Large isotope effect on T_c in cuprates despite a small electron-phonon coupling

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(Received 1 February 2009; revised manuscript received 31 July 2009; published 31 August 2009)

We calculate the isotope coefficients α and α^* for the superconducting critical temperature T_c and the pseudogap temperature T^* in a mean-field treatment of the t-J model including phonons. The pseudogap phase is identified with the d-charge-density wave (d-CDW) phase in this model. Using the small electron-phonon coupling constant $\lambda_d \sim 0.02$ obtained previously in local-density approximation calculations in $YBa_2Cu_3O_7$, α^* is negative but negligibly small, whereas α increases from about 0.03 at optimal doping to values around 1 at small dopings, in agreement with the general trend observed in many cuprates. Using a simple phase fluctuation model where the d-CDW has only short-range correlations, it is shown that the large increase of α at low dopings is rather universal and does not depend on the existence of sharp peaks in the density of states in the pseudogap state or on specific values of the phonon cutoff. Rather, it is caused by the large depletion of spectral weight at low frequencies by the d-CDW and thus should also occur in other realizations of the pseudogap.

DOI: 10.1103/PhysRevB.80.064519 PACS number(s): 74.25.Kc, 71.10.Fd, 71.10.Hf, 74.72.−h

I. INTRODUCTION

An open and rather controversially discussed topic in high-T_c superconductivity is the role played by phonons for the low-energy electronic properties and, in particular, the high transition temperatures T_c. A direct way to show the involvement of the lattice in electronic properties is the study of the isotope effect on T_c.[1] Experimentally, the corresponding isotope coefficient α is very small in high-T_c cuprates near optimal doping but increases strongly in the underdoped region attaining values being comparable or even larger than those in conventional phonon-mediated superconductors. It is often argued that these large observed isotope effects in the underdoped region give direct evidence for a large electron-phonon coupling in the cuprates.[1–3] It even has been suggested that it is so large that Eliashberg theory breaks down and that nonadiabatic and polaronic features play an important role in these systems.[4–7] Other approaches have suggested that large isotope effects may occur in the presence of a pseudogap.[8,9]

Below we show that the essential features of the isotope experiments on T_c can be explained within a mean-field approximation of the t-J model[10–13] using very small values for the electron-phonon coupling. The pure t-J model exhibits in mean-field approximation a competition of d-wave superconductivity and a d-charge-density wave (d-CDW) with transition temperatures T_c and T^*, respectively. The observed pseudogap can be identified with the d-CDW phase in this model.[12,14] Whereas many experiments support the idea of two competing phases,[15–21] the nature of the additional phase remains unclear and many proposals besides of the d-CDW have been considered.[22] Experiments suggest that its order parameter has d-wave symmetry like that of the superconducting phase. This favors an unconventional charge or spin-density wave state with internal d-wave symmetry rather than a conventional one with (anisotropic) s-wave symmetry. The t-J model yields at large N (N is the number of spin components) such a d-CDW but its relevance for the physical case $N=2$, for instance in form of a phase without long-range but strong d-wave short-range order, remains unclear.[23–25]

In Sec. II, we introduce our model, its phase diagram, and numerical results for the competing superconducting and CDW order parameters and the corresponding transition temperatures T_c and T^*. We then add phonons assuming always that the electron-phonon interaction is very small so that they can be treated in the weak-coupling approximation. Explicit formulas for the isotope coefficients α and α^* related to T_c and T^* will be given. In Sec. III, we present numerical results for the doping dependences of α and α^*. In Sec. IV, we extend our treatment by including off-diagonal fluctuations in the d-CDW state using the method of Refs. 26–28. In this way, the pseudogap phase is treated more realistically because the long-range order is removed and self-energy effects are included. Our conclusions are found in Sec. V.

II. THEORETICAL FRAMEWORK

We consider the t-J model[29] with the Hamiltonian H,

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma}c_{j\sigma} - t'\sum_{\langle i,j\rangle',\sigma} c^\dagger_{i\sigma}c_{j\sigma} + \frac{J}{2}\sum_{\langle i,j\rangle}\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}(J-2V_C)\sum_{\langle i,j\rangle} n_i n_j, \quad (1)$$

where $c^\dagger_{i\sigma}, c_{i\sigma}$ are creation and annihilation operators, respectively, for electrons at site i and spin projection σ subject to the condition that double occupancies of sites are excluded. The sums include nearest-neighbor $\langle i,j\rangle$ and next-nearest-neighbor $\langle i,j\rangle'$ sites on a two-dimensional (2D) square lattice and the corresponding hopping elements are t and t', respectively. $\mathbf{S}_i$ and n_i are spin and site-occupation operators, J the Heisenberg coupling constant, and V_C a Coulomb interaction between nearest neighbors.

One way to obtain a mean-field approximation for H is to introduce N spin components in Eq. (1), scale the coupling constants as $t \to 2t/N$, $t' \to 2t'/N$, $J \to 2J/N$, etc., and to consider the large N limit.[30] As a result, t and t' are renormalized yielding the quasiparticle dispersion $\epsilon(\mathbf{k})$. At the same time, the fermionic operators can be treated as usual creation and annihilation operators. Explicitly, one obtains $\epsilon(\mathbf{k}) = -2(\delta t + rJ)[\cos(k_x) + \cos(k_y)] - 4t'\delta \cos(k_x)\cos(k_y) - \mu$, with $r = 1/N_c \Sigma_{\mathbf{q}} \cos(q_x) f[\epsilon(\mathbf{q})]$, where f is the Fermi function, δ the doping away from half filling, and μ a renormalized chemical potential. Here and in the following, we use the lattice constant a of the square lattice as length unit. As previously discussed,[12,32] the relevant order parameters for our mean-field treatment of the t-J model are a CDW order parameter

$$\Phi(\mathbf{k}) = -\frac{i}{N_c}\sum_{\mathbf{q}} J(\mathbf{k}-\mathbf{q})\langle c^{\dagger}_{\mathbf{q}\uparrow} c_{\mathbf{q}+\mathbf{Q}\uparrow}\rangle, \tag{2}$$

with $J(\mathbf{k}) = 2J(\cos k_x + \cos k_y)$ and a superconducting (SC) order parameter

$$\Delta(\mathbf{k}) = \frac{1}{N_c}\sum_{\mathbf{q}} (J(\mathbf{k}-\mathbf{q}) - V_C(\mathbf{k}-\mathbf{q}))\langle c_{\mathbf{q}\uparrow} c_{-\mathbf{q}\downarrow}\rangle, \tag{3}$$

where N_c is the number of primitive cells, $\langle \cdots \rangle$ denotes an expectation value, $\mathbf{Q} = (\pi, \pi)$ is the wave vector of the d-CDW, and $V_C(\mathbf{k}) = 2V_C(\cos k_x + \cos k_y)$. The Coulomb interaction $V_C(\mathbf{k})$ between nearest neighbors has been introduced to prevent an instability of the d-CDW with respect to phase separation in some regions of phase space.[12] From the self-consistency condition for the self-energy, one obtains coupled equations for Φ, Δ, the chemical potential, and a renormalization contribution r to the band dispersion due to J.[12,32] Their most stable solutions have d-wave symmetries in the interesting doping regions, i.e., $\Phi(\mathbf{k}) = \Phi\gamma(\mathbf{k})$ and $\Delta(\mathbf{k}) = \Delta\gamma(\mathbf{k})$, with $\gamma(\mathbf{k}) = (\cos k_x - \cos k_y)/2$.

A similar mean-field approximation as above is obtained by using a slave-boson representation for H in Eq. (1), enforcing the constraint on the average, using usual mean-field decouplings for the third and fourth terms in H and dropping the antiferromagnetic order parameter. The above expressions for $\epsilon(\mathbf{k})$ as well as Eq. (3) are in this way exactly reproduced, Eq. (2), with $J/2 + V_C$ instead of J.

Figure 1 shows the doping dependence of Φ and Δ at zero temperature, calculated fully self-consistently for $t'/t = -0.35$, $J/t = 0.3$, and $V_C/J = 0.2$. In the overdoped region, $\delta \geq \delta_c \sim 0.14$ Φ is zero. In the underdoped region, $\delta \leq \delta_c$ Φ is nonzero and coexists with Δ. Δ shows a maximum near δ_c and decays approximately linearly in δ toward lower and higher dopings. The two order parameters compete with each other which causes the strong decay of Δ with decreasing doping in the underdoped region. Also shown in Fig. 1 are $T^{\star}$ (dash-dotted line) and T_c (dashed line) where Φ and Δ, respectively, vanish. $T^{\star}$ shows near δ_c a reentrant behavior which has a simple explanation: the piece of the $T^{\star}$ line above the T_c curve is unaffected by superconductivity. Discarding superconductivity, the $T^{\star}$ line would continue to the right, decreasing slowly and reaching the x axis only at around $\delta \sim 0.25$. Taking superconductivity into account, $T^{\star}$ and also Φ are suppressed by the presence of a finite Δ, i.e., below the T_c curve. Since Δ increases rapidly with decreasing temperature, $T^{\star}$ even bends back due to the strong repulsion and reaches the critical doping δ_c at zero temperature where Φ becomes nonzero. The re-entrant behavior thus reflects the strong competition of the CDW and SC order parameters. The occurrence of a large coexistence region of Δ and Φ, which extends down to $\delta = 0$, is plausible because the Fermi surface consists in the d-CDW state of arcs around the nodal direction[32] which are unstable against the formation of a BCS gap Δ.

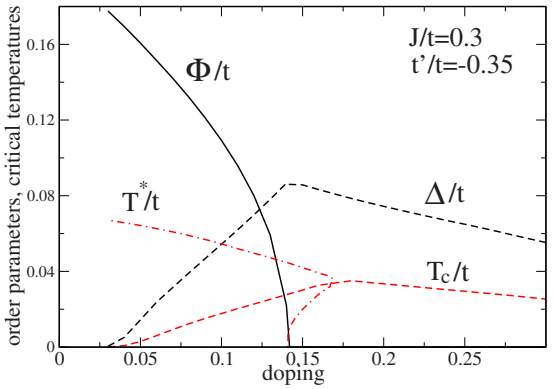

FIG. 1. (Color online) Zero-temperature order parameters Φ and Δ and the critical temperatures $T^{\star}$ and T_c as a function of doping.

In order to discuss the isotope effect, we consider a phonon-induced electronic density-density coupling between nearest neighbors and on the same atom. Approximating its frequency dependence by a rectangular form, as is often done in approximate solutions of the Eliashberg equation,[33] this effective electron-electron interaction has in the d-wave channel the form

$$v(\mathbf{q}, i\omega_n) = -2Vn_d(\mathbf{q}, i\omega_n)n_d(-\mathbf{q}, -i\omega_n), \tag{4}$$

$$n_d(\mathbf{q}, i\omega_n) = \frac{1}{N_c}\sum_{\mathbf{k},\sigma=1,2} \gamma(\mathbf{k})\Theta_n c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}. \tag{5}$$

Similarly, we have in the isotropic s-wave channel

$$w(\mathbf{q}, i\omega_n) = -\frac{W}{2}n(\mathbf{q}, i\omega_n)n(-\mathbf{q}, -i\omega_n), \tag{6}$$

$$n(\mathbf{q}, i\omega_n) = \frac{1}{N_c}\sum_{\mathbf{k},\sigma=1,2} \Theta_n c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}, \tag{7}$$

where V and W are electron-phonon (EP) coupling constants in the d- and s-wave channels, respectively, Θ_n the cutoff function $\Theta(\omega_D - |\omega_n|)$, ω_n the bosonic Matsubara frequency $\omega_n = 2n\pi T$, and ω_D the phonon cutoff frequency. $n_d(\mathbf{q}, i\omega_n)$ and $n(\mathbf{q}, i\omega_n)$ are electronic density operators with d- and s-wave symmetries, respectively. Effects due to a small EP interaction can be taken into account in the curves of Fig. 1 by adding the electronic self-energy due to $v(\mathbf{q}, i\omega_n)$ and $w(\mathbf{q}, i\omega_n)$ in the form of a Fock diagram. The resulting self-consistent equations lead to an equation for the renormalization function $Z(\mathbf{k}, i\omega_n)$ due to W. At $T = T_c$, this equation can be solved directly yielding $Z(\mathbf{k}, i\omega_n) \equiv Z = 1 + \lambda_s$, where λ_s is

the product of W and the electronic density at the Fermi energy and $T=T_c$, i.e., it refers in general to the d-CDW state. A second equation is obtained which determines the SC order parameter $\Delta(\mathbf{k},i\omega_n)$,

$$\Delta(\mathbf{k},i\omega_n) = -4\tilde{J}\gamma(\mathbf{k})\frac{T}{N_c}\sum_{\mathbf{k}'n'}\gamma(\mathbf{k}')g_{12}(\mathbf{k}',i\omega_{n'}) - 4V\gamma(\mathbf{k})\Theta_n\frac{T}{N_c}\sum_{\mathbf{k}'n'}\gamma(\mathbf{k}')\Theta_{n'}g_{12}(\mathbf{k}',i\omega_{n'}), \tag{8}$$

where $\tilde{J}$ is equal to $J-V_C$. g_{12} is the element (1,2) of the 4×4 matrix Green's function g. Its inverse $g^{-1}(\mathbf{k},i\omega_n)$ is given by

$$\begin{pmatrix} i\omega_n Z-\epsilon(\mathbf{k}) & -\Delta(\mathbf{k},i\omega_n) & -i\Phi(\mathbf{k},i\omega_n) & 0 \\ -\Delta(\mathbf{k},i\omega_n) & i\omega_n Z+\epsilon(\mathbf{k}) & 0 & i\Phi(\bar{\mathbf{k}},i\omega_n) \\ i\Phi(\mathbf{k},i\omega_n) & 0 & i\omega_n Z-\epsilon(\bar{\mathbf{k}}) & -\Delta(\bar{\mathbf{k}},i\omega_n) \\ 0 & -i\Phi(\bar{\mathbf{k}},i\omega_n) & -\Delta(\bar{\mathbf{k}},i\omega_n) & i\omega_n Z+\epsilon(\bar{\mathbf{k}}) \end{pmatrix}, \tag{9}$$

with the abbreviation $\bar{\mathbf{k}}=\mathbf{k}-\mathbf{Q}$. $\Phi(\mathbf{k},i\omega_n)$ is the d-CDW order parameter renormalized by the phonons and given by

$$i\Phi(\mathbf{k},i\omega_n) = -4J\gamma(\mathbf{k})\frac{T}{N_c}\sum_{\mathbf{k}'n'}\gamma(\mathbf{k}')g_{13}(\mathbf{k}',i\omega_{n'}) + 2V\gamma(\mathbf{k})\Theta_n\frac{T}{N_c}\sum_{\mathbf{k}'n'}\Theta_{n'}\gamma(\mathbf{k}')g_{13}(\mathbf{k}',i\omega_{n'}), \tag{10}$$

where g_{13} is the element (1,3) of the Green's function matrix g.

For the calculation of T_c, it is sufficient to linearize the right-hand side of Eq. (8) with respect to $\Delta(\mathbf{k},i\omega_n)$. Furthermore, we may neglect the phonon renormalization for Φ in this case. Below, we will be interested only in a small EP constant V yielding also only a small renormalization. Moreover, as will be shown below, this small renormalization is practically independent of the ionic mass M and thus may be neglected in calculating the isotope effect on T_c. We therefore have solved Eq. (10) using only the first term on the right-hand side and use the solution in Eq. (9) to obtain g_{12}. Equation (8) represents an integral equation with two separable kernels which can easily be solved. Writing Eq. (8) as a condition for T_c, we find

$$(1+F_{11})(1+F_{22})-F_{12}^2=0, \tag{11}$$

with

$$F_{11} = -2\tilde{J}\int_0^\infty d\omega\frac{N_d(Z\omega)}{Z\omega}\tanh\left(\frac{\omega}{2T_c}\right), \tag{12}$$

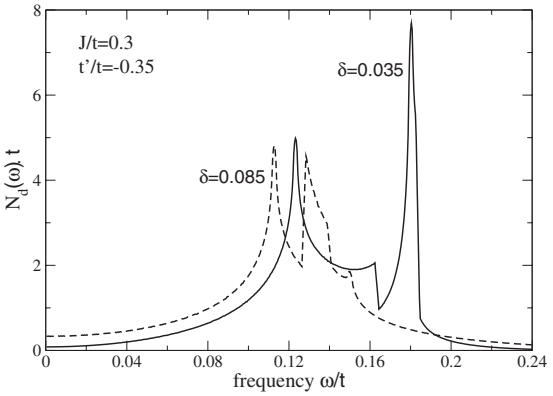

FIG. 2. Weighted density $N_d(\omega)$ of electronic states for two dopings δ.

$$F_{12} = -2\sqrt{V\tilde{J}}\int_0^\infty d\omega\frac{N_d(Z\omega)}{Z\omega}\frac{2}{\pi} \times\Im\left[\psi\left(\frac{1}{2}+\frac{i\omega}{2\pi T_c}\right)-\psi\left(\frac{\omega_D}{2\pi T_c}+1+\frac{i\omega}{2\pi T_c}\right)\right], \tag{13}$$

and $F_{22}=\sqrt{V/\tilde{J}}F_{12}$. ψ is the digamma function and $\Im$ denotes the imaginary part. $N_d(\omega)$ is given by

$$N_d(\omega) = \frac{2\omega}{\pi N_c}\sum_{\mathbf{k}}\gamma^2(\mathbf{k})\Im[G(\mathbf{k},\omega-i\eta)], \tag{14}$$

where η is a positive infinitesimal quantity,

$$G(\mathbf{k},z) = \frac{z^2-\epsilon^2(\bar{\mathbf{k}})-\Phi^2(\mathbf{k})}{[z^2-\lambda_1^2(\mathbf{k})][z^2-\lambda_2^2(\mathbf{k})]}, \tag{15}$$

and

$$\lambda_{1,2} = \frac{\epsilon(\mathbf{k})+\epsilon(\bar{\mathbf{k}})}{2} \pm \frac{1}{2}\sqrt{[\epsilon(\mathbf{k})-\epsilon(\bar{\mathbf{k}})]^2+4\Phi^2(\mathbf{k})}. \tag{16}$$

$N_d(\omega)$ represents a weighted density of electronic states at T_c and is shown in Fig. 2 for two different dopings. It consists of a sharp peak near the energy Φ due to excitations across the d-CDW gap and a structure at lower energies related to the van Hove singularity. It is convenient to characterize V by a dimensionless EP coupling constant

$$\lambda_d = VN_d(0). \tag{17}$$

According to the above equations, phonons affect T_c in a twofold way, namely, via $V=\lambda_d/N_d(0)$ and via $Z=1+\lambda_s$. λ_d and λ_s characterize the phonon-induced pairing interaction of d-wave and s-wave symmetries, respectively. Putting λ_s to zero V increases T_c. To see this, we rewrite Eq. (11) in the form $1+\hat{F}_{11}=0$. $\hat{F}_{11}$ is given by Eq. (12) if one makes there the change $\tilde{J}\to\tilde{J}/(1-F_{12}^2/(1+F_{22}))$. This means that V increases $\tilde{J}$ and thus increases T_c. On the other hand, if we put $V=0$, Eq. (11) reduces to $1+\hat{F}_{11}=0$ with $\hat{F}_{11}$ given by Eq. (12) modified by $\tilde{J}\to\tilde{J}/Z$ and $T_c\to T_cZ$. Each of these two changes diminishes T_c. Thus phonons may lower or may

TABLE I. Isotope coefficient α^* for different dopings δ.

δ	0.028	0.048	0.064	0.090	0.115	0.139	0.164
$100\alpha^*$	−0.20	−0.24	−0.27	−0.34	−0.42	−0.53	−0.66

increase T_c depending which of the above two effects is larger. Numerical calculations indicate that generically, the second effect dominates and that T_c decreases if one couples to phonons.[34] Most important for us is, however, the following observation. Our aim is not to determine the change in T_c when the electron-phonon coupling is turned on but when the ionic mass M is changed. It is well known that λ_s is independent of the ionic mass M, thus there will be no change in Z by isotope substitutions and α will always be positive. For small EP couplings, we may even put $Z=1$ and keep only the linear term in V in the calculation of the isotope coefficient $\alpha=-d\ln T_c/d\ln M$. From Eq. (11), one finds for α in this limit

$$\alpha = \frac{\omega_D}{T_c} F_{12} \left(\frac{\partial F_{12}}{\partial \omega_D}\right)\left(\frac{\partial F_{11}}{\partial T_c}\right)^{-1}, \tag{18}$$

where the derivatives in Eq. (18) are to be taken at the T_c without phonons and we also assumed $\omega_D \sim M^{-0.5}$.

III. RESULTS FOR THE ISOTOPE COEFFICIENTS

In deriving the above formulas, we assumed that the phonon-induced interaction V affects only Δ but not Φ and thus also not T^*. To check this approximation, we have calculated the isotope coefficient $\alpha^\star$ related to $T^\star$ and defined by $\alpha^*=-d\ln T^*/d\ln M$. The calculation of α^* is very similar to that of α.

Numerical values for α^* as a function of doping throughout the underdoped regime are given in Table I for $V/t=0.04$ and $\omega_D/t=0.1$. All values for α^* are negative, i.e., α^* shows an inverse isotope effect. However, this isotope effect is 2 orders of magnitude smaller than the usual BCS value of 1/2 and thus tiny. Furthermore, the absolute value of α^* decreases with decreasing doping quite in contrast to α as will be shown below. The negligible isotope effect on T^* which we found is in agreement with the experiment[8] though there exist also data which have been interpreted in terms of a large isotope coefficient α^*.[35] Strictly speaking, in our calculation of α, the renormalized d-CDW order parameter at $T=T_c$ enters the density of states function $N_d(\omega)$, Eq. (12). Since we have shown that T^* is independent of the ionic mass M, we may conclude that the d-CDW order parameter at $T=T_c$ has also only a negligible isotope effect justifying the above procedure to calculate α.

Figure 3 shows α as a function of doping for $V/t=0.04$ and two phonon cutoffs ω_D corresponding to the buckling and half-breathing phonon modes in $YBa_2Cu_3O_7$.[36] In the overdoped region, α is nearly independent of ω_D and δ and about 0.03, i.e., very small. In the underdoped region, α monotonically increases with decreasing δ and reaches appreciable values, for instance, 1/4 at a T_c which is only reduced by a factor of 2 from its maximum value.

To understand the increase of α at low dopings better, one can rewrite Eq. (18) approximately as $\langle N_d(\omega)\rangle/N_d(0)(-F_{22})$ using a low T_c approximation in the denominator. $\langle N_d(\omega)\rangle$ is an average of $N_d(\omega)$ around the phonon frequency ω_D over an energy interval of about ω_D. This interval is determined by the functions ψ in Eq. (13) and caused by the sharp cutoff in Matsubara frequencies. According to Fig. 2, $N_d(0)$ decreases rapidly with decreasing δ, reflecting the fact that $N_d(0)$ is due to the arcs left over from the Fermi line after formation of the d-CDW gap. The length of the arcs, however, decreases strongly with decreasing δ. From Fig. 2, it is clear that for most phonon frequencies, the large spectral weight near the d-CDW gap will substantially contribute to this average. As a result, $\langle N_d(\omega)\rangle/N_d(0)\gg 1$ and, since $-F_{22}$ is a slowly increasing function with decreasing δ, a large enhancement of α results at low dopings. A sharp cutoff for real frequencies, usually used in BCS theory, would yield $\langle N_d(\omega)\rangle=N_d(\omega_D)$. Consequently, α would exhibit strong resonances for $\omega_D\sim\Phi$ or, more generally, if ω_D is near well-pronounced peaks in $N_d(\omega)$. Implementing the phonon cutoff in terms of Matsubara frequencies, as we did, corresponds to a rather soft cutoff in real frequencies. Such a procedure is closer to an exact solution of Eliashberg equations, yields a finite phonon contribution to Z, and is also free of the above unphysical resonances in α if ω_D and the gap energy Φ are of similar magnitude. Another advantage of our procedure is that α depends only weakly on ω_D, also for $\delta\leq\delta_c$. If there is no pseudogap, $N_d(\omega)$ is rather constant in the phonon energy region which means that the above density ratio $\langle N_d(\omega)\rangle/N_d(0)$ is one and α very small for all dopings.

Qualitatively, the curves for α in Fig. 3 are similar to those in Refs. 8 and 9 where phenomenological pseudogaps were used and the problem of resonances was avoided either by considering only the limit $\omega_D\gg\Phi$ or by a non-states-conserving pseudogap. This as well as the above approxi-

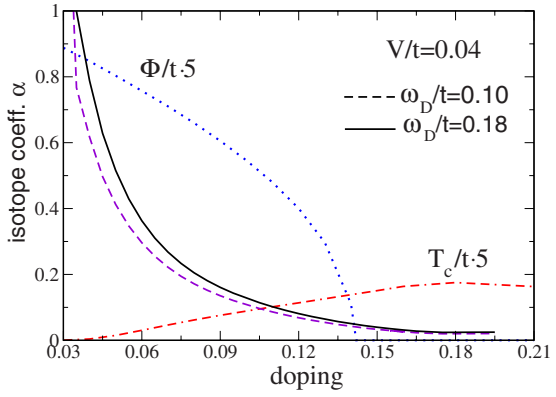

FIG. 3. (Color online) Isotope coefficient α as a function of doping for two phonon cutoffs ω_D. Also shown are the curves for Φ and T_c from Fig. 1

mate expression for α in terms of the density ratio $\langle N_d(\omega)\rangle/N_d(0)$ suggests that the above curves for α are rather independent of the specific features of our model (d-CDW with long-range order) but rather generic for underdoped cuprates with a pseudogap.

Very remarkable in Fig. 3 is the fact that the tiny value of 0.04 for the effective EP coupling V/t is able to produce large values for α comparable to those seen in experiment in the underdoped region. The local-density approximation (LDA) yields $\lambda_d \sim 0.022$ in $YBa_2Cu_3O_7$,[37] which is roughly 1 order of magnitude smaller than λ_s.[38,39] (For a different view on the magnitude of the EP coupling constants in cuprates, see Ref. 40). Using the LDA value $N_d(0)=1.108/\text{eV}$ from Ref. 37, the relation Eq. (17), and $t=0.5$ eV, we get in the LDA $V/t \sim 0.04$ which is the value used in our calculation. This shows that the large experimental values for α in the underdoped region do not contradict, at least in our competing model, the small LDA values for the EP coupling. The case of overdoped samples is presently less clear because of conflicting experimental results.[1,41] An isotope coefficient α which is small throughout the overdoped region[41] would agree with our Fig. 3.

IV. EXTENSION TO FINITE CORRELATION LENGTHS OF THE d-CDW

In the previous sections, our employed mean-field treatment yielded a d-CDW with long-range order and excitations with infinite long lifetimes. Such idealizations are certainly not realized in the cuprates and one may wonder to what degree our previous results depend on them. Generally speaking, we do not expect drastic modifications because the strong increase of α with decreasing doping was due to the rearrangement of spectral weight due to the d-CDW gap. This shift of spectral weight should not be seriously affected by fluctuations or the loss of long-range order as long as the correlation length is sufficiently large. In this section, we will investigate this expectation on a more quantitative level. To this end, we will employ a model[26–28] which allows treating exactly a certain class of semiclassical fluctuation of the off-diagonal order parameter.

First we consider only the d-CDW part of g^{-1}, i.e., the first and third rows and columns of Eq. (9) where we may put $Z=1$ considering again the weak-coupling case. Transforming the part induced by the variation of the order parameter into $\mathbf{r}$ space, we get

$$g^{-1}_{\mathrm{CDW}}(\mathbf{k}-i\nabla, i\omega_n) = \begin{pmatrix} i\omega_n - \epsilon(\mathbf{k}-i\nabla) & -i\gamma(\mathbf{k})\Phi_0 e^{i\beta} \\ i\gamma(\mathbf{k})\Phi_0 e^{-i\beta} & i\omega_n - \epsilon(\bar{\mathbf{k}}-i\nabla) \end{pmatrix}, \tag{19}$$

with $\beta=\mathbf{p}\mathbf{x}+\phi$ and $\bar{\mathbf{k}}=\mathbf{k}-\mathbf{Q}$. $\mathbf{p}$ is a random variable with Cartesian components distributed according to a Lorentzian. ϕ is a random phase which will not enter our final expressions and thus its distribution function has not to be specified. We apply now the unitary transformation

$$U_1(\mathbf{x}) = e^{i\beta\sigma_3/2}, \tag{20}$$

to Eq. (19), where σ_3 is a Pauli matrix. After some algebra, we find

$$\tilde{g}^{-1}_{\mathrm{CDW}}(\mathbf{k}-i\nabla, i\omega_n) = U_1^{\dagger}(\mathbf{x}) g^{-1}_{\mathrm{CDW}}(\mathbf{k}-i\nabla, i\omega_n) U_1(\mathbf{x}) = \begin{pmatrix} i\omega_n - \epsilon(\mathbf{k}) + \epsilon_1 & -i\gamma(\mathbf{k})\Phi_0 \\ i\gamma(\mathbf{k})\Phi_0 & i\omega_n - \epsilon(\bar{\mathbf{k}}) + \epsilon_2 \end{pmatrix}, \tag{21}$$

with the abbreviations $\epsilon_1=\mathbf{v}(\mathbf{k})\mathbf{p}/2$ and $\epsilon_2=-\mathbf{v}(\bar{\mathbf{k}})\mathbf{p}/2$. $v_{x,y}(\mathbf{k})$ are given by $\partial\epsilon(\mathbf{k})/\partial k_{x,y}$. In deriving Eq. (21), we also expanded $\epsilon(\mathbf{k}-i\nabla)$ up to first order in ∇ assuming that the changes in one-particle energies induced by the variation of the order parameter vary slowly in space. To simplify the following, we will take $\epsilon_1=\epsilon_2=\epsilon$ which holds exactly for the case $t'=0$.

The matrix in Eq. (21) can be diagonalized by a second unitary transformation U_2 yielding

$$U_2^{\dagger}(\mathbf{k})\tilde{g}^{-1}_{\mathrm{CDW}}(\mathbf{k}, i\omega_n) U_2(\mathbf{k}) = \begin{pmatrix} i\omega_n - \lambda_1(\mathbf{k}) + \epsilon & 0 \\ 0 & i\omega_n - \lambda_2(\mathbf{k}) + \epsilon \end{pmatrix}, \tag{22}$$

with the eigenvalues $\lambda_{1,2}(\mathbf{k})$ of the unperturbed d-CDW, given by Eq. (16). Taking also superconductivity into account, we note that the Heisenberg interaction is invariant under the gauge transformation U_1. Applying the second unitary transformation U_2 to the Heisenberg interaction and using the BCS factorization, the transformed matrix g^{-1} splits into two 2×2 matrices and the resulting gap equation can easily be calculated. Adding also phonons, one finds that Eqs. (11)–(13) still hold if the density $N_d(\omega)$ of Eq. (14) is replaced by the expression

$$\frac{\omega}{\pi N_c}\sum_{\mathbf{k},\beta}\gamma(\mathbf{k})^2 \Im \frac{1}{(\omega - i\eta + \epsilon)^2 - \lambda_\beta^2(\mathbf{k})}. \tag{23}$$

Finally, Eqs. (11)–(13) have to be averaged over the distribution function $P(\mathbf{p})$,

$$P(\mathbf{p}) = \frac{\kappa^2}{\pi^2(p_x^2+\kappa^2)(p_y^2+\kappa^2)}, \tag{24}$$

where $\kappa=1/\xi$ and ξ is the correlation length of the off-diagonal order-parameter fluctuations. According to Eq. (19), Φ_0 is the equilibrium d-CDW order parameter after omitting the factor $\gamma(\mathbf{k})$. It thus varies in $\mathbf{r}$ space with the momentum $\mathbf{Q}$ because it connects electron states with momenta $\mathbf{k}$ and $\bar{\mathbf{k}}$. The random variable $\mathbf{p}$ modulates the equilibrium total momentum $\mathbf{Q}$ of the d-CDW in an additive way and it is distributed according to a Lorentzian. It is sufficient to apply the necessary average over $\mathbf{p}$ just to the expression of Eq. (23) yielding

$$\bar{N}_d(\omega) = \frac{\omega}{\pi N_c}\sum_{\mathbf{k},\beta}\gamma(\mathbf{k})^2 \times \Im \frac{1}{\{\omega - i/(2\xi)[|v_x(\mathbf{k})| + |v_y(\mathbf{k})|]\}^2 - \lambda_\beta^2(\mathbf{k})}. \tag{25}$$

It is easy to see that the above expression can formally be obtained from $N_d(\omega)$ if one replaces there the infinitesimal η by the finite, $\mathbf{k}$-dependent imaginary part $(|v_x(\mathbf{k})|$

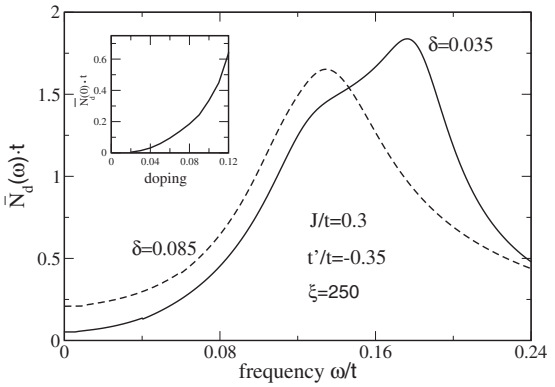

FIG. 4. Weighted density of electronic states $\bar{N}_d(\omega)$ for two dopings δ for a correlation length $\xi=250$. Inset shows $\bar{N}_d(0)$ at low dopings.

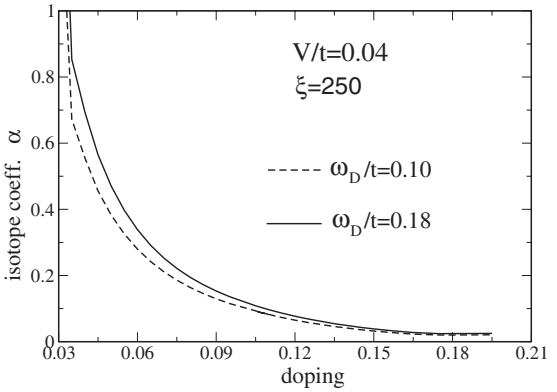

FIG. 5. Isotope coefficient α as a function of doping for two phonon cutoffs ω_D calculated in the presence of short-ranged correlated phase fluctuations with correlation length $\xi=250$.

$+|v_y(\mathbf{k})|)/(2\xi)$. The latter quantity in Eq. (25) is averaged over the Fermi line in the pure d-CDW state, i.e., for $\beta=1$ over the arc around the nodal line and for $\beta=2$ over the remaining small piece near the antinodal point which, however, vanishes for our two considered dopings. Thus the $\beta=2$ contribution in Eq. (25) is negligibly small. In the $\beta=1$ contribution, $(|v_x(\mathbf{k})|+|v_y(\mathbf{k})|)/(2\xi)$ varies only little along the arc so we may replace this quantity by its average over the arc and obtain for $\delta=0.085$ the value $1.15v_F/\xi$, where $v_F\sim 4.6t$ is the square root of the Fermi-surface average of $\mathbf{v}^2(\mathbf{k})$ in the normal state. This allows to describe phase correlations with a finite correlation length ξ as an inverse life time effect with energy $\Gamma/t=1.15v_F/(t\xi)$.

Figure 4 shows $\bar{N}_d(\omega)$ for the two dopings of Fig. 2 and for the case of a correlation length $\xi=250$, corresponding to an inverse lifetime of about $0.02t$. Though such a large correlation length may seem to simulate a rather well-ordered state, most of the fine structures in Fig. 2 are wiped out by phase fluctuations. In particular, the two peaks seen in Fig. 2 have merged into one broad and rather structureless peak. At low frequencies, the changes introduced by phase fluctuations are rather minor. In the inset in Fig. 4, the static value $\bar{N}_d(0)$ is plotted as a function of doping showing the pronounced decrease of $\bar{N}_d(0)$ with decreasing δ similar as in the case without phase fluctuations in Fig. 2. This behavior for the density is rather robust as function of ξ as long as $\xi \gg 1$ holds.

Figure 5 shows the doping dependence of the isotope coefficient α using the same parameter as in Fig. 3 but $\bar{N}_d(\omega)$ instead of $N_d(\omega)$. Comparing Figs. 3 and 5 reveals that this change of densities does hardly affects α so that corresponding curves in these two figures are practically identical. This demonstrates that the steep increase of α with decreasing doping is not related or even caused by the sharp peaks present in $N_d(\omega)$ or by special values for the phonon cutoff ω_D. Instead, it is a rather universal property caused by the large shift of spectral weight toward higher frequency due to the pseudogap. If the correlation length ξ is decreased from large to small values of the order of the lattice constant, the depletion in the density $\bar{N}_d(0)$ at low energies becomes smaller and smaller. In accordance with the decreasing shift of spectral weight from low to high energies, the isotope coefficient α also decreases approaching a similar small value as in the absence of a pseudogap, i.e., in the overdoped region.

Figure 5 can qualitatively be understood in a simple way considering our previously approximate expression $\langle N_d(\omega)\rangle/N_d(0)$ for α. The numerator is essentially given by the area under the density curve in Figs. 2 and 4. Its value thus is independent of the shape of the density curve, i.e., whether it has sharp or broad peaks, as long as the area below the curve is constant. This area is practically the same in Figs. 2 and 4. On the other hand, the $\omega=0$ values of the densities both decrease strongly and in a similar way with decreasing δ. As a result, α should be of similar magnitude in both cases and, in particular, show a strong increase toward low dopings in agreement with Fig. 5. The above approximate expression for α may also explain why the calculated values for α of Ref. 5 are for our electron-phonon coupling V much smaller than ours. Their density of state function at $\lambda_d=0$, plotted in their Fig. 4, is large at $\omega=0$ compared to the modulation due to the pseudogap which implies only a small redistribution of spectral weight by the pseudogap.

V. CONCLUSIONS

We have shown that a mean-field treatment of the t-J model which identifies the pseudogap with the gap of a d-CDW state is able to explain the large isotope effect in underdoped cuprates. Interestingly, a very small EP coupling constant $V/t\sim 0.04$ is sufficient to explain the experimental data. This value is very close to that calculated for $YBa_2Cu_3O_7$ within the LDA. This shows that the large values for α of order 1 found in the underdoped region are, at least in our competing model, compatible with the small EP coupling constants predicted by the LDA. The obtained huge increase of the isotope coefficient α with decreasing doping is rather independent of the phonon cutoff frequency ω_D and the spectral properties of the excitations in the pseudogap state. The latter information is obtained by considering a simple phase fluctuation model where the d-CDW state has only short-range correlations.

Most important for the large increase of α with decreasing doping is in our calculation the large depletion of spectral weight at low frequencies and its shift to high energies by the pseudogap. Because of this, we conjecture that our results are not specific to the employed *d*-CDW providing the pseudogap but also hold for other order parameters such as the antiferromagnet order parameter as long as they lead to a strong depletion of spectral weight at low frequencies. Our calculation shows, in particular, that it is not necessary to assume a large EP interaction in cuprates or extrinsic effects such as pair breaking due to impurities[42,43] to explain the observed isotope effect of T_c.

ACKNOWLEDGMENTS

The authors thank O. Gunnarsson for discussions and A. M. Oleś for a critical reading of the paper.

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