen atoms are larger than for movements of Cu. The magnetic moments on Cu for cells of lengths 8√2a$_0$ and 4√2a$_0$ along [1,1,0] are shown in Table II. The directions and the amplitudes of the distortions are as for the case with the $q$ vectors along [1,0,0] (i.e., the distortions are no longer parallel to $\vec{q}$ for the plane-O and Cu modes). The plane-O mode has large AFM moment fluctuations, as for $\vec{q}$ along [1,0,0], but other modes have grown in importance compared to modulations along [1,0,0]. This is consistent with the observation by Matsuda et al. of a much narrower low-energy part (in the range 15–20 meV) of the spin-excitation spectrum for very low-doped ($x=0.04–0.05$) La$_{2−x}$Sr$_x$CuO$_4$. The correlation between strength of the SPC and wavelength is also evident in the results for modulation along the diagonal, as is shown in Table II by the consistently smaller $m$ for the shortest cell.

According to the mechanism of SPC there is a possibility for increased AFM moment fluctuations at large $T$ where the amplitude of $u$ is increased. But the Fermi-Dirac occupation will catch up with this process and $m$ will go down quickly near $T_\nu$. This can lead to a narrower spin-excitation spectrum for increasing $T$ before the disappearance of clear spin waves near $T_\nu$. A quite strong tendency for shorter $q$ vectors for increasing $T$ was reported by Matsuda et al. at low energy and low doping. This appears to be stronger than the expected variation in SPC, but on the other hand, an extreme sensitivity is expected when the exchange enhancement diverges at such low doping. The exact behavior for $T$ closer to $T_\nu$ is hard to predict because of the rapid weakening of the spin waves in that $T$ range.

Isotope shifts on the spin excitations have been proposed, but no significant shift of energy due to exchange of O isotopes ($O^{16}→O^{18}$) has been observed in LSCO. This may seem surprising in view of the model for strong SPC if the phonon frequency $\omega=\hbarM^{−1/2}$. However, many intervened dependencies make isotope shifts compli-
cated here. For instance, the force constant for vibrations depend on several atoms and the use of an effective mass instead of the mass of one type of atoms will attenuate isotope shifts. Furthermore, heavier O isotopes should not only decrease the frequencies for the phonons and the coupled spin waves but they should also decrease $u$. At low temperature $u \sim M^{-1/4}$, which in the model for SPC will make $V_q^p$ smaller. This implies two things. First, since SPC also predicts a sizeable phonon softening (by 15%–20%) (Ref. 23), there will be less softening for a heavy isotope when $u$ is smaller, so that the downward isotope shift of $\omega$ is reduced. Second, smaller $u$ and $V_q^p$ will move the pseudogap toward lower energy, away from $E_F$. The SPC at the original $q$ will no longer be supported if the gap is not at $E_F$, but other shorter $q$ vectors will move in and restore a pseudogap at $E_F$ (it is assumed that the doping is unchanged by isotope shifts.) Since SPC is a bit weaker for shorter waves, it will again renormalize $V_q^p$, $q$, and $u$ to lower values, and in the end there will be less phonon softening. This is a complicated self-consistent process and a quantitative prediction of the total reduction will be uncertain, but all effects tend to reduce the original isotope shift.

The possibility of indirect SPC may cause even more complicated isotope shifts, especially for changes in the heavy La/Ba atoms. The associated phonon frequencies are low, and the promotion of fast spin waves can be reduced if the distortion amplitudes of La/Ba are reduced through the change in isotopes. The high-energy excitations show little structure and evidence of isotope shifts from indirect SPC might be seen in the linewidths more than in the $q-\omega$ characteristics.

### IV. SUPERCONDUCTIVITY

Undoped cuprates are generally stable AFM insulators. The exchange enhancement for spin waves in doped cuprates is moderately large in the absence of phonons, and as has been shown, it becomes peaked by the interaction with phonon distortions, especially at low doping. This unusual mechanism can be translated into a large spin-polarized contribution to the phonon deformation potential, which therefore has to be associated with $\lambda_u$ for AFM spin fluctuations. This can work in two ways. Many phonon modes are excited at a certain $T_c$ and a spin fluctuation can profit from the SPC to the available modes. A calculation of $\lambda_u$ can in this case be done without the phonon excitation but with the lattice distortion taken into account. The second mechanism is when the virtual excitations involve the phonon and the spin fluctuation together. The coupling constant for such a process, denoted by $\lambda_{\text{SPC}}$, is estimated later from the change in spin-polarized potential when an atom is displaced by $\Delta u$. A third coupling constant, $\lambda_{\text{coul}}$, is for conventional electron-phonon coupling. It turns out that the ingredients for all of these coupling constants are related to the same $V_q^p$ parameters for phonons and spin excitations as determined above. Thus, there is a link between the key parameters for spin excitations and theories for superconductivity. For instance, $\langle V_q^p \rangle$ corresponds to the monopolar matrix element in electron-phonon coupling, $\lambda_{\text{ph}}$. The good agreement between the calculated spin excitations and experiment suggests that the calculated $V_q^p$’s are of the correct order. Thus, on the basis of the band results obtained above, we consider contributions from pure phonons, from spin fluctuations coupled to phonons, and from independent spin fluctuations in estimations of $\lambda$ and $T_c$

Assume first that $T_c$ depends exclusively on (harmonic) phonons without SPC. The rigid muffin-tin approximation (RMTA) leads to a simple estimate of $\lambda = N \lambda_u^2 K_{\text{av}}$, where $N$ is the DOS at $E_F$ and $I_u$ is the dipolar matrix element for the deformation potential,

$$I_u = \int \Psi^*(r) dV(r)/dr\Psi(r) d^3r = \langle dV/\text{dr} \rangle$$

where the last simplification is done if $\Delta V(r)$ is nearly constant within the contributing volume, i.e., for a rigid shift of the potential within one Cu. This matrix element is the first-order change in the energy at $E_F$, which in the NFE model is equivalent to $\langle V_q^p / \Delta u \rangle$. With $N \approx 0.9 (\text{eV Cu spin})^{-1}$ from the DOS near optimal doping (when the pseudogap is not much developed), $\Delta V^p$ from Table I, the $K$ values from Table III, and with $a_0 = 3.78$ Å, this makes an average (averaged over the number of sites per cell) of $\lambda_{\text{ph}} \approx 0.36$. The plane-O phonon alone would make $\lambda_{\text{ph}} \approx 1.12$. This is in qualitative agreement with a recent calculation of the total (Brillouin zone averaged) $\lambda_{\text{ph}}$ for LSCO of 0.4 where the electron-phonon matrix elements are “by far the largest” for the breathing modes, which corresponds to the plane-O mode here. A similar calculation for YBCO gives an even smaller total $\lambda_{\text{ph}} \approx 0.2$. The conclusion of these two works

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<th>pl-O$_{\text{c}}$</th>
<th>La$_{\text{c}}$</th>
<th>ap-O$_{\text{c}}$</th>
<th>Cu$_{\text{c}}$</th>
<th>Average</th>
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</tbody>
</table>
Next we consider spin fluctuations induced by phonons through SPC. Phonons are emitted and absorbed by the electrons as before but with the difference that the change in potential is now in the spin-polarized part. Such deformation potentials can be much larger than the conventional nonpolarized deformation potential for a system such as this since AFM fluctuations are strong at underdoping. Probably AFM order could even be stable if the lattice distortions were static and large. In contrast, AFM fluctuations would be rather weak in the absence phonons, in particular at overdoping. The spin-polarized $\Delta V^m(r)$ is essentially monopolar for modulations with long wavelengths with contributions mainly coming from Cu sites and is of the same order as $\Delta V^p$ for O modes (see Table I). The SPC analog to $\lambda_{ab}$ can be estimated on the same level of approximation, $\lambda_{SPC} = N^2_{ph} \langle \Delta V^p \rangle / K_{SPC}$, where $I_m = \langle \Delta V^m(r)/\Delta u \rangle = V^m_q/\Delta u$. (6)

The quantity $\Delta V^m/\Delta u$ is constant in the harmonic approximation and can be estimated from the results shown in the tables. For instance, for the plane-O mode at 120 $\mathrm{K}$, $u$ is 0.014 $\mathrm{Å}$, $m$ is about 0.15 $\mu_B$/Cu, and $V_m \approx 13 \mathrm{mRy}$. The force constants $K_{SPC}$ should be modified so that the total energy in $d^2E/du^2$ includes also the energy needed to create the spin wave ($K_m$). This is difficult to calculate because the total energy for spin fluctuations goes to zero near the singular point for diverging exchange enhancement, i.e., exactly for the interesting case of SPC. But some experimental facts are useful. For example, phonons in the energy range of oxygen modes can be $\approx 20\%$ softer in the doped high-$T_c$ materials. This is an indication of a negative $K_m$. Phonon softening and a negative contribution from $K_m$ have been estimated for a coexisting phonon and spin wave. By assuming zero energy from the spin wave for all modes ($K_m = 0$), this gives $\lambda_{SPC} \approx 0.6$ (and $T_c \approx 95 \mathrm{K}$ in BCS). The results are summarized in Table III. The contribution from different modes are not so different as in the case with $\lambda_{ph}$, but plane-O is still strongest. If no phonon softening exists for La and Cu modes, then $K_m$ could be positive and perhaps large for such modes. If, in an extreme case, it is assumed that La and Cu modes have $K_m \gg 0$, so that such modes give zero contribution to $\lambda_{SPC}$, then $\lambda_{SPC}$ will be reduced to 0.35.

The third possibility, a pure $\lambda_{sf}$ without simultaneous excitations of phonons, (but calculated for lattices with phonon distortions), should be available from

$$
\lambda_{sf} = N(dV_m/dm)^2/K_m.
$$

(7)

The matrix element in the numerator $dV_m/dm$ can be large near the AFM instability. It can increase with $T$ because of the increasing distortion amplitudes of the existing phonons up to $T = T_c$. As was noted before, $K_m$ is small for O distortions, and it will go down for increasing $u(T)$. But $K_m$ is difficult to calculate, and corrections to the LSDA are needed. Therefore, no calculated values of $\lambda_{sf}$ for LBCO are presented here. A calculation including LSDA corrections for the shortest possible wave in HBCO with half-breathing distortions led to $K_m \approx 0.7 \mathrm{eV}/\mu_B$ (i.e., no phonon softening) and a $\lambda_{sf}$ of about 0.5.

Clearly, these estimates are very approximate and should not be used for quantitative conclusions. But the point is that the order of magnitude is large enough for being interesting for high $T_c$. It is not clear if the total $\lambda$ can be a combination of the three different mechanisms. However, the spin enhancement is sensitive to doping and it is likely that $\lambda_{SPC}$ and $\lambda_{sf}$ increase faster than $\lambda_{ph}$ when the doping goes down. Many other facts suggest that $\lambda_{SPC}$ could be larger. For instance, in addition to being larger for longer waves at less doping, it can also increase because of larger $u$ through a “feedback” mechanism from SPC. The calculations are made for pure modes with one atom at the time, while hybridization in real phonons could make the deformation potentials stronger. Finally, as was indicated, probable corrections to LSDA are needed for realistic values. Such corrections tend to increase the exchange enhancement for AFM fluctuations.

The SPC and spin fluctuations become very large at underdoping when the wave modulations are longest, so $N$ (and $\lambda$) are reduced because of the pseudogap, and hence the pseudogap competes with superconductivity. Other reasons for competition between superconductivity and pseudogap have been proposed. On the overdoped side $\lambda$ is reduced because of a smaller $\Delta V$, and $T_c \rightarrow 0$. Another reason for vanishing $T_c$ at larger doping is that the wavelength for phonons and SPC will be too short to fit within the lattice. In addition, signs of weak ferromagnetic order have been seen in calculations for LBCO with clustering of dopants. The different limitations at extreme dopings leave out a range of intermediate doping for optimal conditions for large $\lambda$’s and high $T_c$.

V. CONCLUSION

These calculations suggest that the hour-glass-shaped dispersion of the spin-wave spectrum is a consequence of different degrees of SPC for different phonon modes. The “half-breathing” O-mode in the midpart of the phonon spectrum is found to be the most efficient one, which explains the waist in the spin-wave dispersion. The amplitude of the $q$ vectors agree reasonably with experiments, which means that the amplitude of the parameters in the NFE model is of the correct order. These parameters are derived from results of ab initio calculations, but many assumptions and approximations are made. On the other hand, if the SPC-NFE model were used to fit the experimental data, it would give $V_q$ parameters not too far from what is shown here. Moreover, other normal-state properties fit surprisingly well with the SPC-NFE simulation based on these parameters. Therefore, since it can be argued that the parameters are closely related to parameters for electron-phonon coupling and spin fluctu-
tions, there is a possible link between spin excitations and superconductivity. One important fact is that spin fluctuations may become peaked through the interaction with phonons, in particular at low doping. This makes spin fluctuations largely responsible for the pseudogap at low doping but also for the mechanism of superconductivity. The parameters for SPC are sufficiently large for high $T_c$ at intermediate doping when the pseudogap is not much developed. Isotope effects will normally show up in both frequency and $q$ dependencies, but many coincidences in the mechanism for SPC make them much reduced. There is no reason why they should cancel exactly, and it would be useful to pursue precise experiments where fine effects from phonons and isotope shifts can be seen in spin excitations.

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