PHYSICAL REVIEW B VOLUME 50, NUMBER 10 1 SEPTEMBER 1994-II

Spin-phonon renormalization of the excitation energy in a dilute two-dimensional antiferromagnet

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(Received 7 June 1993; revised manuscript received 15 November 1993)

The contribution of spin-lattice coupling to the phonon self-energy is calculated in a dilute two-dimensional antiferromagnet. The calculations are based on a bond percolation model of the CuO_2 plane of high-T_c copper oxides recently proposed by some of the authors. Numerical results are presented for the dampings of phonon excitations relating to three different situations. They are two magnons (Case A), one magnon and one fracton (Case B), and two fractons (Case C) involved in the phonon self-energy process. At low temperatures, the damping rate is much smaller than the frequency of excitations, leading to well-defined phonons for all the cases. The overall features of the $\Gamma_q \sim q$ curves possess similar characteristics: Γ_q increases linearly with q in the small-q region, reaching a maximum at an intermediate q, and after that scales nearly as q^{-2} until q approaches the edge of the Brillouin zone. The temperature-dependent phonon linewidths arising from spin-lattice coupling are also presented. We point out the sensitivity of the interaction involving fractons on bond concentration of the network. Relevance of the calculated results to experimental data are discussed.

I. INTRODUCTION

Since the discovery of high-T_c cuprate superconductors, the two-dimensional (2D) Heisenberg antiferromagnet has received much attention. It has become well-known that the parent materials of the cuprate superconductors are antiferromagnetic (AF) insulators which undergo a phase transition to superconductors when dopant holes are introduced. The interplay between AF ordering and hole doping is considered important to the mechanism of high-T_c superconductivity. While hole doping strongly reduces the effective intralayer Cu-Cu superexchange coupling constant, and destroys quickly the long-range AF order,[1,2] experiments[3–5] suggest that there are still short-range AF fluctuations in the metallic regime. The effect of spin dynamics of the CuO_2 plane on physical properties of the cuprate superconductors is an interesting subject. Many theories[6] have considered the spin-wave renormalization of a hole in Heisenberg antiferromagnets though this is not the purpose of this paper. The investigations of Bucher *et al.*[7] indicated that the CuO_2 plane transport in the normal state is governed by the spin dynamics. Tyč and Halperin[8] studied the damping of spin waves due to magnon-magnon scattering in a 2D Heisenberg antiferromagnet at low temperatures and obtained rich understandings about the dynamical properties of the 2D antiferromagnet. Canali, Girvin, and Wallin[9] computed the spin-wave velocity renormalization in the 2D Heisenberg antiferromagnet and show that the $O(1/S^2)$ correction term makes the agreement between the spin-wave theory result and the series-expansion estimate almost perfect. Also the effects of cyclic four-spin exchange in the CuO_2 plane have been studied by Honda, Kuramoto, and Watanabe[10] who discussed the effects of J_c upon magnetic Raman scattering and upon properties of the ground state. However, the possible influence of spin dynamics on lattice dynamics in the CuO_2 plane still remains to be investigated. Recently, Tsai[11] calculated the modified magnon spectrum of the CuO_2 plane due to phonon-magnon interaction and studied the possibility of phonon-induced antiferromagnetic magnons in the cuprates at low temperatures. Generally speaking, one can also expect an influence on the phonon excitations themselves by a coupling to magnetic degrees of freedom. Recent experiments[12] have revealed a correlation between the anomalies of phonons and spin excitations in the Y-Ba-Cu-O system but the significance of spin-lattice coupling on phonon excitations has not been appreciated.

In this paper, we present a study of the spin renormalization of phonon excitations in high-T_c copper oxides. Especially, we will discuss the change of phonon lifetime due to the coupling to spin excitations. We do this by calculating the contribution of spin-lattice coupling to the phonon self-energy in the CuO_2 plane. The model we use is described in Sec. II, where the interaction Hamiltonian is introduced and the effective-medium approximation is used to deal with the randomly broken superexchange coupling. In Sec. III, we present a study of the effect of the interaction on phonon self-energy at low temperatures. The $\Gamma_q \sim q$ curves are plotted there and they show that the spin-lattice coupling is strongly **q** dependent. The calculations of temperature-dependent phonon self-energy are contained in Sec. IV, which includes a discussion of the relevance of the calculated phonon linewidths to Raman experiments. We point out the sensitivity of the interaction involving fractons on the

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bond concentration of the network. The conclusions of this work are given in Sec. V.

II. MODEL

We start from a bond percolation model of the CuO_2 plane recently proposed by some of the authors.[13] Since the superexchange interaction of adjacent localized spins (which is presented on the Cu sites) is mediated *via* the oxygen atoms, the hole doping which is believed to be on the oxygen sites[14] will have a drastic effect on the destruction of the AF couplings. So far as we consider the magnetic properties, the effect of adding holes to the CuO_2 plane may be accounted by randomly breaking some of the superexchange couplings between two adjacent localized spins. This picture can be modeled as a bond percolation network in a dilute 2D antiferromagnet. We further assume that the effective exchange coupling constant J_{ij} obeys the probability density

$$P(J_{ij})=p\delta(J_{ij}-J)+(1-p)\delta(J_{ij}) , \quad (1)$$

where the bond concentration is p and the broken bonds $1-p$. J is the exchange coupling constant in the undoped regime.

Percolation networks are known to be homogeneous at long length scales (L longer than the percolation correlation length ξ_p), and exhibit fractal characteristics at shorter length scales ($L<\xi_p$).[15,16] Excitations on a fractal lattice are termed fractons.[15] Existence of fractons in dilute magnets has been confirmed by experiments[17] and it has been shown that fractons play an important role in many stages of physics for topologically disordered systems.[18–22] Thus, there are two types of magnetic excitations in this dilute 2D antiferromagnet, namely magnons and magnonlike fractons. Based on the *s-d* exchange interaction Hamiltonian, Li *et al.*[13] calculated the temperature-dependent resistivity arising from the scattering of electrons off fractons and magnons in this dilute 2D antiferromagnet. They found that the existence of fractons lead to a linear temperature dependence of the resistivity over a wide temperature range, which is consistent with experimental results in high-T_c cuprates. We further study in this paper the spin renormalization of phonon excitations in this dilute 2D antiferromagnet.

The dominant spin-phonon interaction arises from the strain modulation of the exchange integral between copper d electrons. To lowest order in power of the atomic displacement, this interaction is described by the following Hamiltonian:

$$H_I=\sum_{ij}[\nabla J(r_i-r_j)\cdot(u_i-u_j)]\mathbf{S}_i\cdot\mathbf{S}_j \quad (2)$$

with

$$\mathbf{u}_i=\sum_{q\lambda}\frac{\epsilon_{q\lambda}}{\sqrt{2MN\Omega_{q\lambda}}}e^{iq\cdot r_i}(b_{q\lambda}+b^{+}_{-q\lambda}) . \quad (3)$$

Here M is the mass of the Cu atoms, N the total number of the Cu sites, $\epsilon_{q\lambda}$ is the polarization vector, $\Omega_{q\lambda}$ is the phonon frequency, $b^{+}_{q\lambda}$ and $b_{q\lambda}$ are the phonon creation and annihilation operators. Here and thereafter $\hbar$ will be set equal to 1. In fact, a Hamiltonian similar to that described by Eq. (2) has been used recently by Tucker and Dyre[23] to study phonon excitations in Heisenberg magnets, though their studies have different emphasis than ours.

Introducing the Dyson-Maleev transformation

$$S_i^-=a_i^+ , \quad S_i^+=(2S-a_i^+a_i)a_i , \quad S_i^z=S-a_i^+a_i , \quad (4a)$$

$$S_j^-=-b_j , \quad S_j^+=-b_j^+(2S-b_j^+b_j) , \quad S_j^z=b_j^+b_j-S , \quad (4b)$$

into Eq. (2), one has

$$H_I=S\sum_{ij}[\nabla J(r_i-r_j)\cdot(u_i-u_j)] \times(a_i^+a_i+b_j^+b_j-a_ib_j-a_i^+b_j^+) , \quad (5)$$

where a_i and b_j are bose operators. Then we go to collective coordinates, and make a unitary transformation to the new operator set α_k,β_k:

$$a_i=\sqrt{2/N}\sum_k e^{ik\cdot r_i}a_k , \quad b_j=\sqrt{2/N}\sum_k e^{-ik\cdot r_j}b_k , \quad (6a)$$

$$a_k=u_k\alpha_k+v_k\beta^{+}_{-k} , \quad b_k=u_k\beta_k+v_k\alpha^{+}_{-k} . \quad (6b)$$

Following the usual way of choosing u_k,v_k,

$$u_k=\cosh\theta_k , \quad v_k=\sinh\theta_k , \quad (7a)$$

$$\tanh(2\theta_k)=-\gamma_k , \quad \gamma_k=\frac{1}{Z}\sum_\delta e^{ik\cdot\delta} , \quad (7b)$$

we find

$$H_I=\sum_{q\lambda}{}'\frac{1}{\sqrt{2MN\Omega_{q\lambda}}}(b_{q\lambda}+b^{+}_{-q\lambda})\sum_k H_k , \quad (8)$$

with

$$H_k=(a^{+}_{k-q}a_k-b^{+}_{k+q}b_k)j_q -(a_{k+q}b_k-a^{+}_{k-q}b_k^{+})(j_k-j_{k-q}) . \quad (9)$$

The prime in the sum of Eq. (8) means that the wave vectors $\mathbf{q}$ are confined to the $\mathbf{k}$ set. In obtaining Eq. (9), we have defined j_k as

$$j_k=\sum_j[\nabla J(r_i-r_j)\cdot\epsilon_{q\lambda}]e^{ik(r_i-r_j)} , \quad (10)$$

which is expected to be independent of $\mathbf{r}_i$ because of the periodic boundary condition. As a preliminary step to evaluate j_k, we define another quantity J_g by

$$J_g=\sum_j J(r_i-r_j)e^{ig(r_i-r_j)} , \quad (11)$$

then one finds

$$j_k=-(ik\cdot\epsilon_{q\lambda})J_k . \quad (12)$$

In obtaining Eq. (12), we defined $J_{ii}=0$ to extend the sum over i,j without restriction. The calculation of J_k is not simple since we have assumed the randomly broken exchange coupling constant for adjacent Cu spins. However, one can rewrite Eq. (11) by using the nearest-neighbor approximation

$$J_g=\sum_\delta J(\delta)e^{ig\cdot\delta}\ , \tag{11a}$$

the sum here runs over the nearest-neighbor Cu sites. Then $J(\delta)$ is treated in the effective-medium approximation,[24] in which $J(\delta)$ is replaced by a uniform coupling constant $\bar{J}$. Following Ref. 24, we get

$$\bar{J}=2J(p-p_c)\left[1-\frac{\Omega G_0(\epsilon)}{2J(p-p_c)}+\frac{\Omega G_0(\epsilon)}{4J(p-p_c)^2}\right]\ , \tag{13}$$

for the bond percolation network on a 2D lattice. Here Ω is the phonon frequency, and $G_0(\epsilon)$ is given by

$$G_0(\epsilon)=\int_0^\infty \exp[-(2+\epsilon)x][I_0(x)]^2dx\ ,$$

where $\epsilon=\Omega/\bar{J}$ and $I_0(x)$ is the modified Bessel function of order 0. We are now able to obtain from Eq. (11a)

$$J_k=\bar{J}Z\gamma_k\ , \tag{14}$$

which produces the result

$$j_k=-i\bar{J}Z\gamma_k(k\cdot\epsilon_{q\lambda})\ . \tag{15}$$

On combining Eqs. (7), (8), (9), and (15), one gets

$$H_I=\sum_{q\lambda,k}{}'(b_{q\lambda}+b^+_{-q\lambda})\{M^\alpha_{q\lambda,k}\alpha^+_{k-q}\alpha_k+M^\beta_{q\lambda,k}\beta^+_k\beta_{k-q}+M^\zeta_{q\lambda,k}\alpha^+_{k-q}\beta^+_k+M^\eta_{q\lambda,k}\alpha_k\beta_{k-q}\}\ . \tag{16}$$

The phonon-magnon (magnonlike fracton) coupling constants $M^\alpha_{q\lambda,k}$, $M^\beta_{q\lambda,k}$, $M^\zeta_{q\lambda,k}$, and $M^\eta_{q\lambda,k}$ are given in Appendix A.

III. LOW TEMPERATURES

In order to gain a conceptual understanding of the effect of spin-lattice coupling on phonon excitations, we perform a calculation of the phonon self-energy using the zero-temperature Green's function techniques. For simplicity as well as clarity, we study one term of Eq. (16), which presents the interaction between phonons and the β mode spin-wave excitations:

$$H_{I\beta}=\sum_{q\lambda,k}{}'M^\beta_{q\lambda,k}(b_{q\lambda}+b^+_{-q\lambda})\beta^+_k\beta_{k-q}\ . \tag{17}$$

It is easy to see that this term is similar to that of electron-phonon interaction. The proper self-energy of a phonon arising from this interaction is given by[25]

$$P^\beta(q,\Omega)=\frac{i}{2\pi}\int d\omega'\sum_k|M^\beta_{q\lambda,k}|^2G^0(k-q,\omega'-\Omega)G^0(k,\omega')\ . \tag{18}$$

Here $G^0(k-q,\omega'-\Omega)$ and $G^0(k,\omega')$ are the Green's functions of bare magnetic excitations (magnon and magnonlike fractons). They have the form[12]

$$G^0(k,\omega')=\frac{1}{\omega'-\omega_k+i\delta}\ , \tag{19}$$

where δ is a positive infinitesimal number. The polarization subscript λ in the phonon self-energy has been omitted in the conventional way, since the Hamiltonian does not mix polarization and we are interested in just one kind of phonon. By making use of the identity

$$\frac{1}{x+i\delta}=P\left[\frac{1}{x}\right]-i\pi\delta(x)\ ,$$

where P stands for the principle part, one has

$$P^\beta(q,\Omega)=\text{Re}P^\beta(q,\Omega)+i\ \text{Im}P^\beta(q,\Omega)\ . \tag{20}$$

The real part of the phonon self-energy $\text{Re}P^\beta(q,\Omega)$ leads to shift of excitation energy. We have calculated this quantity, which results as a small increase in the long-wavelength sound velocity. This effect is, however, not significant at low temperatures. So the following study concentrates on the imaginary part of the phonon self-energy, which expresses the damping or inverse lifetime of the phonon excitations arising from the spin-lattice coupling:

$$\Gamma^\beta_q=\text{Im}P^\beta(q,\Omega)|_{\Omega=\Omega_q}\ . \tag{21}$$

Then one finds it convenient to obtain from the above equations:

$$\Gamma^\beta_q=\sum_k|M^\beta_{q\lambda,k}|^2\delta(\Omega+\omega_{k-q}-\omega_k)\ . \tag{22}$$

This allows us to carry out numerical calculations. In the CuO_2 plane, Cu atoms form a square lattice with O atoms bridged between each nearest-neighbor Cu pair. When $\epsilon_{q\lambda}$ is in either x or y direction, the couplings will be maximum.

Thus we choose $\epsilon_{q\lambda}$ to be in the x direction. We further restrict the study to those phonons with **q** parallel to $\epsilon_{q\lambda}$. Then

$$|M^{\beta}_{q\lambda,k}|^2=\frac{J^2Z^2S^2}{2MN\Omega_q}\{(v_kv_{k-q}-u_ku_{k-q})q\gamma_q+(u_{k-q}v_k+u_kv_{k-q})[\gamma_k k\cos\theta-\gamma_{k-q}(k\cos\theta-q)]\}^2 . \quad (23)$$

Here θ is the angle between **k** and $\epsilon_{q\lambda}$, u_k, v_k, and γ_k are defined in Eqs. (6) and (7). The sum over **k** in Eq. (22) can be transformed into an integral. In doing this, we shall discuss several different situations in the interaction process.

As noted above, we have assumed that there are two kinds of magnetic excitations (magnons and magnonlike fractons). It has been predicted[15] and confirmed by experiment[16,26] that in a percolating network, propagating phonons or magnons at long wavelengths and low energies should crossover (at the crossover frequency ω_c) to localized fractons at higher energies and shorter length scales where the network has a fractal geometry. The fractons exhibit some interesting characteristics which are quite different from that of phonons and magnons (for details, please see Refs. 15 and 18). Whether magnons or fractons are involved in the phonon self-energy process depends on the frequency of the magnetic excitations (greater or less than ω_c). Considering this, we now come to the three cases:

Case A. $\omega_{k-q}<\omega_c$, and $\omega_k<\omega_c$, which means that two magnons are participating in the phonon self-energy process. In this regime, the excitation energy of a magnon is[27]

$$\omega_k=2\sqrt{2}Jm_1ka \quad (\omega_k<\omega_c) \quad (24)$$

and the sum over **k** in Eq. (22) can be transformed into an integral according to

$$\frac{1}{N}\sum_k=\frac{a^2}{2\pi^2}\int_0^{k_{\max}}k\,dk\int_0^{\pi}d\theta . \quad (25)$$

Here $m_1=S+0.078\,974$ and a the distance between two adjacent Cu atoms.

Case B. $\omega_{k-q}<\omega_c$, while $\omega_k>\omega_c$, that is, one magnon and one fracton are involved in the phonon self-energy process. For a magnon of frequency ω_{k-q}, its dispersion relation is expressed by Eq. (24). For a fracton, however, we have[28]

$$\omega_k=\omega_c(k\xi_p)^{D/\bar{d}}=\omega_f(ka)^{D/\bar{d}} \quad (\omega_k>\omega_c) , \quad (26)$$

where D is the fractal dimensionality and equals 1.9 for $d=2$,[15] $\bar{d}$ is the fracton dimension and is expected to be 1.33 for a 2D percolation network, ω_f is the fracton cutoff frequency defined in terms of the crossover frequency ω_c by $\omega_f=\omega_c(\xi_p/a)^{D/\bar{d}}$. ξ_p is the percolation correlation length which depends on the concentration p for the bond occupancy

$$\xi_p=a|p-p_c|^{-4/3} . \quad (27)$$

For a quantum percolation problem, p_c has been found to be 0.76 for the bond percolation on a square lattice.[29] The sum of Eq. (22) in this regime will be transformed to an integral according to[11]

$$\frac{1}{N}\sum_k=\frac{2K_{D-1}a^D}{(2\pi)^D}\int_{1/\xi_p}^{1/a}k^{D-1}dk\int_0^{\pi}(\sin\theta)^{D-2}d\theta , \quad (28)$$

with $K_D=\pi^{D/2}/\Gamma(D/2)$.

Case C. $\omega_{k-q}>\omega_c$, and $\omega_k>\omega_c$, then two fractons are taking part in the phonon self-energy process. In this regime, one expects that Eq. (26) holds for both ω_{k-q} and ω_k, the transformation from the sum in Eq. (22) to an integral should be done according to Eq. (28).

In the numerical calculations, we make use of parameters of the Y-Ba-Cu-O system, they are $J=0.12$ eV,[30] $a=3.8$ Å,[31] $v_s=5\times10^3$ ms^{-1}.[32] A Debye spectrum is assumed for the phonon excitations. In each case, the damping is calculated for three different bond concentrations, i.e., $p-p_c=0.01$, 0.02, and 0.03. The calculated results are shown in Figs. 1, 2, and 3.

The primary result is that the ratio of the phonon damping rate Γ_q to the phonon frequency Ω_q satisfies $\Gamma_q/\Omega_q \ll 1$, leading to well-defined phonon excitations in all the situations. From the curves, one finds that there exists a universal characteristic for the overall features: Γ_q increases linearly with q in the small-q region, reaching a maximum at an intermediate q, and after that scales nearly as q^{-2} until q approaches the edge of the Brillouin zone. Therefore, the spin-lattice coupling is strongly q dependent. Another observation is that the peak position has a shift for different situations. The most interesting, however, occurs at the p (bond concentration) dependence of the damping rate Γ_q. For Case A, Γ_q does not change much with the change of p. On the contrary, Γ_q decreases drastically with the variation of p from p_c for both Case B and C. In other words, the damping of pho-

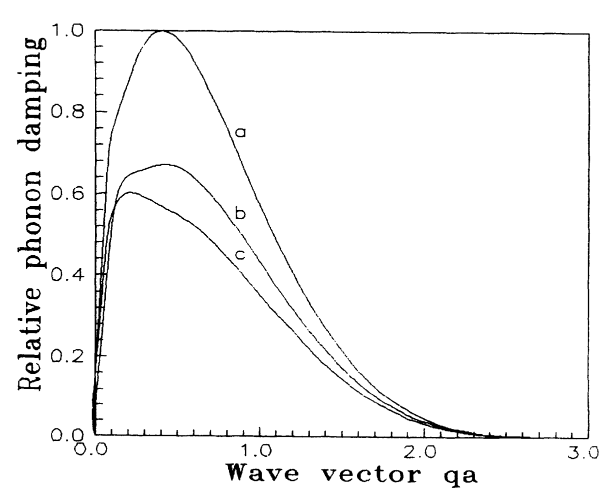

FIG. 1. Relative phonon damping $\Gamma^{\beta}_q/\Gamma^{\max}_q$ as a function of wave vector qa for Case A. Curves a, b, and c correspond to $p-p_c=0.01$, 0.02, and 0.03, respectively. $\Gamma^{\max}_q$ is 1.44×10^{-2} meV.

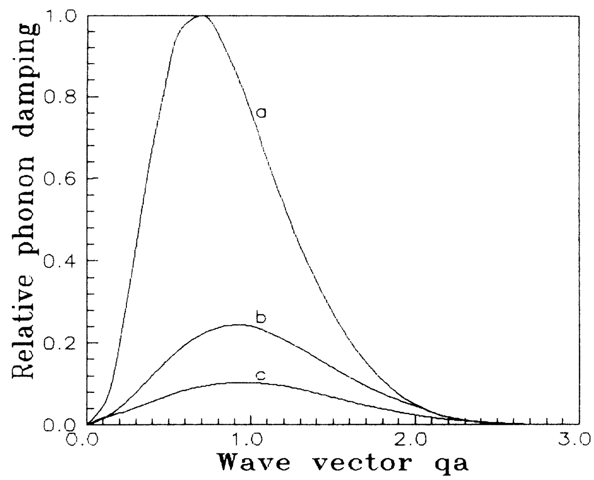

FIG. 2. Results as in Fig. 1 but for Case B. $\Gamma_q^{\max}$ is 7.13×10^{-3} meV.

nons involving fractons has a more significant p dependence than that involving only magnons. This can be understood in relation to the sharp p dependence of the percolation correlation length ξ_p. The percolation network appears to be self-similar or exhibits a fractal nature on length scales smaller than ξ_p. As is indicated by Eq. (27), when p approaches p_c, ξ_p increases as $|p-p_c|^{-4/3}$. If $p-p_c$ is small, the percolation network can be regarded as a fractal on a large length scale and one would expect that the phonon damping involving fractons be large in this situation. While when p deviates from p_c, the correlation length becomes shorter and shorter, and on a larger length scale, the system is regarded as being homogeneous. Therefore, the phonon damping involving fractons will decrease sharply with the deviation of p from p_c. In Case A, where only magnons are taking part in the phonon self-energy process, the less significant p dependence is easily understood because the magnons' contribution changes very slightly with the deviation of p from p_c. This indicates a strong sensitivity of the interaction involving fractons on bond concentration. One can further conclude that when $p-p_c$ is small, Cases B and C will dominate the phonon self-energy process, while for large $p-p_c$, Case A will contribute most to the phonon self-energy.

IV. TEMPERATURE-DEPENDENT PHONON SELF-ENERGY

In the following, we shall compute the phonon self-energy resulting from the spin-lattice coupling as a function of temperature. To proceed, we consider the total Hamiltonian of the coupled spin-lattice system in the bond percolation network

$$H=\sum_{q\lambda}\Omega_{q\lambda}(b_{q\lambda}^{+}b_{q\lambda}+\tfrac{1}{2})+\sum_{k}\omega_k\{(\alpha_k^{+}\alpha_k+\tfrac{1}{2})+(\beta_k^{+}\beta_k+\tfrac{1}{2})\}+H_I\ , \quad (29)$$

and H_I is given by Eq. (16). Defining the one-particle retarded Green's function for phonons

$$D(q,\Omega)=\langle\langle A_{q\lambda}|A_{-q\lambda}\rangle\rangle=\frac{2\Omega_{q\lambda}}{\Omega^2-\Omega_{q\lambda}^2-2\Omega_{q\lambda}\Pi(q,\Omega)}\ , \quad (30)$$

where $A_{q\lambda}=b_{q\lambda}+b_{-q\lambda}^{+}$ and $\Pi(q,\Omega)$ is the phonon self-energy, we are able to get from the equation of motion (EOM) of $D(q,\Omega)$:

$$\Omega D(q,\Omega)=\Omega_{q\lambda}G(q,\Omega)\ . \quad (31)$$

Equation (31) contains the new Green's function

$$\langle\langle B_{q\lambda}|A_{-q\lambda}\rangle\rangle=G(q,\Omega)\ ,$$

where $B_{q\lambda}=b_{q\lambda}-b_{-q\lambda}^{+}$. The EOM of $G(q,\Omega)$ yields

$$\Omega G(q,\Omega)=2+\Omega_{q\lambda}D(q,\Omega)+2\sum_k\{M_{-q\lambda,k}^{\alpha}G_k^{\alpha}(q,\Omega)+M_{-q\lambda,k}^{\beta}G_k^{\beta}(q,\Omega)+M_{-q\lambda,k}^{\xi}G_k^{\xi}(q,\Omega)+M_{-q\lambda,k}^{\eta}G_k^{\eta}(q,\Omega)\}\ , \quad (32)$$

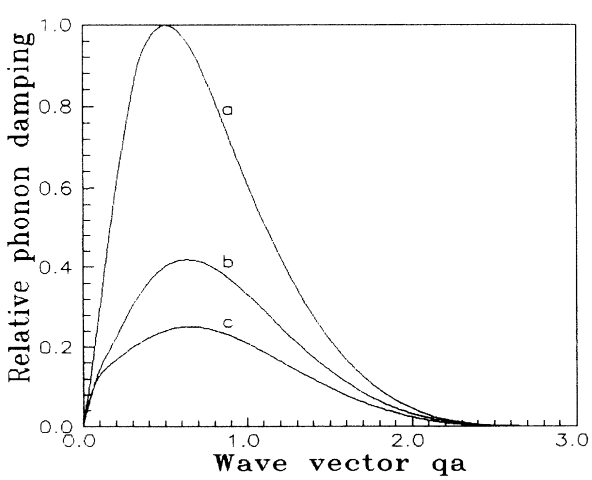

FIG. 3. Results as in Fig. 1 but for Case C. $\Gamma_q^{\max}$ is 1.26×10^{-2} meV.

where we have defined

$$G_k^{\alpha}(q,\Omega)=\langle\langle\alpha_{k+q}^{+}\alpha_k|A_{-q\lambda}\rangle\rangle\ ;$$

$$G_k^{\beta}(q,\Omega)=\langle\langle\beta_k^{+}\beta_{k+q}|A_{-q\lambda}\rangle\rangle\ ;$$

$$G_k^{\xi}(q,\Omega)=\langle\langle\alpha_{k+q}^{+}\beta_k^{+}|A_{-q\lambda}\rangle\rangle\ ;$$

$$G_k^{\eta}(q,\Omega)=\langle\langle\alpha_k\beta_{k+q}|A_{-q\lambda}\rangle\rangle\ .$$

After making some decoupling approximations

$$\langle\langle A_{q'\lambda}\alpha_{k+q}^{+}\alpha_{k+q'}|A_{-q\lambda}\rangle\rangle\simeq\langle\alpha_{k+q}^{+}\alpha_{k+q'}\rangle\langle\langle A_{q'\lambda}|A_{-q\lambda}\rangle\rangle=n_{k+q}\langle\langle A_{q'\lambda}|A_{-q\lambda}\rangle\rangle\delta_{qq'}\ ,$$

$$\langle\langle A_{q'\lambda}\alpha_{k+q-q'}^{+}\alpha_k|A_{-q\lambda}\rangle\rangle\simeq n_k\langle\langle A_{q'\lambda}|A_{-q\lambda}\rangle\rangle\delta_{qq'}\ ,$$

$$\langle\langle A_{q'\lambda}\alpha_k\beta_{k+q-q'}|A_{-q\lambda}\rangle\rangle\simeq0\ ,$$

$$\langle\langle A_{q'\lambda}\alpha_{k+q-q'}^{+}\beta_k^{+}|A_{-q\lambda}\rangle\rangle\simeq0\ ,$$

we get from the EOM of $G_k^\alpha(q,\Omega)$:

$$G_k^\alpha(q,\Omega)=\frac{1}{\Omega-\omega_k+\omega_{k+q}}(n_{k+q}-n_k)M^\alpha_{q\lambda,k+q}D(q,\Omega)\ . \tag{33}$$

Here n_k is the Bose-Einstein distribution function of magnons (or magnonlike fractons) with frequency ω_k. The other three can be obtained in the same way and the results are given in Appendix B. Combining these equations, one finds the phonon self-energy:

$$\Pi(q,\Omega)=\sum_k\left\{\frac{1}{\Omega-\omega_k+\omega_{k+q}}(n_{k+q}-n_k)M^\alpha_{-q\lambda,k}M^\alpha_{q\lambda,k+q}-\frac{1}{\Omega+\omega_k-\omega_{k+q}}(n_{k+q}-n_k)M^\beta_{-q\lambda,k}M^\beta_{q\lambda,k+q}\right.$$
$$\left.-\frac{1}{\Omega+\omega_k+\omega_{k+q}}(n_{k+q}+n_k)M^\xi_{-q\lambda,k}M^\eta_{q\lambda,k+q}+\frac{1}{\Omega-\omega_k-\omega_{k+q}}(2+n_{k+q}+n_k)M^\eta_{-q\lambda,k}M^\xi_{q\lambda,k+q}\right\}\ . \tag{34}$$

In order to make a link with experimental results, we then perform numerical calculations. Experimentally the Raman- and infrared-active phonons have been widely studied because they can provide much information about the magnitude of the superconducting energy gap. For example, measurements of the temperature dependence of the linewidth and frequency of the 340-cm^{-1} Raman-active $YBa_2Cu_3O_7$ phonons show significant anomalies with the opening of superconducting gap.[33–35] These transverse optical (TO) vibrational modes have the energies of the same order of the exchange coupling J, i.e., the same order as the magnetic excitations. Therefore, one can expect the coupling between them be strong. Experimentally observed phonon softenings occurring at T_c in high-T_c superconductors have been explained within the framework of strong-coupling Eliasberg theory by Zeyher and Zwicknagl.[36] Besides, some authors reported observation of phonon softenings taking place well above T_c in $YBa_2Cu_3O_7$.[12,37] These phonon softenings correspond to negative increase in the phonon shifts with decreasing temperature. The changes occur in a rather sudden way[12,37] and one should not expect that the present spin-lattice coupling mechanism be responsible for them because our assumption of the spin dynamics does not account for any sudden change, such as a gap formation in the spectrum of spin excitations. We have calculated the phonon shifts due to spin-lattice coupling. They result as a smooth negative increase with increasing temperatures, which must be considered as a background in the experimental curves.

The theoretical temperature dependence of the 340-cm^{-1} TO phonon linewidth $2\Gamma_q/\Omega_q$ arising from the spin-lattice coupling is given in Figs. 4, 5, and 6 for Cases A, B, and C, respectively. The parameters used are given in Sec. III and we study those phonons with $qa=0.1$, since the phonons measured in the Raman experiments often have small but nonzero vectors.[34] The wave-vector dependence of the optical phonon frequencies is ignored in the calculations. One can see from Figs. 4–6 that the relative phonon widths increase drastically with the increase of temperature for all three cases, indicating a more significant influence of spin dynamics on phonon excitations at elevated temperatures. The same tendency of temperature dependence had been obtained by Psaltakis and Cottam[38] in the study of magnon damping due to the spin-wave interaction in $S=1$ two-sublattice uniaxial magnets. This general feature agrees with experimental measurements in $YBa_2Cu_3O_7$.[12,33–35] However, if one compares the theoretical results with the Raman data (Fig. 2 of Ref. 34, for example) quantitatively, some discrepancies will be found: (1) when the temperature approaches zero, the theoretical linewidth tends to zero quickly, while the experimental result has a finite width; (2) the theoretical value for linewidth at 300 K is smaller than 10 cm^{-1}, a quantity smaller by a factor of 2 or more than the experimental measurements: (3) the calculated contribution of spin-lattice coupling to phonon linewidth behaves smoothly with the change of temperature, while Raman data show drastic broadening below T_c. However, we argue that these discrepancies show nothing but the soundness of our theoretical results. As we know, besides the spin-lattice coupling, some other mechanisms such as electron-phonon coupling, phonon anharmonic interaction, and defect-phonon scattering can also contribute to the change of phonon self-energy. In fact, the electron-phonon coupling has been shown to be responsible for the anomalous change of phonon linewidths occurring below the critical temperature.[36] The anhar-

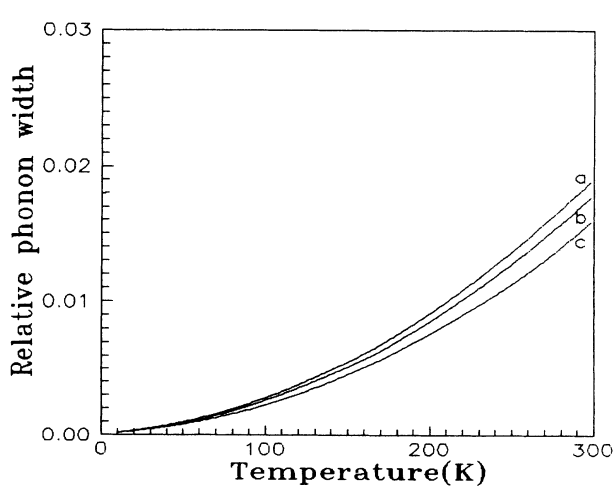

FIG. 4. Temperature dependence of relative linewidth $2\Gamma_q/\Omega_q$ of the 340-cm^{-1} TO phonons for Case A. Curves a, b, and c correspond to $p-p_c=0.01$, 0.02, and 0.03, respectively.

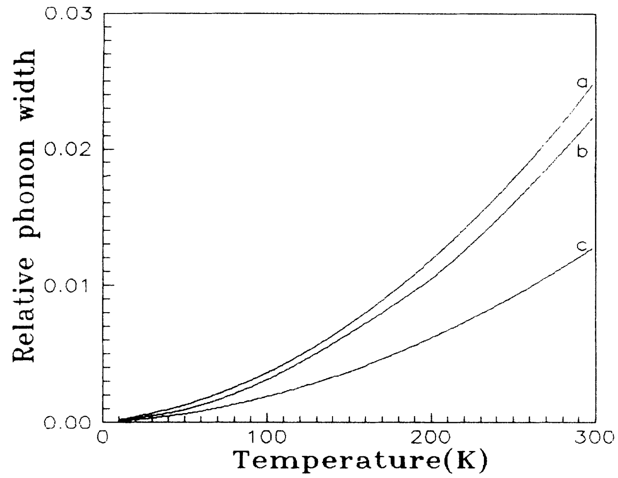

FIG. 5. Results as in Fig. 4 but for Case B.

monic decay of the zero wave-vector phonons into two phonons with opposite q vectors has been used to explain some of the experimental results.[33] And the defect-phonon interaction in high-T_c materials containing isotope defects was studied by Tao and Singh,[39] who demonstrated that the phonon relaxation effect resulting from this interaction may be an alternative explanation of the anomalous T^2 behavior of thermal conductivity of high-T_c cuprates. It seems likely that the electron-phonon coupling, phonon anharmonic decay and defect-phonon interaction, which we have not considered, account for the discrepancies between our theoretical results and experimental data. When they work together with the spin-lattice coupling, one could expect that the result gives the right magnitude compared with experimental measurements. We therefore think that our theoretical calculations are in fact supported by experiment.

If one seeks to find the p (bond concentration) dependence of linewidths for different cases, one can see from Figs. 4–6 a similar sensitivity of the interaction involving fractons on bond concentration with that observed in the previous section: for Case A where only magnons are involved, the width does not change much with the deviation of p from p_c; while for Cases B and C, this change is significant. Which process dominates the phonon self-energy depends strongly on the bond concentration. As has been discussed in Sec. III, this can be understood in relation to the p dependence of the percolation correlation length ξ_p.

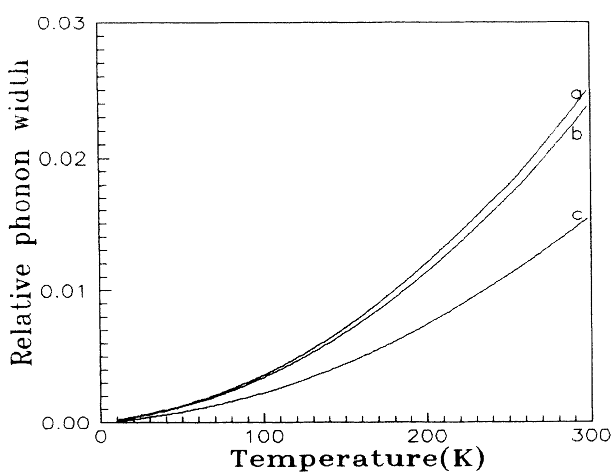

FIG. 6. Results as in Fig. 4 but for Case C.

V. CONCLUSIONS

In this paper we have studied the effect of spin-lattice coupling on phonon self-energy in a dilute 2D antiferromagnet. The effective-medium approximation has been used to treat the randomly broken superexchange couplings. Numerical results of phonon damping using the parameters of the Y-Ba-Cu-O system are presented for three different situations. The results indicate that the spin-phonon coupling is strongly q dependent. Interactions involving fractons are very sensitive to the bond concentration of the network. Raman-active phonons have the same energy scale with the magnetic excitations in the Y-Ba-Cu-O system, and they can influence each other strongly. The calculated results show that the spin-lattice coupling can have more significant influence on phonon self-energy in elevated temperatures. We compare the theoretical phonon linewidths with experimental Raman data and argue that our results are, in fact, supported by experiments though there exists some discrepancies between them.

It should be mentioned that we have ignored the oxygen phonon modes in our calculations. Thus our model seems to be describing an ideal dilute 2D antiferromagnet rather than the CuO_2 plane. Nevertheless, the adjacent Cu d electrons interact with each other *via* the O atoms, so the modulation of superexchange energy due to the displacement of O atoms is a high-order term, which has not been taken into consideration in the present study. Another point to be noted is the spin dynamics that we have assumed. Our calculations are based on the assumption that there exists a crossover from magnons to fractons in the dilute 2D antiferromagnet. In high-T_c cuprates, there is no direct experimental confirmation on this point. However, other considerations of the spin dynamics would not change the results qualitatively but amount to little more than small modifications, unless one supposes a gap formation in the excitation spectrum at a certain temperature. Recently Nagaosa and Lee[40] proposed a mean-field phase diagram for the CuO_2 plane where there is a spin-gap state, and some authors also interpreted their experimental results as the effect of a spin-gap formation.[7,12] But the study concerning the origin of a spin gap in the CuO_2 plane is still debated. Research in this direction will be worthwhile though, we believe that the results obtained from our model system are essentially adequate: the coupling of phonons to magnetic excitations strongly varies with the wave vector and has its maximum weight at intermediate q values; the coupling has a more significant influence on phonon self-energy at elevated temperatures; and the spin-phonon coupling involving fractons has a strong sensitivity on the bond concentration of the network.

ACKNOWLEDGMENTS

One of us (X.B.W.) would like to acknowledge J. W. Tucker for useful correspondence. D. C. Tian is grateful to Professor S. T. Chui of Bartol Research Institute, Delaware University for hospitality and discussions. This work is supported by the National Natural Science Foundation of China and the National Center for Superconductivity of China.

APPENDIX A

Phonon-magnon (magnonlike fracton) coupling constants:

$$M^{\alpha}_{q\lambda,k}=\frac{S}{\sqrt{2MN\Omega_{q\lambda}}}[(u_k v_{k-q}+u_{k-q}v_k)(j_k-j_{k-q})+(u_k u_{k-q}-v_k v_{k-q})j_q] ,$$

$$M^{\beta}_{q\lambda,k}=\frac{S}{\sqrt{2MN\Omega_{q\lambda}}}[(u_k v_{k-q}+u_{k-q}v_k)(j_k-j_{k-q})-(u_k u_{k-q}-v_k v_{k-q})j_q] ,$$

$$M^{\zeta}_{q\lambda,k}=\frac{S}{\sqrt{2MN\Omega_{q\lambda}}}[(u_k u_{k-q}+v_k v_{k-q})(j_k-j_{k-q})-(u_k v_{k-q}-u_{k-q}v_k)j_q] ,$$

$$M^{\eta}_{q\lambda,k}=\frac{S}{\sqrt{2MN\Omega_{q\lambda}}}[(u_k u_{k-q}+v_k v_{k-q})(j_k-j_{k-q})+(u_k v_{k-q}-u_{k-q}v_k)j_q] .$$

APPENDIX B

By making use of some decoupling approximations, we obtain from the EOM's of $G^{\alpha}_k(q,\Omega)$, $G^{\beta}_k(q,\Omega)$, $G^{\zeta}_k(q,\Omega)$, and $G^{\eta}_k(q,\Omega)$:

$$G^{\alpha}_k(q,\Omega)=\frac{1}{\Omega-\omega_k+\omega_{k+q}}(n_{k+q}-n_k)M^{\alpha}_{q\lambda,k+q}D(q,\Omega) ,$$

$$G^{\beta}_k(q,\Omega)=-\frac{1}{\Omega+\omega_k-\omega_{k+q}}(n_{k+q}-n_k)\times M^{\beta}_{q\lambda,k+q}D(q,\Omega) ,$$

$$G^{\zeta}_k(q,\Omega)=-\frac{1}{\Omega+\omega_k+\omega_{k+1}}(n_{k+q}+n_k)\times M^{\eta}_{q\lambda,k+q}D(q,\Omega) ,$$

$$G^{\eta}_k(q,\Omega)=\frac{1}{\Omega-\omega_k-\omega_{k+q}}(2+n_{k+q}+n_k)\times M^{\zeta}_{q\lambda,k+q}D(q,\Omega) .$$

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