Spin-Phonon Coupling in High-\(T_C\) Copper Oxides.

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Abstract. Band calculations on HgBa\(_2\)CuO\(_4\) and La\(_{2-x}\)Sr\(_x\)CuO\(_4\) with phonon and spin-waves within the CuO planes show that partial gaps are created at various energies depending on wavelengths. Spin and phonon gaps appear at different energies when the modulations are along \([1,1,0]\), while they are at the same energy for modulations along \([1,0,0]\). It is shown that the ability to form gaps and antiferromagnetic waves is correlated with the strength of the interaction parameter \(\lambda_{sf}\) for spin fluctuations. Many unusual properties of the high-\(T_C\) oxides can be understood from spin-phonon coupling.

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INTRODUCTION

Properties of high-\(T_C\) superconductors have been seen to depend both on phonons \([1,2]\) and magnetic fluctuations \([3,4]\). Therefore it is expected that the mechanism for high-\(T_C\) superconductivity should involve phonons as well as magnetic fluctuations. Here, band results show that spin-phonon coupling (SPC) is important and many results are compatible with observations.

Band calculations on the high-\(T_C\) cuprates HgBa\(_2\)CuO\(_4\) and La\(_{2-x}\)Sr\(_x\)CuO\(_4\) show that gaps or pseudo gaps appear near the Fermi energy, \(E_F\), when the potential has a modulation within the CuO-plane \([5]\). The calculations are made for long unit cells oriented either along \([1,1,0]\) or \([1,0,0]\) containing so-called half-breathing (bond-stretching) phonons. The planar O-atoms on both sides of a Cu-atom are alternatively displaced towards ("compressed") or away from the Cu ("diluted"). Calculations with anti-ferromagnetic (AFM) field on the Cu atoms are made to model spin-waves. When the calculations are made for co-existing phonon and spin waves, it turns out that the magnetic moments are largest on the "diluted" Cu-sites. The nodes of modulated spin waves coincide with "compressed" Cu-sites. The phonon mode creates a potential modulation of the CuO plane \([5]\). Spin waves induce a modulation in the spin-polarized part of the potential and magnetic moments on the Cu. Gaps appear at different energies depending on the wave length of the modulation. The gain in kinetic energy is maximized when the gap is at \(E_F\). The position of \(E_F\) is controlled by doping (calculations use the virtual crystal approximation). The wavelength of the spin wave is twice that of the phonon, because the spin can be up or down at "diluted" Cu-positions. Hence, for modulations along \([1,1,0]\), the band structure has two gaps, one due to the phonon and one at a higher energy because of the spin wave, and there is no direct SPC for electrons at \(E_F\). However, for modulations along \([1,0,0]\) one realizes that two rows of CuO are required along the unit cell, so that the phase of the spin wave along each row will differ by \(\pi\). The band results show in this case a constructive SPC, where the gap from separate phonon and AFM-modulations will open a gap at the same energy, i.e., at \(E_F\) for the correct doping. In addition, a phonon with large atomic displacements will increase the moments of the spin wave, and both waves contribute to a common gap.

The abovementioned results can be found in refs, \([5,7]\), where it also is shown that a small correction to the band structure (which affects the potential and the localization) will stabilize a gapped AFM state instead of the metallic non-magnetic state for the undoped system. The same correction will increase the mass enhancement from spin fluctuations in doped cases \([7]\).

RESULTS AND DISCUSSION

The calculated density of states (DOS) at \(E_F\), \(N \approx 1.5(Cu \cdot eV)^{-1}\). The atomic displacement \(u^2 = 1.5\hbar\omega/K\) at low \(T\) and \(u^2 = 3k_BT/K\) at high \(T\) (relative to the Debye temperature). The force constant \(K = 25\ eV/Å^2\) for a typical O phonon with \(\hbar\omega \sim 80\ meV\) makes \(u\) about 0.06 Å at room temperature. Spin waves can, in analogy with phonons, be assigned a magnetic moment \(m^2 = k_BT/K_m\), where \(K_m = d^2E_{tot}/dm^2\). This gives \(m \approx 0.3\ \mu_B/Cu\) at room temperature for the co-existing case. A partial gap removes roughly half of the DOS within an energy \(\Delta = 100\ meV\) around \(E_F\). The gain in kinetic energy is approximately \(\frac{1}{2}N\Delta^2 = 8\ meV/Cu\), i.e., about 15-20 percent of the elastic energy \(U = \frac{1}{2}K\cdot u^2\) at the average \(u\). Thus, the phonon energy is expected to decrease by this percentage because of the coupling to the spin wave, but only in the doped case when \(E_F\) is at the gap.
These results compare reasonably well with experiment. Less doping implies coupling at longer wavelengths so that the softening moves away from the zone boundary and finally disappears. The softening should also disappear when the pseudo gap disappears. This is expected when the Fermi-Dirac occupation, $f$, becomes too wide to separate the occupied majority spins at $E_F$ − $\Delta$ from the unoccupied minority spins at $E_F$ + $\Delta$. As function of $T$, $m(T) = N \cdot \Delta \cdot [f(\frac{E_F}{k_B T}) - f(\frac{E_F + \Delta}{k_B T})]$, while from the band calculations $\Delta \approx \text{const} \cdot m$. By solving iteratively the two last equations as function of $T$, one finds a stable gap (and $m$) up to a $0.9 \cdot T_{\text{max}}$ after which $\Delta$ and $m$ drop to zero at $T_{\text{max}}$, as is the case with the pseudo gap near $T^*$. The reason is the strong exponential $T$-dependence of $f$, and the feedback of $m$ on $\Delta$.

Isotope shifts are expected. The zero-point motion makes a mass ($M$) dependence $u \sim (K \cdot M)^{-1/4}$. A lower $M$ will also decrease $K$ because of the phonon softening due to the promotion of spin waves at larger $u$ (see above), so the isotope effect will be stronger than is suggested from a constant $K$. The effect on the pseudogap will be moderated at large $T$, when there is no explicit mass dependence of $u$, $u^2 \sim K^{-1}$. The effect on the superconducting $T_c \sim \omega \exp(-1/\lambda)$ is complex. Pure phonon $\omega \sim \sqrt{K/M}$, but with SPC also $K$ will drop when phonon amplitudes increase because of lower $M$. A pure $\lambda_{s\text{f}}$ from spin fluctuations tend to increase at increased phonon amplitudes. The mass dependence of $\omega_{s\text{f}}$ and $\lambda_{s\text{f}}$ may act oppositely on $T_c$. Anharmonic effects are expected, which will mix phonon and spin contribution. Experiments show small isotope effects on $T_c$. The mass dependence of $u$ is largest at low $T$, which suggests comparison with isotope shifts of the penetration depth $\Lambda$ measured at low $T$. Some assumptions lead to $\Lambda^{-2} \sim N \cdot v^2$, where $v$ is the Fermi velocity. The band crossing $E_F$ along $\Gamma$-$M$ has larger $v$ than at the crossing along $X$-$M$. Phonon and spin waves along $[1,0,0]$ will produce the gaps in the latter region, so that $v$ will increase. If $16\Omega$ are substituted by $O^{16}$ it will decrease $u$ for half-breathing phonons by 3 percent. The band results tell that the DOS is reduced roughly by a factor $\frac{1}{2}$ by spin fluctuations if a pseudo gap distortion is present and by 20-25 percent if no distortions are present. By simple interpolation from these results one can estimate that reducing $u$ by 3 percent will increase $N$ by 1-2 percent. As $N \sim v^{-1}$ this suggests a decrease of $\Lambda^{-2}$ by 1-2 percent. This is smaller but of the same order as in ref [11]. It can be noted that the gap starts in the $X$-$M$ region from waves along $[1,0,0]$ (and $[0,1,0]$). This fits to the observation of ‘destruction’ of the Fermi surface in this region of k-space [3], while it remains along $\Gamma$-$M$ if no waves are oriented along $[1,1,0]$.

Photoemission and tunneling spectra show the pseudogap and a ‘dip’ in the DOS about a tenth of an eV below $E_F$. The position of this dip relative to the main gap at $E_F$ depends on doping according to tunneling data [2]. A projection of these data on to the calculated DOS suggests that the dip is located at a fixed energy (a fixed wavelength in our mechanism), while the main gap moves to higher energy for decreased doping. This is consistent with a type of perpendicular spin-phonon coupling as follows: Consider the shortest possible coexisting SPC along $[1,0,0]$. The half-breathing phonon creates maximum ‘diluted’ distortions for two out of four pairs of Cu, where condition for magnetism is optimal (while magnetic nodes fall on the two other pairs of Cu). The perpendicular rows of (optimally magnetized) Cu can develop spin waves along $[0,1,0]$, possibly coupled with phonons along the same direction. Complete band calculations are more difficult because very large unit cells are needed to cover even the smallest configuration. However, band results for a simplified case, with only a half-breathing mode with large and small moments (no full spin wave) along $[1,0,0]$ together with longer complete spin waves along $[0,1,0]$, show that two gaps form simultaneously at two different energies. At low energy the gap is due to the short wave along $[1,0,0]$, while at larger energy a second partial gap develops because of a longer spin wave along $[0,1,0]$. The doping dependence of the two gaps fits with data in ref. [9], but the energy scale is too large, almost by a factor of two. This could be explained if the DOS was larger, if all wavelengths were larger or if the real doping, $x$, is not what it is supposed to be.

In conclusion, it is shown that many properties of high-$T_c$ materials are consistent with SPC, although more precise works are needed for quantitative results. More detailed results will be published elsewhere [10].

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