Spin-phonon coupling in the single-layer extended t-J model

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We consider the implications of spin-phonon coupling within the slave-boson, mean-field treatment of the extended t-J model of a high-temperature superconductor. In materials such as YBaCuO, where the CuO_2 plane is buckled, this interaction is linear in O displacement along the c axis, and the coupling constant is found to be large. We calculate the spin effects on phonon dynamics, finding at and below the spin singlet formation temperature changes in frequency shift and linewidth broadening for certain, key phonon modes which correspond well with experiment near the optimal doping level. Furthermore, the theory predicts that phonon anomalies in underdoped compounds should show evidence of spin-gap phenomena with the same characteristic temperature as that found in NMR studies; this is exactly as observed in YBaCuO systems, suggesting a possible unified understanding of the anomalies in magnetic and lattice properties. Finally, such a coupling affords the possibility of a small isotope effect, and our estimate is in good agreement with recent site-selective O-substitution experiments.

I. INTRODUCTION

Since the discovery of high-temperature superconductivity in oxide-based ceramics, a wide variety of experiments has shown strong evidence of a link between anomalies in the lattice structure and the onset of superconductivity in these materials. A comprehensive overview of the techniques available and their results is contained in Ref. 1. More specifically, a number of local probes has shown this connection: neutron-scattering studies[2,3] of the probability distribution function for atoms in the CuO_2 plane show clear local distortions at the transition temperature T_c in several systems; ion channeling[4] shows anomalous changes in the oscillation amplitudes of Cu and O atoms not only at T_c, but also at temperatures above it; extended x-ray absorption fine-structure experiments[5] show changes in the environments of both Cu and apical O atoms; ultrasound measurements[6] show alterations of the elastic constants of the crystal. Among the more general probes, there have been various reports from Raman-scattering and infrared reflectivity investigations[7–9] which indicate anomalous temperature dependences in the frequency shift and linewidth of phonons around and above the superconducting transition. A separate manifestation is the existence of an isotope effect,[10,11] albeit one which appears to have very different forms as a function of sample doping. Strikingly, infrared reflectometry measurements of both the in-plane conductivity σ_{ab} (Ref. 12) and the c-axis conductivity σ_c (Ref. 13) also illustrate a connection between c-axis phonon modes and the properties of charge carriers.

In this work we will be particularly interested in the issue of phonon anomalies, which are one direct consequence of the spin-phonon coupling under consideration. Anomalies in phonon mode frequencies and linewidths at T_c in the $YBa_2Cu_3O_{7-\delta}$ (YBCO) system have been examined since very early in the history of high-T_c superconductivity,[14] because of the light they can shed on both the magnitude and the symmetry (from mode polarization) of the electron-phonon interaction. Studies by Raman spectroscopy have centered largely on the 340 cm^{-1} mode of planar oxygen which shows a particularly large effect in the O_7 compound, and we will encounter its importance throughout the present work. However, it is essential to note, using the well-characterized case of this mode, that not all early measurements of the anomalies, performed on a variety of systems, reached the same result; detailed investigations of high-quality samples have since verified the anomaly, but have shown that its magnitude is very sensitive to both oxygen content,[8] falling sharply as the O depletion δ increases from zero, and to impurities.[15] Because samples with non-zero δ are non-stoichiometric, a considerable amount of disorder may be present, acting to suppress the observed effects; thus the stoichiometric materials $Y_2Ba_4Cu_7O_{15}$ and $YBa_2Cu_4O_8$ will represent important benchmarks of the variation in anomalies with doping level. In other classes of the high-T_c materials there remain debates about sample purity, and rather few crystals of any single compound, so particular care will be required in interpreting results from these.

On the theoretical side, anomalies in the transport and magnetic properties, observed in both normal and superconducting states of the high-temperature superconductors,[16] are considered to be manifestations of a metallic state arising near the Mott transition due to strong correlations. While there remains no consensus on the appropriate theoretical description of the phenomena associated with this anomalous metallic state, in this work we will pursue an approach based on the t-J model[17] treated by the slave-boson mean-field theory.[18–21] This framework has been shown to contain ingredients essential to an understanding of both transport properties,[22] including the temperature dependence of the resistivity and Hall coefficient, and spin excitations,[23–29] such as the different temperature dependences[30,31] of the shift and rate of nuclear magnetic resonance between high- and low-doping regions. On this last point, such models appear to contain a consistent description of the "spin-gap" behavior,[31,28,29] noted first by Yasuoka[30] and subsequently the subject of much investigation. However, while some aspects of the link between these features and the phonon prob-

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lem have been studied theoretically, to our knowledge there have not so far been any efforts to understand all of the low-lying excitations on a unified basis.

The application of conventional electron-phonon coupling to the problem of high-temperature superconductivity was made by Zeyher and Zwicknagel,[32] in a model which required a number of basic assumptions about the nature of the system, including Fermi-liquid behavior of quasiparticles, an *s*-symmetric superconducting gap and a cylindrical Fermi surface. These authors computed the form of the superconductive phonon anomalies, and found that a very strong coupling constant $\lambda \simeq 3$ was required to reproduce the experimental features, which appears to be inconsistent with later studies of transport phenomena within the same framework.[33] At the band-structure level, the resonant frequencies of many phonon modes of the YBCO structure were computed in an extensive local-density approximation study by Andersen *et al.*,[34] who concluded that good qualitative agreement with experimentally observed anomalies would be given on application of the conventional model. These authors drew particular attention to the ''dimpling'' modes of planar O(2) and O(3) atoms, not only due to the strong anomaly in their out-of-phase oscillatory mode (340 cm^{-1}), but also because they cause ''extended saddle points'' near the Fermi surface of the electron dispersion in the region of the $(\pi,0)$ points in k space, which contribute strongly to the calculations of many physical properties. Further studies also based on conventional electron-phonon coupling[35,36] have given detailed descriptions of the Fano line shape, and pointed out how phonon anomalies may be used to deduce the gap symmetry. We note briefly that in contrast to most of the conventionally based treatments,[32] the present analysis is based on strong correlations, encoded by the *t-J* model, and takes a simple, mean-field approach containing no further assumptions about the nature of the system.

We emphasize that this is not a study of a phononic mechanism for superconductivity. In the *t-J* and related models, quasiparticle pairing is the consequence of the spin interaction, and so its origin is entirely electronic. In this work we investigate the effects of phonon oscillations of the host lattice on the parameters of the model itself, showing that they cause an effective spin-phonon coupling. As explained in the following section, while the coupling constant is large, the net interaction depends also on the magnitude of the phonon oscillation, and is found to be small. However, its results are clearly observable in a variety of experimental properties, which may in turn shed much light on the behavior of the system itself.

The structure of this paper is as follows. In Sec. II we introduce the concept of a coupling between the spin and lattice degrees of freedom, and deduce the quantitative form of the interaction vertices. In Sec. III is given a complete account of the application of the single-layer theory to phonon anomalies in $YBa_2Cu_3O_7$. In Sec. IV we present a qualitative discussion of the extension of the same ideas to underdoped YBCO materials, leading to a connection with the mean-field phase diagram and spin-gap behavior. Section V contains an analysis of the isotope effect, and Sec. VI a concluding discussion.

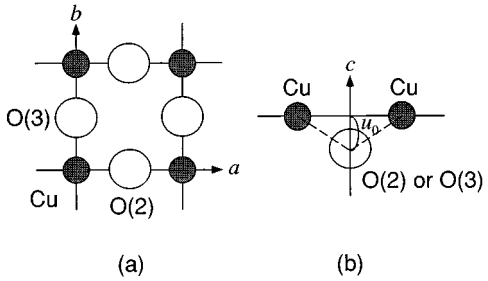

FIG. 1. Schematic representation of the CuO_2 layer. (a) Planar structure. (b) ''Buckling'' deformation of the equilibrium positions of O(2) and O(3) atoms out of the plane of the Cu atoms, appropriate for YBCO. a, b, and c represent the crystal axes (assuming tetragonal symmetry).

II. SPIN-PHONON COUPLING

We consider the spin-phonon coupling arising naturally within the extended *t-J* model of a single CuO_2 layer, which has been shown[24,29] at the mean-field level to give a good account of many features of the spin excitations in both $La_{2-x}Sr_xCuO_4$ (LSCO) and $YBa_2Cu_3O_{7-\delta}$ (YBCO), based on realistic Fermi surface shapes for each class of material. The Hamiltonian is

$$H=-\sum_{ij,\sigma} t_{ij}a^{\dagger}_{i\sigma}a_{j\sigma}+\sum_{\langle ij\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{1}$$

where the Hilbert space is that without double occupancy, t_{ij} corresponds to the transfer integrals used to reproduce the Fermi surface, and the superexchange interaction J_{ij}, which is usually taken to be a constant at fixed doping, is assumed to be finite only between nearest neighbors.

In YBCO, the CuO_2 layer is ''buckled,'' by which is meant that the oxygen atoms O(2) and O(3) lie out of the plane of the Cu atoms, as shown schematically in Fig. 1. Let $u_0+u_i^{\alpha}$ represent the magnitude of the oxygen displacement along the c axis, with u_0 the equilibrium buckling and u_i^{α} the phonon coordinate, in which i refers to the Cu sites on the square lattice, and α to either O(2) ($\alpha=x$) or O(3) ($\alpha=y$). Then t_{ij} and J_{ij} between nearest-neighbor Cu sites have contributions linear in u_i^{α} which may be written as

$$t_{i,i+\alpha}=t[1-\lambda_t(u_i^{\alpha}/a)], \tag{2}$$

$$J_{i,i+\alpha}=J[1-\lambda_J(u_i^{\alpha}/a)], \tag{3}$$

with a the distance between Cu sites, and λ_t and λ_J the corresponding coupling constants. Microscopic estimates of λ_t and λ_J are somewhat involved, and we proceed to detail the steps required in their derivation.

The degree of buckling may be deduced from the structural data of Ref. 37, which shows the equilibrium O displacement to be $u_0=0.256$ Å; these data were taken at 10 K, but the temperature dependence is thought to be very weak, even at the superconducting transition. We neglect the 5% anisotropy between a and b axes in the pseudotetragonal system, and thus continue also with the assumption that the atomic levels of the σ and π orbitals on O(2) and O(3) are

the same. Although the degree of buckling is small, $u_0/a \ll 1$, its inclusion is crucial in providing a coupling which is strong and linear.

The dependence on interatomic separation of the transfer integral t_σ (t_π) between Cu:$d_{x^2-y^2}$ and O:p_σ (O:p_π) is given, following Ref. 38, by

$$\begin{aligned} t_\sigma &= \frac{\sqrt{3}}{2} V_{pd\sigma} \left[1 - \frac{3}{2} \left(\frac{2u}{a} \right)^2 \right] + \left(\frac{2u}{a} \right) V_{pd\pi} \\ &= \frac{\sqrt{3}}{2} V_{pd\sigma} \left[1 - 2.03 \left(\frac{2u}{a} \right)^2 \right] \\ &= \frac{\sqrt{3}}{2} V^0_{pd\sigma} \left[1 - 3.78 \left(\frac{2u}{a} \right)^2 \right], \end{aligned} \tag{4}$$

$$t_\pi = \frac{\sqrt{3}}{2} \frac{2u}{a} V^0_{pd\sigma} \left(1 - \frac{V^0_{pd\pi}}{V^0_{pd\sigma}} \right) = 1.53 \left(\frac{2u}{a} \right). \tag{5}$$

Here $(\sqrt{3}/2)V_{pd\sigma}$ ($V_{pd\pi}$) is the transfer integral between $d_{x^2-y^2}$ (d_{xz}) and p_σ (p_z) orbitals with separation $d = \{[(1/2)a]^2 + u^2\}^{1/2}$, directed along $\hat{x}$ according to definition, and we have taken the distance dependence to be

$$V_{pd}(d) = V^0_{pd} \left(\frac{d}{d_0} \right)^{-7/2}. \tag{6}$$

By writing $u = u_0 + \delta u$, where δu ($\equiv u_i^\alpha$) denotes the oscillation amplitude, for the value of u_0 above one obtains to lowest order $t_\sigma(u)/t_\sigma(u_0) = 1 - 2.03\delta u/a$ and $[t_\pi(u) - t_\pi(u_0)]/t_\sigma(u_0) = 3.06\delta u/a$.

The final requirement is the dependence on t_σ and t_π of t_{ij} and J_{ij}, and here we must consider in detail a model of the CuO_2 plane. Following Eskes and Jefferson,[39] J_{ij} can be given by the perturbative expression

$$J = \frac{4(t^4_{pd,\sigma} - 2t^2_{pd,\sigma} t^2_{pd,\pi})}{(\Delta_{\rm CT} + U_{pd})^2} \left[\frac{1}{U_d} + \frac{2}{2\Delta_{\rm CT} + U_p} \right], \tag{7}$$

where U_d and U_p are on-site interactions for the participating Cu and O orbitals, U_{pd} is a Coulomb interaction between holes on neighboring sites and $\Delta_{\rm CT}$ is the charge-transfer energy. Application of this formula alone yields a very large coupling constant $\lambda_J = 10.4$, because of the quartic power law and because the contributions from σ- and π-hopping processes in the numerator combine ferromagnetically. However, use of the lowest-order perturbation form (7) is not well justified, as there are no small parameter ratios, and in particular the direct O-O hopping integral t_{pp} will have a strong effect. A detailed investigation of the influence of higher-order terms[39] has found for the parameters of the CuO_2 layer the effective relationship $J \propto t_{pd}^x$, with $x \simeq 2.3$, when all overlap integrals are taken to vary uniformly [$t_{pp} \propto t_{pd}^{2/3}$ (Ref. 38)] and $\Delta_{\rm CT}$ is held fixed. However, this result depends upon the variation of the transfer integrals with the bond distortion associated with each phonon mode, and for a mode in which t_{pp} remains constant (A_{1g} and A_{2u} symmetries, Sec. III), the effective power is reduced to $x \simeq 1.7$.[40]

The case of the hopping terms t_{ij} is complicated further by the fact that it requires consideration of the many intersite transfer integrals which contribute to the hopping of a Zhang-Rice singlet, and not simply of the motion of a hole. This problem has been considered within a cell-perturbation method,[41] and the results for the effective power in $t \propto t_{pd}^y$ are $y \simeq 1.0$ for uniform variation, and $y \simeq 0.7$ when t_{pp} is held constant.[40] In this study, our primary aim is to elucidate the effects of spin-phonon coupling in the t-J model at a semiquantitative level, with attention paid to the vertex magnitudes mainly to ensure that the consequences discussed are not irrelevant to experiment. Thus for the current purposes we accept possible errors of order 20–30% in adopting the values $x = 2.0$ and $y = 1.0$, so that $\lambda_J = 5.2$ and $\lambda_t = 2.6 = (1/2)\lambda_J$, and errors of similar magnitude incurred by neglecting any modulation of the extended singlet hopping terms. [In fact, the first set are likely to lead to an overestimate, while the second, in the most naive approximation, would give a similar underestimate, although this depends on the mode symmetry.] An independent indication of the validity of these values is provided by the agreement they yield with the measured isotope shift in YBCO (Ref. 46) (Sec. V).

In this discussion we have disregarded changes in the charge-transfer energy $\Delta_{\rm CT}$ as the bond length varies, because we believe this to be appropriate for the deformation processes associated with a phonon oscillation, which are both local and screened. This situation is to be contrasted with that in experiments in which the bond length is made to vary by application of hydrostatic pressure,[42] or by atomic substitution,[43,44] where one finds the weaker relation $J \propto d^{-\alpha}$, $4 < \alpha < 6$. In these cases long-range forces are brought into play, the Madelung energy of the system is altered, and it is found that a d dependence of $\Delta_{\rm CT}$ is required to account for experiment.[45]

In the slave-boson treatment of the t-J model (1), the spin and charge degrees of freedom carried by the quasiparticles are represented by the explicit decomposition $a_{i\sigma} = f_{i\sigma} b_i^\dagger$, where $f_{i\sigma}$ is a fermionic spinon, in terms of which the spin is given by $\mathbf{S}_i = (1/2) f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta}$, and b_i is a bosonic hole, or holon. With these operators, the coupling in H (1) of the phonon coordinate u_i^α to the spin degrees of freedom may be expressed in the mean-field approximation as

$$\begin{aligned} -\sum_i \sum_{\alpha = x,y} \Bigg\{ & t\lambda_t \left(\frac{u_i^\alpha}{a} \right) \langle b_i b_{i+\alpha}^\dagger \rangle \chi_{i,i+\alpha} + \tfrac{3}{8} J \lambda_J \left(\frac{u_i^\alpha}{a} \right) \\ & \times [\langle \chi_{i,i+\alpha}^\dagger \rangle \chi_{i,i+\alpha} + 2 \langle \Delta_{i,i+\alpha}^\dagger \rangle \Delta_{i,i+\alpha} + \text{H.c.}] \Bigg\}, \end{aligned} \tag{8}$$

where $\chi_{i,j} = \Sigma_s f_{is}^\dagger f_{js}$ and $\Delta_{ij} = (f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow})/\sqrt{2}$. The first two terms, containing $\chi_{i,j}$, will contribute in the normal, or uniform resonant valence band (RVB),[29] state, and will be termed the u-RVB vertex, while the last appears only below the singlet RVB transition, so constitutes an s-RVB vertex. At the onset of singlet order there will be additional contributions to any physical quantity due to the appearance of a finite particle-particle vertex represented by the third term, as well as to changes in the quasiparticle propagators joining the particle-hole terms. In this analysis of the t-J model[29] we do not include a density-density ($n_i n_j$) decoupling of the spin interaction term $J\mathbf{S}_i \cdot \mathbf{S}_j$, because it has been found[47] to have a small coefficient in the derivation from the d-p

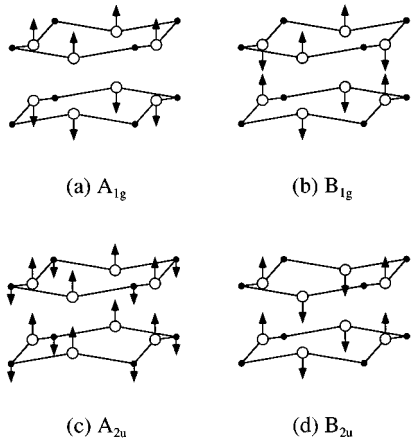

FIG. 2. Schematic representations of phonon modes involving c-axis oscillations of in-plane oxygen atoms in the YBCO bilayer structural unit: (a) A_{1g}, (b) B_{1g}, (c) A_{2u}, and (d) B_{2u}.

model. In principle, the phonon-holon coupling vertex, which is also contained in the t term, may contribute to physical processes, but this will be neglected because in the normal state a boson polarization term vanishes at $q=0$, while in the Bose-condensed state corresponding to true superconductivity in this model the holon has no dynamics.

While the coupling constants λ_t and λ_J have been found to be large, the overall strength of the spin-phonon coupling depends also on the magnitude of the phonon oscillations u_i^α/a, and so remains small. It can be estimated from the root-mean-square (rms) fluctuations of the relative magnitudes of t and J [(2) and (3)], by using $\sqrt{\langle (t_{i,i+\alpha}-t)^2\rangle}/t=(\lambda_t/a)\sqrt{\langle (u_i^\alpha)^2\rangle}$, and similarly for J. The rms fluctuation of $\delta u \equiv u_i^\alpha$ is given by $\langle \delta u^2\rangle=(\hbar/2M\omega_0)$, where ω_0 is taken for the phonon frequency of interest and M is the mass of the O atom. Taking as a typical frequency that of the 340 cm^{-1} mode, to which we will devote most attention in the following section, $\langle \delta u^2\rangle=(0.055\ \text{Å})^2$, and the relative fluctuations in t and J are 3.8 and 7.5%, respectively. These values appear surprisingly large, but are consistent with the estimates of Haas *et al.*,[48] who considered only the effect of a fluctuating J term on the linewidth in electronic Raman scattering. In what follows we will find also that the changes in physical quantities arising from the combined effects of these fluctuations are of the order of their square.

III. PHONON ANOMALIES

Having derived a coupling between spin and lattice modes, we consider first its modification of phonon dynamics. In Fig. 2 are shown the four mode symmetries of a CuO_2 bilayer in which the O(2) and O(3) atoms may oscillate in the c direction. We will use throughout the nomenclature of the D_{4h} symmetry obeyed by the pseudotetragonal CuO_2 planar unit in the slightly anisotropic YBCO system, and refer the reader to Ref. 14 for full details. Here we will be concerned mainly with the 340 cm^{-1} B_{1g} mode in $YBa_2Cu_3O_7$, which is an out-of-phase oscillatory motion of the planar oxygen atoms ($u_i^x=-u_i^y$), and is also out of phase

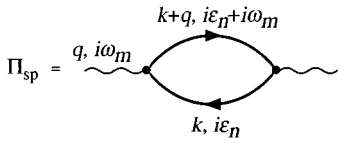

FIG. 3. Diagrammatic form of the lowest-order contribution to the phonon self-energy Π_{sp} due to coupling to spinons. The thick line denotes the spinon propagator in Nambu representation, and the dot the corresponding 2×2 spinon-phonon vertex.

between the planes of the bilayer.[14] This mode has attracted experimental interest because it shows the largest effects in the superconducting state, and there are available both detailed Raman[7–9] data, which are taken at wave vector $q=0$, and inelastic neutron-scattering results,[49] which can probe all q. The primary quantity of experimental interest is the T dependence of the frequency shift and linewidth at $q=0$, in addition to which we will illustrate the dependence of the results on mode frequency and wave vector. The 193 cm^{-1} B_{2u} mode is identical at the single-layer level, although in the real crystal the atomic motions are in-phase between layers, and so is also amenable to description by the same model at this lower frequency. Because this mode is infrared silent, it may be studied only by neutron scattering, and it has recently been investigated in $YBa_2Cu_3O_7$.[50] We will also show the results of the single-layer model for the in-phase ($u_i^x=u_i^y$) A_{1g}- and A_{2u}-symmetric oscillations, and discuss the relevance of the model to experiment for these.

A. Theory

The effect of the coupling on the dynamical properties of the phonon is calculated from the lowest-order spinon polarization correction to the phonon self-energy $\Pi_{sp}(\mathbf{q},i\omega_n)$, shown in Fig. 3; the full phonon propagator is given by $\Pi_{ph}^{-1}(\mathbf{q},i\omega_n)=\Pi_0^{-1}(\mathbf{q},i\omega_n)-\Pi_{sp}^{-1}(\mathbf{q},i\omega_n)$, where the bare propagator has the conventional form $\Pi_0(\mathbf{q},i\omega_n)=2\omega_0/i\omega_n^2-\omega_0^2$. Thus when $|\mathrm{Re}\,\Pi_{sp}|\ll\omega_0$, the superconductivity-induced phonon frequency shift is given to lowest order by $\delta\omega=\mathrm{Re}\,\Pi_{sp}$, and the correction to the linewidth Γ is $\delta\Gamma=\mathrm{Im}\,\Pi_{sp}$. Second-order perturbation theory in terms of the interaction strength results in a frequency shift which is given at $q=0$ by

$$\delta\omega=c(\lambda_J J)^2\frac{4}{N}\sum_k F_k\frac{1}{\omega^2-(2E_k)^2}\frac{\tanh(E_k/2T)}{E_k}, \quad (9)$$

where $c=(3/4a)^2\langle\delta u^2\rangle$, with $\langle\delta u^2\rangle$ defined at the end of Sec. II, and has the value $c=1.18\times10^{-4}$ for the B_{1g} phonon. E_k is defined by $E_k=[\xi_k^2+\Delta_k^2]^{1/2}$, with ξ_k the spinon band energy relative to the chemical potential, and $\Delta_k=-(3\sqrt{2}/4)J\Delta(\cos k_x-\cos k_y)$ the singlet order parameter, which has been shown to have $d_{x^2-y^2}$-wave symmetry in the lowest-energy state in the present framework;[19,20] the negative branch given by $-E_k$ is illustrated in Fig. 4 for the parameters of the YBCO system used in this study. Finally, F_k is a form factor which depends on the mode symmetry,

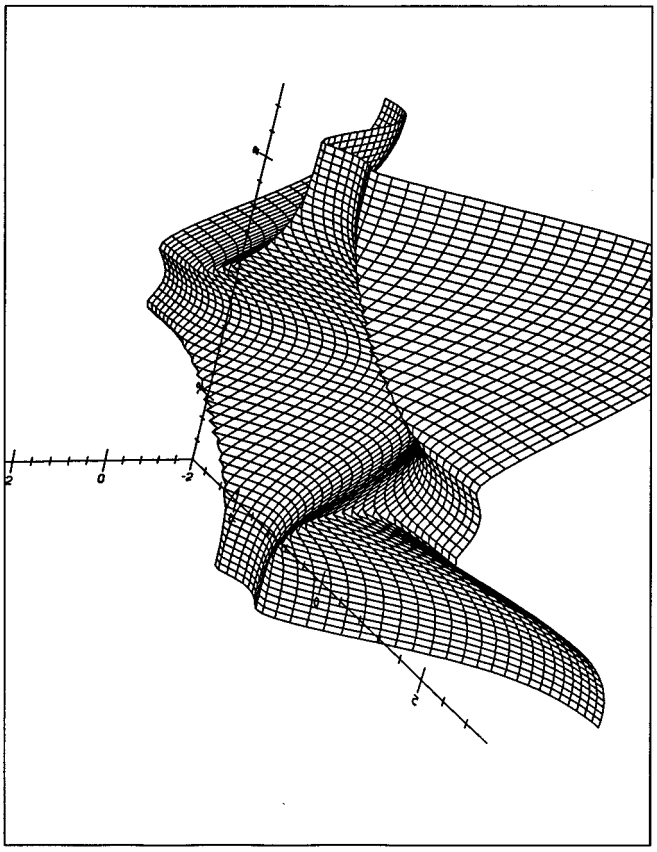

FIG. 4. Energy dispersion $E_k = -\sqrt{\xi_k^2 + \Delta_k^2}$ for a YBCO-like system, where the transfer integrals in the extended t-J model are $t = 4J$, $t' = -(1/6)t$ and $t'' = (1/5)t$, corresponding, respectively, to nearest-, second-, and third-neighbor hopping processes.

$$F_k = 2\Delta^2 \left(\gamma_k \xi_k + \frac{3J}{4} \bar{\chi} \eta_k^2 \right)^2, \quad B_{1g},\ B_{2u} \text{ modes},$$

$$F_k = 2\Delta^2 \eta_k^2 \left(\xi_k + \frac{3J}{4} \bar{\chi} \gamma_k \right)^2, \quad A_{1g},\ A_{2u} \text{ modes}, \quad (10)$$

where $\gamma_k = \cos k_x + \cos k_y$, $\eta_k = \cos k_x - \cos k_y$, $\Delta = \langle \Delta_{ij} \rangle$ and $\bar{\chi} \equiv \langle \chi_{ij} \rangle + (2t\delta/3J)$ is written to contain the effects of the particle-hole vertices from both J and t terms; δ is the hole concentration. In Eq. (10) one has $F_k \propto \Delta^2$, so that there is no phonon energy correction due to spin coupling in the normal state: this result applies only at $q = 0$ for the optic phonon modes under consideration. By a similar analysis, the linewidth broadening is given by

$$\delta\Gamma = -c(\lambda_J J)^2 \frac{\pi}{N} \sum_k F_k [\delta(\omega - 2E_k) - \delta(\omega + 2E_k)] \times \frac{\tanh(E_k/2T)}{E_k^2}. \quad (11)$$

B. Results

For the following calculations we use the self-consistent solutions to the mean-field equations of the extended t-J model[24] for the temperature dependence of the parameters $(\bar{\chi}, \Delta, \mu)$ for

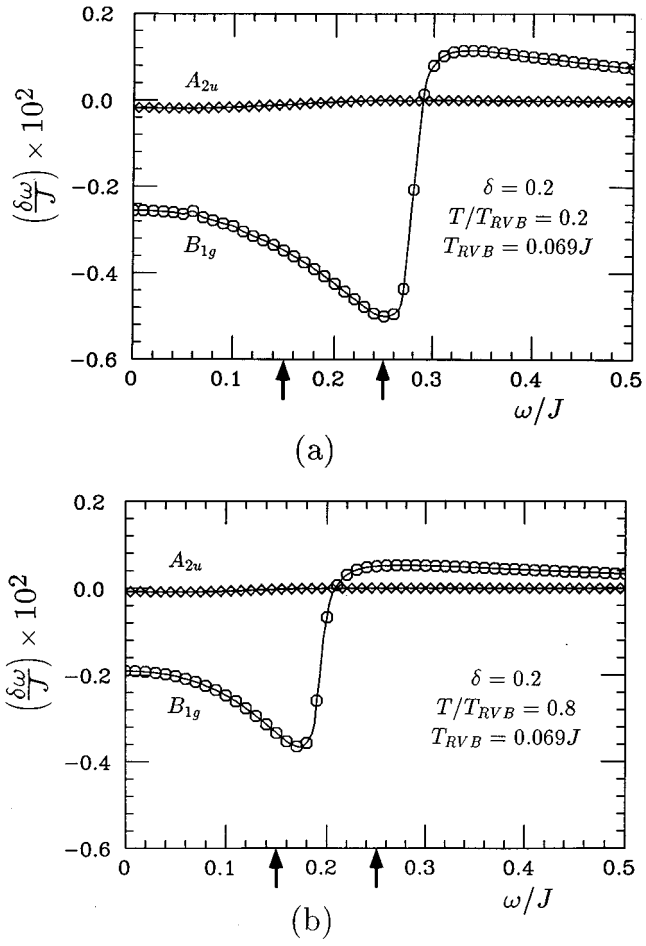

FIG. 5. Phonon frequency shift $\delta\omega$ for B_{1g} ($\bigcirc$) and A_{2u} ($\times$) modes at $q = 0$ as a function of frequency at (a) $T = 0.2T_{\rm RVB}$ and (b) $T = 0.8T_{\rm RVB}$. The arrows indicate the frequencies whose T dependence is illustrated in Fig. 7.

(i) the transfer integrals appropriate to YBCO: $t = 4J$, $t' = -(1/6)t$ and $t'' = (1/5)t$ (corresponding to hopping processes between nearest, next-nearest, and third neighbors, respectively), giving the spinon dispersion shown in Fig. 4, and

(ii) a doping level $\delta = 0.2$, corresponding approximately to optimal doping, or $YBa_2Cu_3O_7$ in this model.[29]

We note here that in the t-J models with the superexchange J calculated in the random-phase approximation, the doping cannot be taken to be a parameter which may be varied to reproduce experimental observations. The chosen doping level is taken neither too near nor too far from the antiferromagnetic instability of the system, so that the quantities calculated may be considered to be a reasonable reflection of the effects of spin-fluctuation enhancement, without being singular.[29] Thus we will not have any semiquantitative statements to make with regard to doping dependence. Throughout the calculations we have assumed a Lorentzian broadening of the spinon spectrum $\gamma = 0.12 k_B T_{\rm RVB}$, and we find that the results depend very little on value of this parameter: specifically, a reduction of γ by a factor of 10 is required to enhance the frequency shift by a factor of 2, for mode frequencies close to the maximum shift [Fig. 5(a) below].

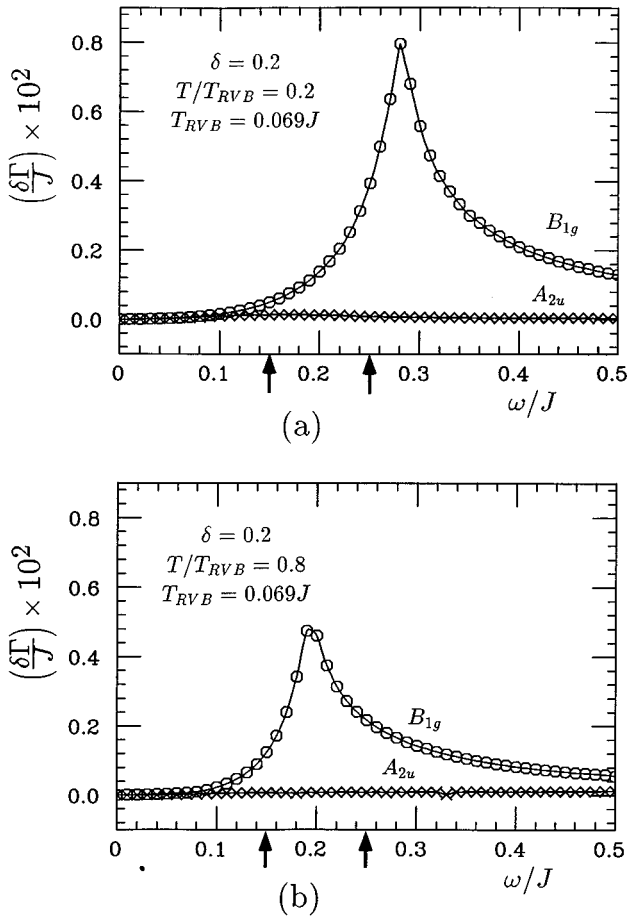

FIG. 6. Phonon linewidth broadening $\delta\Gamma$ for B_{1g} ($\bigcirc$) and A_{2u} ($\times$) modes at $q=0$ as a function of frequency at (a) $T=0.2T_{\rm RVB}$ and (b) $T=0.8T_{\rm RVB}$. The arrows indicate the frequencies whose T dependence is illustrated in Fig. 8.

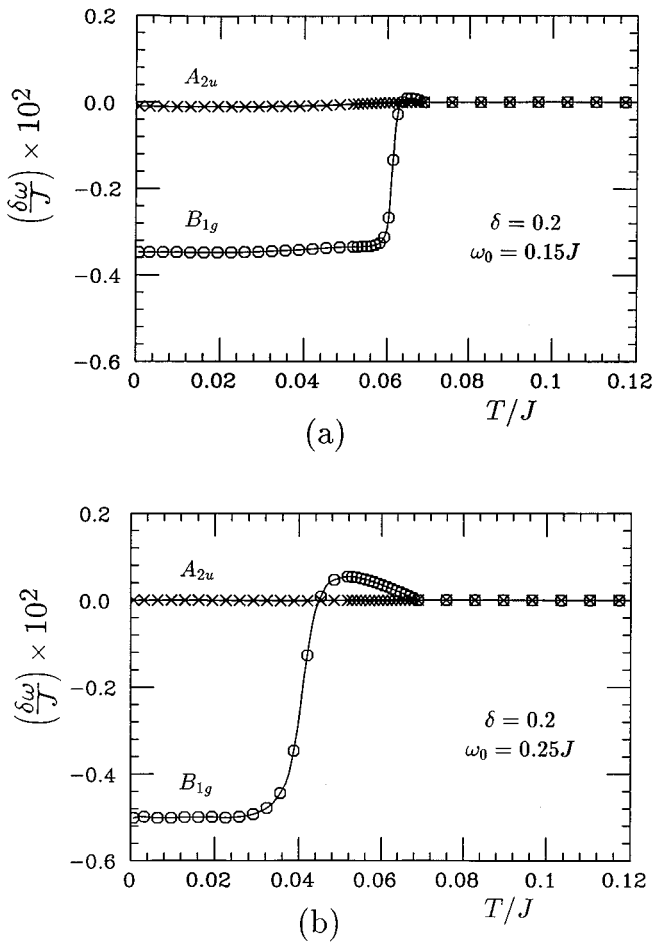

FIG. 7. Phonon frequency shift $\delta\omega$ for B_{1g} ($\bigcirc$) and A_{2u} ($\times$) modes at $q=0$ as a function of T for mode frequencies (a) $\omega_0=0.15J$ and (b) $\omega_0=0.25J$.

ω dependence

Using the mean-field parameters, the frequency dependence of $\delta\omega$, given by Eq. (9), has been evaluated numerically at $T/T_{\rm RVB}=0.2$ and $T/T_{\rm RVB}=0.8$, where $T_{\rm RVB}=0.069J$ is the onset temperature for the singlet RVB order parameter Δ, and the results are shown by the $\bigcirc$ symbols in Fig. 5 for $q=0$. The change in sign with frequency for $\delta\omega$ of the B_{1g} mode is a result of the ω-dependent denominator in Eq. (9). The frequency of the crossing is an approximate measure of the value of $2\Delta_k(T)$ near the $(\pi,0)$ points, where the gap is maximal, as these regions are favored by the B_{1g} symmetry. As the temperature is increased towards $T_{\rm RVB}$, the ω dependence of $\delta\omega$ remains qualitatively the same, but the sign change occurs at lower frequencies as the gap magnitude falls. The experimental mode frequency $\omega_{\rm ph}=340\ {\rm cm}^{-1}\simeq 0.3J$ for the B_{1g} mode is near, but just below, the frequency of the crossing at low temperatures, so this mode can be expected to show a maximal effect.

The linewidth broadening $\delta\Gamma$ is shown in Fig. 6 for the same two temperatures, and has the form to be expected for an imaginary part of the quantities whose real part is shown in Fig. 5, namely a peak at the frequency of the sign change in $\delta\omega$. Note that because the gap is d symmetric (point nodes on the Fermi surface) there is no region at low frequencies where the imaginary part vanishes.

T dependence

The temperature dependence of $\delta\omega$ is shown in Fig. 7 for $q=0$ and the frequency choices $\omega_0/J=0.15$ and 0.25, which are indicated by arrows in Fig. 5: the former is in the regime where the mode frequency is considerably less than $2\max[\Delta_k(T=0)]\equiv$ "2Δ," and shows a sharp transition; the latter value has reasonable quantitative agreement with the 340 $\rm cm^{-1}$ mode, and shows clearly that as the mode frequency approaches 2Δ, the shift in frequency occurs at a temperature somewhat below $T_{\rm RVB}$. This corresponds well to the observations of Ref. 8, where the full frequency shift develops over a range of temperatures below the onset. In fact, at the value $\omega_0=0.3J$, closest to the exact experimental mode frequency $\omega_{\rm ph}$, there is a small, positive frequency shift because $\omega_0>2\max[\Delta_k(T=0)]$; however, we illustrate the anomalous effects for a mode frequency just below this value, as is shown to be the case in experiment, and in general regard the degree of correspondence between model and experimental mode and gap energies as a success of the initial mean-field formulation.

Comparison with the experimental result[8] for the temperature-dependent broadening of the B_{1g} mode shows

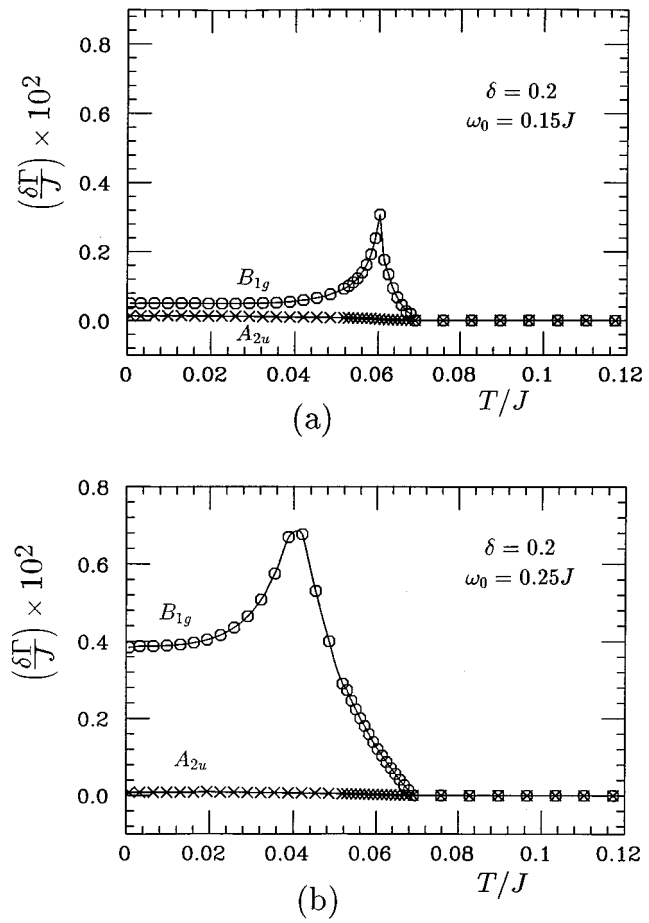

FIG. 8. Phonon linewidth broadening $\delta\Gamma$ for B_{1g} ($\bigcirc$) and A_{2u} ($\times$) modes at $q=0$ as a function of T, for mode frequencies (a) $\omega_0=0.15J$ and (b) $\omega_0=0.25J$.

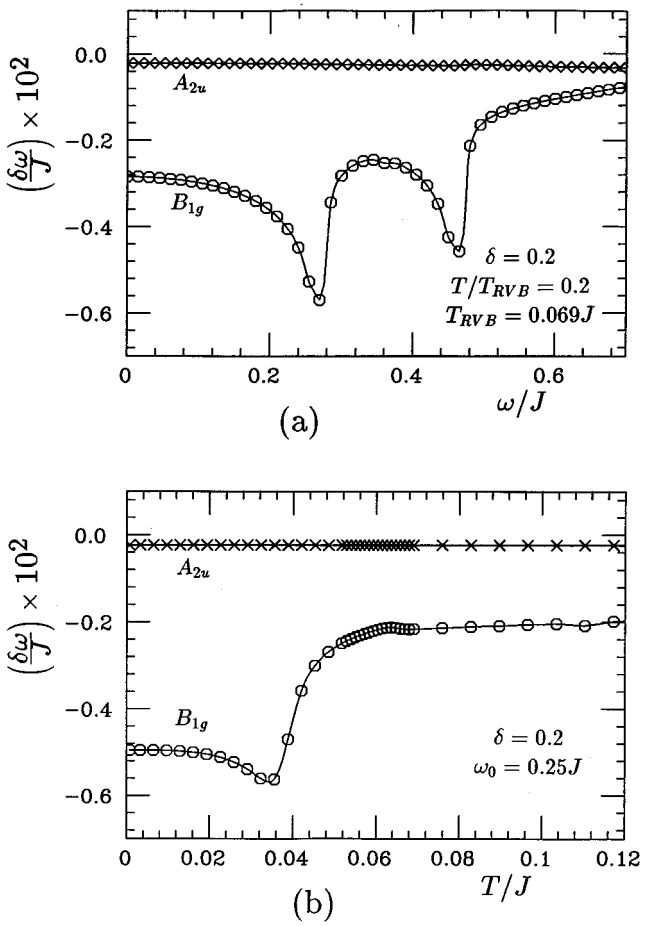

FIG. 9. Phonon frequency shifts $\delta\omega$ for B_{1g} ($\bigcirc$) and A_{2u} ($\times$) modes at wave vector at $\mathbf{q}=(0.2,0)\pi$; (a) as a function of frequency at $T=0.2T_{\mathrm{RVB}}$ and (b) as a function of T for mode frequency $\omega_0=0.25J$.

extremely good agreement in functional form and in magnitude ($\delta\omega\simeq\delta\Gamma\simeq 0.01\omega_0$) for a frequency ω_0 close to ω_{ph} [Fig. 8(b)]. At lower frequencies, away from the ''resonance'' energy set by the low-temperature gap, $\delta\Gamma$ is suppressed [Fig. 8(a)]. Note that in Figs. 7(a) and 8(a) [and 10(a)] we retain the labeling B_{1g} for the symmetry of the phonon distortion, although in fact the frequency is chosen to be close to that of the B_{2u} mode.

Quantitatively, the magnitude of the effects given by the model with the chosen values of λ_t and λ_J is within a factor of 1.5 of the Raman measurements[8] on $YBa_2Cu_3O_7$. In the light of the approximations detailed in the preceding section, such correspondence may be taken as justification for these, and appears eminently satisfactory within a mean-field treatment using no adjustable parameters. We note also that the magnitude of the anomalies in frequency and broadening appear to drop quickly with doping δ, and that neutron measurements at $q=0$ (Ref. 49) suggest a somewhat smaller frequency shift than is seen by Raman scattering.

Gap symmetry

The frequency shift and linewidth results obtained for the B_{1g} and B_{2u} modes are consistent only with predominantly $d_{x^2-y^2}$-wave singlet pairing, as this has a constructive combination with the phonon symmetry in the expression (10) for the form factor. By contrast, a conventional extended s-symmetric gap is found to give an immeasurably small frequency shift for both B- and A-type mode symmetries, because the form factors (F_k) are small for B symmetry, while both thermal and the form factors are small for A. While a pairing state characterized by an intermediate phase $\Delta_y/\Delta_x=e^{i\phi}$,[21,52] with ϕ different from but close to π, so that the system is close to d symmetry, cannot be excluded by the present analysis alone, it appears that all forms of anisotropic s-wave gaps are ruled out by their antiphase combination with the phonon symmetry (see also Ref. 36).

q *dependence*

We have extended our analysis to the case where the phonon has a finite wave vector, and will consider here only the variation of the frequency shift, $\delta\omega$, as this has been measured. $\delta\omega(\mathbf{q},\omega,T)$ exhibits a wealth of features as $\mathbf{q}$ is varied, because the quantitative effects are sensitive to the detailed shape of the spinon dispersion E_k (Fig. 4), as well as to the bare phonon frequency as illustrated above. When the phonon has finite wave vector $\mathbf{q}$, one may show that the components of $\mathbf{u}(\mathbf{q})$ obey the relations $u_x(\mathbf{q})=\pm u_y(\mathbf{q})$ for every $\mathbf{q}$ as a consequence of $u_i^x=\pm u_i^y$, and the expression (9) takes the more general form

$$\delta\omega(\mathbf{q}) = -c(\lambda J)^2 \frac{2}{N}\sum_k \left\{ F^{(+)}[f(E_+)-f(E_-)]\frac{(E_+-E_-)}{\omega^2-(E_+-E_-)^2} - F^{(-)}[1-f(E_+)-f(E_-)]\frac{(E_++E_-)}{\omega^2-(E_++E_-)^2}\right\}, \quad (12)$$

where the form factors for the normal and anomalous processes are given by

$$F^{(\pm)} = \tfrac{1}{2}(c_1^2+c_3^2) \pm \frac{1}{2E_+E_-}[(c_1\Delta_+ + c_3\xi_+)(c_1\Delta_- + c_3\xi_-) - (c_1\xi_+ - c_3\Delta_+)(c_1\xi_- - c_3\Delta_-)], \quad (13)$$

in which the subscripts $\pm$ denote momentum labels $\mathbf{k}\pm(1/2)\mathbf{q}$ throughout, and $(c_1,c_3)=(\sqrt{2}\Delta_0\gamma_k,\bar{\chi}\eta_k)$ for the B_{1g} mode, and $(\sqrt{2}\Delta_0\eta_k,\bar{\chi}\gamma_k)$ for the A_{2u} mode. We assume for simplicity that the phonon is nondispersive, i.e., that the mode frequency changes little with q, and this appears to be borne out by experiment.

In Fig. 9 are shown the frequency shifts at $\mathbf{q}=(0.2,0)\pi$ as a function of ω at low T [(a), cf. Fig. 5(a)], and of T at $\omega_0=0.25J$ [(b), cf. Fig. 7(b)]. In the ω dependence there is a clear additional contribution at $\omega\simeq 0.45J$ which is found to grow and then disappears as q_x is varied between 0 and 0.4π. This feature is readily explained by the fact that the strongest contributions, from the $(\pi,0)$ and $(0,\pi)$ regions, have a second characteristic energy separation related to the sum of the maximum gap and the energy of the flat part of the spinon dispersion at $(\pi,0)$ (Fig. 4): the general denominator $\omega^2-(E_{k+q/2}+E_{k-q/2})^2$ in (12) remains negative at these values.

In the T dependence, the most distinctive feature is that the contribution to $\delta\omega$ from the u-RVB state is no longer vanishing, so that the anomaly at $T_{\rm RVB}$, which is the difference between this and the phonon self-energy in the s-RVB state, becomes smaller. It also appears somewhat sharper as a function of temperature, and both of these features agree well with the finite-q results from inelastic neutron scattering.[49]

In Fig. 10 is shown the difference in the self-energy correction between low ($T=0.1T_{\rm RVB}$) and high ($T=1.1T_{\rm RVB}$) temperatures as a function of q_x (a,b) and of q along the (1,1) direction (c). The peak features have a simple explanation on the basis of E_k: viewing the integral to be performed as an exercise in maximizing the contact between two spinon dispersion surfaces (one inverted for the anomalous scattering contribution), the initial peak comes from a considerable improvement in surface overlap around the $(\pi,0)$ points as soon as q is offset. The peak around $q/\pi\sim 0.3$ is due to overlap between opposite sides of the low-energy part of the dispersion, which is spanned by this wave vector, or scattering processes across the ''neck'' of the open Fermi surface. Both features are strongly dependent on the exact shape of E_k, and while we suspect that the first is unlikely to be observed in a real experiment, it is possible that the second will appear. The contrast between Figs. 10(a) and 10(b) suggests that the latter peak would only be discernible for the 340 cm^{-1} phonon mode, where the anomalies are most pronounced due to the proximity of the mode frequency to ''2Δ.'' Comparison with the experimental results of Ref. 49, where fewer wave-vector points could be sampled, shows some correspondence to the decreasing trend seen in the O_7 material, although this decrease is somewhat more rapid in the calculation. A very recent study of the q dependence of $\delta\omega$ for the 193 cm^{-1} B_{2u} mode suggests a similar q dependence for this, in that it varies little with wave vector in the region of the zone center.

C. Application to other modes

The 193 cm^{-1} B_{2u} mode (Fig. 2) is also an out-of-phase oscillation of O(2) and O(3) atoms in the plane, although in this case the motion is in-phase between the planes of the bilayer. This mode has recently been analyzed in $YBa_2Cu_3O_7$ by Harashina *et al.*,[50] and they observed a sharp frequency shift occurring close to the superconducting transition temperature, with a relative magnitude $\delta\omega/\omega_0\simeq 1\%$. These features are in very good agreement with the results of the single-layer model shown in Fig. 7(a) for a similar frequency ω_0. However, the authors also find that the phonon linewidth Γ narrows significantly below the transition, which leads to the model-independent conclusion of a strong electron-phonon coupling. Here we have taken the intrinsic linewidth to be a constant, independent of the spinon spectrum, because no spinon spectral weight is expected for optic phonon frequencies at $q=0$, so the experimental result cannot be obtained. The correction, Fig. 8(a), from the imaginary part of the phonon self-energy (Fig. 3), is always positive and nonzero for a d-symmetric gap choice in the approximation used. For a quasiparticle density of states corresponding to a d-symmetric gap state, it is easy to argue that in the presence of a coupling, phonon modes of frequencies close to the maximal value of the gap will be broadened by the quasiparticles, while those at low frequencies will narrow, in accord with the standard picture for acoustic phonons.[51] However, in the present case a mechanism for the applicability of this scenario remains to be elucidated.

In Figs. 5–10 are shown not just results for B_{1g} and B_{2u} modes, but also those for modes at the same frequencies with in-phase O(2) and O(3) oscillations, which in the single-layer case would correspond to A_{1g} (Raman-active) or A_{2u} (infrared-active) symmetry. The A_{1g} mode appears at 440 cm^{-1}, above 2Δ, and so if its response was similar to B_{1g} [Fig. 5(b)] would show at best a small positive frequency shift and broadening, similar in fact to the observation of Ref. 8. The A_{2u} mode occurs at 307 cm^{-1}, well positioned to show strong effects. However, one sees immediately that in the current approximation these have negligible anomalies, a qualitative difference from the B-symmetric modes which emerges from the form factors F_k (10) appropriate to d-wave singlet pairing.

Experimentally, the situation surrounding the strongly infrared-active A_{2u} mode appears not to be clearly understood, since neutron studies[49] report a ''mysteriously'' small shift $\delta\omega/\omega_0\simeq 0.4\%$, whereas far infrared spectroscopy[7] reveals a strong shift $\delta\omega/\omega_0\simeq 1.2\%$. The result from infrared

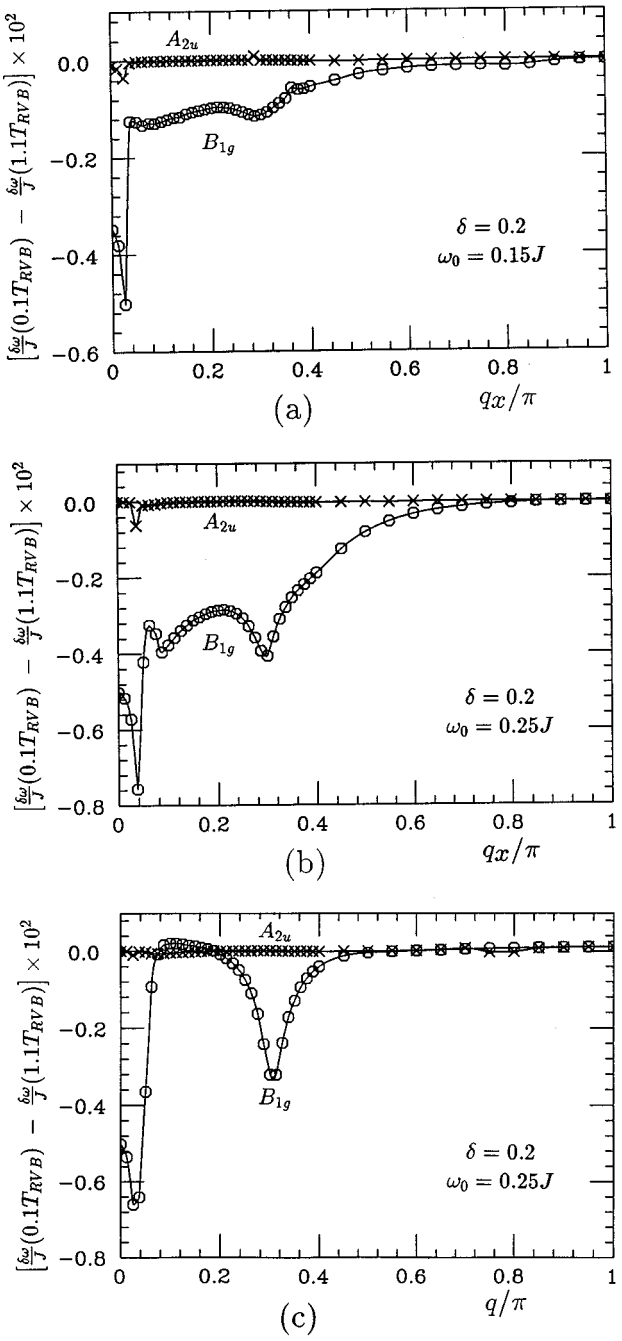

FIG. 10. Phonon frequency shift $\delta\omega$ for B_{1g} ($\bigcirc$) and A_{2u} ($\times$) modes of wave vectors (a) q_x in the (1,0) direction, for a phonon of bare frequency $\omega_0 = 0.15J$, (b) q_x in the (1,0) direction, for a phonon of bare frequency $\omega_0 = 0.25J$, and (c) $q/\sqrt{2}$ in the (1,1) direction, for a phonon of bare frequency $\omega_0 = 0.25J$.

reflectivity has recently been reproduced on a single crystal of optimally doped YBCO,[56] while the neutron-scattering experiment suffers in that this mode appears as an extremely broad peak. The failure of the present model to reproduce these effects is directly attributable to its single-plane nature: the A_{2u} mode develops a very strong dipole moment, so is accompanied by significant interplane charge transfer, and a bilayer formulation including interband processes in a weak-coupling scheme has already been shown[53] to contain this physics. Extension of the model to a system of two coupled planes is an area of active research, and leads to nontrivial questions about the allowable symmetries of the superconducting gap in a bilayer which are themselves of intrinsic interest. In the case of the A_{1g} mode, its atomic motions will also cause charge motion within the CuO_2 plane, the treatment of which is beyond the basic t-J framework.

Finally, the effects studied will be strongly suppressed in the E-symmetric phonon modes of O(2) and O(3), where atomic displacements are parallel to the plane, as the modulation of t_{ij} and J_{ij} will be only quadratic in the phonon coordinate [cf. (2,3)]. In addition, we would not expect to find significant superconductive anomalies in phonon modes involving motions of atoms in the unit cell which are not located in the CuO_2 layers, with the possible exception of apical O(4), which is strongly coupled to the planar system as indicated in Ref. 54. In large part these qualitative expectations are borne out by experiment, where no other strong anomalies are observed, except indeed for a moderate feature in the 500 cm^{-1} A_g-symmetric mode of O(4),[8] and a very curious, low-frequency mode in some YBCO compounds which appears to involve the c-axis motion of the Ba atom[55] (which we note lies also in the plane of apical O).

A concluding comment is in order on the possibilities for phonon anomalies in other classes of high-T_c ceramics. The most extensively studied groups of compounds are the $La_{2-x}Sr_xCuO_4$ and the related $Nd_{2-x}Ce_xCuO_4$ series with variable doping x, and the parent R_2CuO_4 series with a selection of elements R; in these cases there is now well-documented evidence for the link between superconductivity and local structural anomalies.[57] However, neither spectroscopic nor neutron investigations have revealed, in the modes examined so far, any clear signature of phonon anomalies[58] of the type we consider, even in the B-symmetric distortion of the single CuO_2 layer in the unit cell (although this occurs above the characteristic value of "2Δ"). While this result is exactly that predicted by the theory, because the CuO_2 plane is essentially unbuckled above T_c [high-temperature tetragonal (HTT) phase], so that phonon modulation of the t and J terms would be quadratic, and thus small, it is by no means certain that the observations correspond to an intrinsic property of the materials, rather than being an effect of impurities (Sec. I) or, more fundamentally for Raman studies, the lack of true inversion symmetry. In the low-temperature orthorhombic (LTO) and low-temperature tetragonal (LTT) phases, the plane does undergo a distortion, consisting of alternating tilts of the CuO_6 octahedral units in the [1,1] and [1,0] directions, respectively, but against this background equilibrium configuration of positive and negative u_0 values (Sec. II), the net coupling for any combination of A- and B-symmetric gap and phonon symmetries at $q = 0$ will cancel at linear order.

The Bi-Sr-Ca-Cu-O group of compounds also shows a buckling distortion. While exact structural determinations are complicated by the presence of dislocations, modulations and disorder, there have been satisfactory characterizations of $Bi_2Sr_2CaCu_2O_8$ (Refs. 59 and 60) which show the nature of the CuO_2 plane buckling to be that of the LTO distortion of the single plane in LSCO compounds. From the theory, we would expect no observable anomalies due to the cancellation of linear terms in such a structure (above), and this is

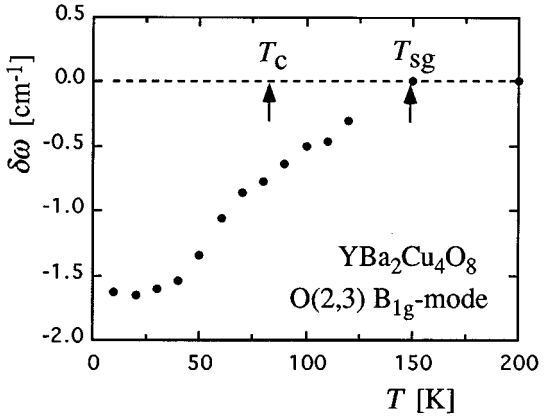

FIG. 11. Schematic representation of the frequency shift of the 340 cm^{-1} B_{1g} phonon mode as a function of temperature in the underdoped compound $YBa_2Cu_4O_8$, from the data of Ref. 55. $T_c = 82$ K is the temperature of the superconducting transition, and $T_{sg} \simeq 150$ K denotes the onset of the anomalous frequency shift.

consistent with experimental reports,[61] which indicate that a frequency shift for the 336 cm^{-1} B_{1g} mode is absent in $Bi_2Sr_2CaCu_2O_8$-related materials. Given the sensitivity to impurities of the anomalous effects documented in YBCO materials, these results are yet to be verified. There remains no data on phonon anomalies also for the Tl- and Hg-containing materials, although there has been a detailed investigation of the local structural anomaly in the former.[2]

IV. UNDERDOPED PHASE AND SPIN GAP

In the preceding sections we have detailed the predictions of a model where the phonon anomalies are coupled to spin singlet formation, which gives as their onset temperature not the superconducting critical temperature T_c but the s-RVB condensation temperature T_{RVB}. This result raises the interesting possibility of probing the spin-gap behavior found in members of the YBCO class in the low-doping regime, by which is meant doping levels below that required for the optimal T_c, by considering the frequency shifts of particular phonons. The definition of the spin gap varies among authors and experiments, but we take it to mean the loss of spectral weight in the spin response which sets in at some temperature T_0 above T_c, and has been best characterized by observations of the temperature dependence of the NMR relaxation rate,[30] which is maximal at this T_0.

There exist already several experimental reports[7–9] of anomalies in the frequency shift well above T_c, whose onset temperature corresponds closely to that where the NMR rate exhibits a maximum. Recent, highly accurate Raman-scattering studies of phonon anomalies in the stoichiometric underdoped YBCO compounds $Y_2Ba_4Cu_7O_{15}$ and $YBa_2Cu_4O_8$ (Ref. 55) add considerable weight to these considerations as they show clearly the onset of a frequency shift at some $T_0 \simeq 150$ K, followed by growth of this shift as temperature is lowered, until a saturation below T_c, as shown schematically in Fig. 11. Such features may be understood on the basis of the mean-field phase diagram of the extended t-J model,[29] reproduced in Fig. 12, in which T_{RVB} is indeed higher than T_c only in the low-doping region. In

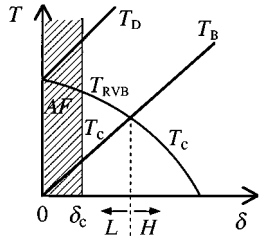

FIG. 12. Mean-field phase diagram for the extended t-J model in the slave-boson formulation, showing the existence of a spin gap at doping levels below that for the optimal T_c (after Ref. 24).

this framework, there is an onset of short-ranged singlet RVB order around T_0, which is then identified with the crossover temperature T_{RVB},[22] and an increasing correlation length of the coherent regions with decreasing temperature until fully coherent, long-range order is attained at T_c. The saturation of the magnitude of the phonon frequency shift below T_c is a consequence of the finite-frequency nature of the excitation [Fig. 7(b)]. We speculate that studies of phonon anomalies at higher wave vectors might show full development of the energy correction at temperatures closer to T_0, but on the basis of Fig. 10 we doubt that these would be measurable.

These results for the change in nature of the transition between low- and high-doping regimes are consistent with the observation that the specific-heat anomalies at T_c in each case are qualitatively different.[62,63] The existence of two temperature scales may provide an explanation for the contrasting low-q behavior of the energy shifts in nominal $O_{6.92}$ and O_7 compounds observed in Ref. 49: here the authors took as their high temperature for comparison a value of 100 K, which if the lower-doped compound were to possess a spin gap above T_c could very well remain in the regime with a phonon anomaly, i.e., below T_0. We note also that there have been some experimental reports which indicate a true transition, as opposed to a crossover, around the higher temperature in several material classes, notably low-doped phases of YBCO, and it is possible that this may be identified with a lattice instability.[6,64,65]

In conclusion to this section we comment that the present theory contains only one temperature scale, T_{RVB}, and thus a detailed quantitative explanation of the low-doping regime remains beyond its scope (see the related note in the introduction to Sec. III). Within the same framework, a more accurate account of the features reproduced in outline here will require additional physics, perhaps in the form of an improved treatment of the boson degrees of freedom, to restore the lower temperature scale of the true superconducting transition.

V. ISOTOPE EFFECT

The isotope effect was one of the critical pieces of evidence which pointed the way to the formulation of the BCS theory for superconductivity in conventional metals. In the high-T_c materials the situation is somewhat complex, and a comprehensive review with a wealth of experimental evidence and a summary of theoretical models to date is given in Ref. 66. In brief, the qualitative trend in each material class appears to be a situation where the oxygen isotope

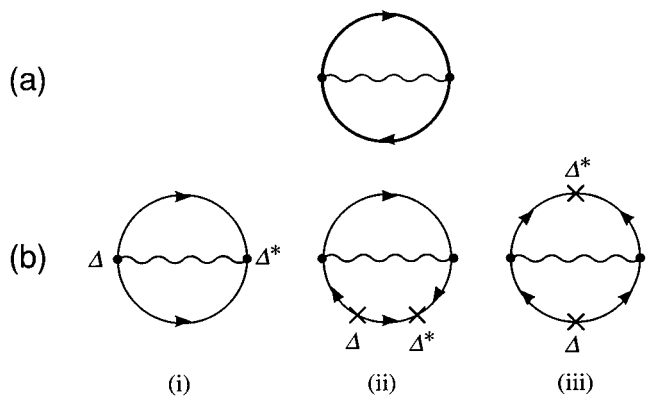

FIG. 13. Diagrammatic representation of (a) the free-energy contribution due to the lowest-order spinon-phonon coupling term, and (b) those parts of order Δ^2, to be evaluated in the normal state at T_{RVB}.

effect, parametrized by $\alpha=-d\ln T_c/d\ln M\simeq-(\Delta T_c/T_c)(M/\Delta M)$, is close to vanishing at the optimal doping level, but rises smoothly to values of at least $\alpha=0.5$ on sufficient under- and overdoping. The question of sample purity and randomness away from the stoichiometric compounds (Sec. I) may be pertinent here once again, but this form has been observed in almost all types of system. In general, electronic models such as the current one do not address the question of the isotope effect at all, and in this work we will have the modest aim only of elucidating the influence of the spin-phonon coupling at the near-optimal doping level.

The thermodynamic properties of the coupled system may be studied self-consistently by including phonon-spinon terms in the free energy F [Fig. 13(a)]. In a Ginzburg-Landau expansion, the free-energy difference between a normal state and a superconducting one with a single order parameter Δ has the form $F_S-F_N=A(T)\Delta^2+B(T)\Delta^4+\ldots$. It is tempting to postulate that the Δ^2 contribution of the additional parts acts to enhance the stability of the spin singlet state, providing a natural linkage of the spin gap to the lattice structure which might account for the variety of characteristic temperatures discussed in the previous section. However, the relative magnitude of the effective phonon-spinon vertex may be estimated as shown at the end of Sec. II, and because the contributions due to fluctuations in t and J require two such vertices, their effect can be expected to be of order 10^{-2}. Here we estimate this effect by evaluating the Δ^2 contributions from the lowest-order phonon-spinon coupling term at T_{RVB}, using the spinon propagators for the normal, or u-RVB, state.

Omitting details of the lengthy but straightforward calculation, the free-energy contributions from phonon coupling are shown in Fig. 13(b) for the terms (i), the s-RVB vertex part, (ii), a pair of diagrams corresponding to a spinon self-energy correction by the phonon, and (iii) phonon vertex correction of the u-RVB vertex. Near the transition, F_S-F_N may be linearized in temperature, so that the coefficient of the Δ^2 term becomes $A(T)=a(T-T_{\mathrm{RVB}})$. The phonon contributions are approximately T independent, so have the schematic form $-b\Delta^2$, and can be written as a constant shift $\delta T_{\mathrm{RVB}}=b/a$; in Table I are given the values of the relative shifts $\delta T_{\mathrm{RVB}}/T_{\mathrm{RVB}}$ arising from each of the diagram types in Fig. 13(b), and for the four phonon symmetries and frequencies (Fig. 2). One observes from the figures that the anomalous vertex part remains approximately constant for all of the modes, while each of the other two parts is small for the A-symmetric modes, but has large contributions from the B-symmetric ones, as would be expected on the basis of the phonon anomalies computed in Sec. III. The figures can be shown to be approximately constant by performing the same calculation at different temperatures, using the slightly different self-consistent values of the u-RVB order parameter $\bar{\chi}$ and chemical potential μ at each. The total free-energy shift for these four modes of a bilayer is compared with twice the free energy of the single-layer system.[29] The net contribution corresponds to a 1.1% enhancement of T_{RVB}, a magnitude exactly in line with the qualitative expectation, which to the same degree of accuracy is a 1.2 K enhancement. The isotope shift for $^{16}\mathrm{O}\rightarrow{}^{18}\mathrm{O}$ on this quantity is approximately -6%, leading to the prediction of a total shift due to in-plane oxygen of -0.07 K. The equivalent α parameter is 0.005. We would expect the quantitative agreement to be improved when interplane hopping processes are taken into account (Sec. III), in order to describe correctly the contributions from the A-symmetric modes (Table I).

This result may be compared with a recent site-selective substitution study of YBCO near optimal doping, performed by Zech *et al.*[46] These authors were able to achieve high exchange rates of $^{16}\mathrm{O}$ by $^{18}\mathrm{O}$ during crystal preparation, while discerning with good resolution the location of the exchange, whether it was on planar O(2) and O(3) sites, or apical O(4) and chain O(1) sites. They measured a total O isotope shift (complete exchange) of -0.25 K, of which at least 80%, or -0.20 K, was found to be due to modes of in-plane oxygen. Qualitatively, this conclusion contains im-

TABLE I. Lowest-order spinon-phonon coupling contributions to the s-RVB transition temperature. The magnitude is relative to $T_{\mathrm{RVB}}=0.069J$, and the sign is chosen so that a positive contribution corresponds to an enhancement of T_{RVB}. Figures are given at T_{RVB} for the four modes involving c-axis motion of planar O(2) and O(3) atoms (Fig. 2), and for the three types of process shown in Fig. 13(b).

	(i)	(ii)	(iii)	total
A_{1g}	1.545×10^{-3}	3.453×10^{-4}	-3.588×10^{-4}	1.532×10^{-3}
B_{1g}	1.319×10^{-3}	-1.775×10^{-4}	3.210×10^{-3}	4.351×10^{-3}
A_{2u}	1.812×10^{-3}	3.755×10^{-4}	-4.223×10^{-4}	1.765×10^{-3}
B_{2u}	1.718×10^{-3}	-2.558×10^{-3}	4.547×10^{-3}	3.708×10^{-3}

portant agreement with the current picture, that it is the planar O modes which are most strongly coupled to the superconducting interaction. At the quantitative level, the theoretical result from the c-axis modes appears to be too small by a factor greater than 2, which, while constituting an acceptable level of agreement given the nature of the model, is not in as good accord as the phonon anomaly results within the same approximation.

We have shown that a realistic spin-phonon coupling within an electronic model for superconductivity can show the small isotope effect consistent with experimental observation in the high-T_c superconducting ceramics at optimal doping. In the present theory we would not expect to see significant alterations in the magnitude of this shift on changes in doping, which will act to move the chemical potential and cause minor changes in the spinon dispersion (Fig. 4) away from the optimally doped level. From the phase diagram discussed in Sec. IV, one observes that T_c falls with increasing doping in the overdoped region, where it is given by $T_{\rm RVB}$, and with decreasing doping in the underdoped region, where it is given by T_B (Fig. 12). With ΔT_c ($\Delta T_{\rm RVB}$) approximately constant, the threefold reductions in T_c achieved experimentally by overdoping in some systems[66] would give a commensurate increase in α; in the underdoped regime, the changes in T_B with doping have not been estimated.

From these considerations, it seems unlikely that the t-J framework alone contains the origin of the spectacular changes in isotope effect with doping reported in experiment, or that a purely electronic picture could account for the apparent changeover to large values ($\simeq 0.5$) of α which these data present. However, the situation is complicated due to questions of O disorder, and even equilibrium position, on doping and isotope substitution, the actual fraction of O in the plane sites, and the sensitivity of charge fluctuations to these uncertainties. At minimum, we may suggest that the results show once again the spin-phonon interaction to be a detectable effect which can be used to probe the physics of the high-T_c materials, but to be only a small perturbation on the dominant processes. In the case of the isotope effect, this perturbation is seen clearly at the optimal doping level where the dominant contribution vanishes, but a full explanation of the latter will require additional or separate physics. Ideas which have been put forward[66] include van Hove singularities, interlayer pair tunneling, bipolaron formation, strong Coulomb correlations and isotope-dependent hole concentration, but many models based on these contain a conventional, often phenomenological, electron-phonon interaction, and suffer from other weaknesses which this entails.

VI. CONCLUSION AND DISCUSSION

We have proposed a theory of spin-phonon coupling, based on the mean-field approximation to the extended t-J model of a single CuO_2 plane, which provides good agreement with a variety of experimental observations on high-T_c cuprates of the YBCO class. A key element is the buckling of the CuO_2 plane present in these materials, which causes the coupling to be linear in O displacement along the c axis. The model contains the following features.

(i) It gives, without recourse to parameter fitting, a semiquantitative account of the frequency and linewidth anomalies observed in the important and well-characterized B_{1g}- and B_{2u}-symmetric phonon modes of planar oxygen atoms in the stoichiometric O_7 compound.

(ii) The symmetry of the superconducting gap consistent with experiment is found to be predominantly $d_{x^2-y^2}$.

(iii) The conclusions are supported by the results obtained for different phonon mode types, and from observations in other materials.

(iv) Those features of the phonon anomalies which are not given by the present treatment are expected to be readily described within the same framework by consideration of a bilayer structural unit, and by a more sophisticated treatment of the intrinsic phonon linewidth.

(v) At lower doping levels, away from that for optimal T_c, there is good qualitative agreement, which provides additional strong evidence, consistent with the results from NMR and inelastic neutron scattering, for the origin of the spin gap.

(vi) There is a satisfactory degree of correspondence with the measured isotope shift near optimal doping, and the phonon modes giving the most important contributions to this are identified.

The single-layer t-J model for the strongly correlated CuO_2 system has thus been shown to contain an additional class of physical phenomena, namely those related to structural anomalies. The theory is found to be well suited to illustrating a variety of interesting properties observed in experiment, and to constitute a basis for further development.

Based on the results for alteration of phonon dynamics by spin excitations, it would seem logical also to seek the alteration of spin dynamics by their interaction with the phonon degrees of freedom. In fact this study was motivated initially by the failure of the extended t-J model to reproduce at the mean-field level some features of the YBCO spin excitation spectrum, notably the 41 meV peak in the O_7 compound.[67,68] The close coincidence of this resonance energy with the frequency of the B_{1g} mode, whose superconducting anomalies are the strongest, and the T dependence of the peak intensity, which scales with $\Delta^2 \propto \rho_s$, the superfluid density, make the present spin-phonon coupling theory appear well suited to explain these features. However, as in Secs. III and V, the phonon contributions to the spin susceptibility through the spin-phonon coupling vertices of Sec. II are of the order of a few percent, while the 41 meV peak dominates the entire spin response.[69] One may consider instead direct coupling of the phonon to spin-flip processes via the spin-orbit (Dzyaloshinskii-Moriya) interaction in the buckled CuO_2 plane,[70] but this will be two orders of magnitude smaller still. We note also that the exact position of the resonance depends on the doping δ, with the energy declining on moving to lower doping,[71] while the frequency of the B_{1g} mode appears to remain approximately constant. In addition, there is no trace of an analogous feature in the spin response associated with the B_{2u} phonon mode, which also shows a considerable anomaly.

While we have explored in some detail the consequences of a spin-phonon coupling in this class of model, many questions remain. One of the major shortcomings of the theory is its failure to deal systematically with a physical range of hole-doping levels, as explained in Secs. III and V, but de-

spite this it does provide a consistent description of the spin gap, as discussed in Sec. IV. Another issue which remains a drawback of the slave-boson formulation is the treatment of the holon degrees of freedom: in the model they have an intrinsic tendency towards Bose condensation, and thus contribute little to the dynamical phenomena, even within a gauge-field scheme where the appropriate spin- and hole-backflow requirements are enforced, leading to the Ioffe-Larkin composition rules for transport properties.[72,22] Some studies indicate that the holes also possess a Fermi surface,[73,74] which suggests that the appropriate physical description will require hard-core bosons or secondary statistical transmutation. In the present context, this would lead to the introduction of a meaningful second temperature scale in the low-doping regime (Sec. IV), and the possibility of a realistic account not only of the development of the phonon anomalies, but also of the features in the spin response detailed by NMR and inelastic neutron-scattering experiments.

To elaborate on the observable consequences of a gauge-theory approach to describing fluctuations around a mean-field solution, we have considered the possibility of gauge-field screening[22] of the phonon anomalies. This is discussed briefly in the appendix for the massive, longitudinal gauge modes, which can in principle have a Fano-type coupling to phonons. We show that the corrections due to gauge fluctuations are small or vanish, depending on the phonon mode symmetry. However, the effects of the massless, transverse gauge modes in providing quasiparticle self-energy and vertex corrections have been studied only briefly in the context of their influence on the dynamical properties of the spin degrees of freedom,[75] and remain an open question.

In conclusion, we propose that the model discussed represents a useful step in the formulation of a coherent theory of spin excitations, transport properties and lattice degrees of freedom. The agreement between theory and experiment achieved at the current level is encouraging in efforts to construct a unified picture of the anomalous metallic state, whose characterization is vital to a full understanding of high-temperature superconductivity.

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APPENDIX

Fluctuations about the mean-field solution of the order parameters in a model of the type we consider may be taken into account by the introduction of a gauge field,[22] whose transverse components, corresponding to phase fluctuations, turn out to be massless, and whose longitudinal component, originating in the temporal part of the fluctuation coordinate and corresponding to density fluctuations, is massive. Without going into the full details of the gauge-field formulation, we may consider the effect of possible gauge-field screening in the spin-phonon coupling problem as follows.

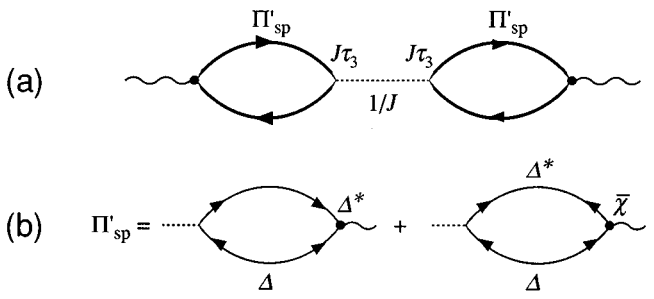

FIG. 14. Gauge-field correction to the lowest-order spinon polarization. (a) Representation of all orders of correction due to gauge field. (b) End bubbles in diagrammatic sequence, showing $O(\Delta^2)$ nature.

The bare gauge field is merely a restatement of boson-fermion coupling within the slave-boson decomposition, and has no dynamics, but the boson and fermion polarization terms, occurring in sequences of any length, act to generate effective dynamical properties.[22] Restricting the discussion to Fano-type processes, the full gauge-field correction by polarization terms to the lowest-order spinon-phonon diagram shown in Fig. 3 is then simply the diagram in Fig. 14(a), where the dotted line is the full dynamical gauge-field propagator $-1/(\Pi_B+\Pi_F)$. Because the phonon vertex, from t and J terms, contains only spin-spin and density-density components, it may couple only to the longitudinal part of the gauge field, whose propagator is simply that of a mass $M_0 \sim J$, while the magnitude of the gauge-field vertex is approximately J; these considerations may be made more quantitative, but the important feature of the result is unaffected. As only the spinon coupling to the phonon is considered, each end ''bubble'' in the full gauge-field-mediated sequence, with one k-dependent phonon and one constant gauge vertex, may be denoted by Π'_{sp}, in which case the total corrected expression at the order of Fig. 3 is $\Pi_{sp}-\Pi'^2_{sp}$.

Brief examination of the diagram [Fig. 14(b)] for Π'_{sp} shows that at $q=0$ the expression must be $O(\Delta^2)$: with a u-RVB vertex the anomalous propagators are required, while with an s-RVB vertex, of $O(\Delta)$, a single anomalous propagator appears, so the correction will unavoidably be $O(\Delta^4)$, and unimportant. One may write down an expression analogous to (9) for Re Π'_{sp}, and find that the form factor is

$$F'_k = 2\Delta^2 \eta_k \left(\gamma_k \xi_k + \frac{3J}{4} \bar{\chi} \eta_k^2 \right), \quad B_{1g},\ B_{2u} \text{ modes},$$

$$F'_k = 2\Delta^2 \eta_k \left(\eta_k \xi_k + \frac{3J}{4} \bar{\chi} \gamma_k \eta_k \right), \quad A_{1g},\ A_{2u} \text{ modes}. \tag{A1}$$

This is odd in η_k for the B-symmetric modes (in fact for both s and d symmetry of the singlet order parameter), and so

vanishes upon k integration, while for A-symmetric modes it remains of the order of Π_{sp}, and so becomes irrelevant on taking the square. Thus the consequence of considering fluctuations through a gauge-field coupling, which will involve only massive longitudinal modes with no singularities in momentum space, is that their correction is small or vanishing.

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