Phase-fluctuation-induced reduction of the kinetic energy at the superconducting transition

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(Received 11 March 2003; published 14 July 2003)

Recent reflectivity measurements indicated a possible *violation* of the in-plane optical integral in the underdoped high-T_c compound $Bi_2Sr_2CaCu_2O_{8+\delta}$ up to frequencies much higher than expected by the standard BCS theory. The sum rule violation may be related to a loss of in-plane kinetic energy at the superconducting transition. Here, we show that a model based on phase fluctuations of the superconducting order parameter introduces a change of the in-plane kinetic energy at T_c. The change is due to a transition from a phase-incoherent Cooper-pair motion in the pseudogap regime above T_c to a phase-coherent motion at T_c.

DOI: 10.1103/PhysRevB.68.014505 PACS number(s): 74.72.Hs, 71.10.Fd, 71.27.+a, 74.25.Jb

I. INTRODUCTION

The key idea of the phase-fluctuation scenario in the high-T_c superconductors (HTSC) is the notion that the pseudogap, observed in a wide variety of experiments, arises from phase fluctuations of the superconducting gap.[1–7] In this scenario, below a mean-field temperature scale T_c^{MF}, a $d_{x^2-y^2}$-wave-gap amplitude is assumed to develop. However, the superconducting transition is suppressed to a considerably lower transition temperature T_c by phase fluctuations.[1,7] In the intermediate temperature regime between T_c^{MF} and T_c, phase fluctuations of the superconducting order parameter give rise to the pseudogap phenomena. Recently, we have shown that indeed, a two-dimensional (2D) BCS-like Hamiltonian with a $d_{x^2-y^2}$-wave gap and phase fluctuations, which were treated by a Monte Carlo simulation of an XY model, yields results that compare very well with scanning-tunneling measurements over a wide temperature range.[7,8] Thus, they support the phase-fluctuation scenario for the pseudogap.

There is also increasing evidence from a number of recent experiments for the relevance of phase fluctuations, such as the measurements by Corson *et al.*,[9] of the high-frequency conductivity, which track the phase correlation time. XY vortices are probably responsible for the large Nernst effect.[10,11] The evolution of T_c with electron irradiation, found very recently,[12] also emphasizes the importance of phase fluctuations. In this paper, we argue that phase fluctuations should have yet another, rather unexpected, consequence: they should induce a reduction of the kinetic energy at the superconducting transition. This reduction is due to a transition from a ‘‘disordered,’’ i.e., phase-incoherent Cooper-pair motion in the pseudogap regime above T_c to an ‘‘ordered,’’ i.e., phase-coherent motion at T_c. Comparison of our results, based on the BCS phase-fluctuation model, with optical experiments[13,14] support this idea.

In ordinary BCS superconductors the optical conductivity is suppressed at frequencies within a range of about twice the superconducting gap. The corresponding low-frequency spectral weight W_{low} is transfered to the zero-frequency delta peak W_D,[15] associated with the dissipationless transport (and the superfluid weight D) in the superconducting state. This is the Glover-Ferrell-Tinkham (GFT) sum rule. On the other hand, the *total* frequency integral of the optical conductivity is conserved when decreasing the temperature across the superconducting transition, due to the f-sum rule,[15] i.e., $W_{tot}^{sc}=W_{tot}^{n}$.

However, recent measurements of the in-plane optical conductivity[13,14] have indicated a violation of the GFT optical sum rule for frequencies up to 2 eV in underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$. By entering the superconducting state, not only spectral weight W_{low} from the microwave and far infrared, but also from the visible optical spectrum, i.e., high-frequency spectral weight W_{high} contributes to the superfluid condensate W_D. That is, in contrast to ordinary BCS superconductors, a ‘‘color change’’ is introduced at the superconducting transition. The interpretation of this unusual result may require the inclusion of local-field effects and other (such as excitonic) many-body effects. They are known to play a crucial role already in weakly correlated systems (such as semiconductors) and introduce a shift of order of the Coulomb correlation energy between single-particle and two-particle, i.e., optical excitations.[16] Therefore, they may partly account for the ‘‘high-energy’’ features observed in $\sigma(\omega)$. On the other hand, within a tight-binding one-band model, the anomalously large energy scale, which contributes to the superfluid weight, and the corresponding color change can be attributed to a reduction of kinetic energy[17] at the superconducting transition. This is rather surprising, since one would expect that in a conventional (BCS) pairing process, it is the potential energy which is reduced at the expense of the kinetic energy, with the latter being increased due to particle-hole mixing.

The full optical integral, when integrated over all frequencies and *energy bands*, is proportional to carrier density (n) over bare mass (m)

$$W_{tot}\equiv W_{low}+W_D+W_{high}=\int_0^\infty \mathrm{Re}\,\sigma_{xx}(\omega)\,d\omega=\frac{ne^2}{2m} \tag{1}$$

and, thus, is conserved. When the optical integral is restricted over a finite (low) range of frequencies Ω, in the HTSC typically of the order of eV, one may consider the weight $W_{low}+W_D$ as being essentially due to a single band around the Fermi energy, i.e.,

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$$W_{low}+W_D=\int_0^\infty \mathrm{Re}\,\tilde{\sigma}_{xx}(\omega)d\omega=(\pi e^2a^2/2\hbar^2V)E_K, \quad (2)$$

where $\tilde{\sigma}$ is the single-band conductivity, a the lattice constant, and V the unit-cell volume. With this single-band assumption, the frequency integral of the optical conductivity is proportional to the inverse mass tensor ($\partial^2\epsilon_k/\partial k_x^2$, $\hat{x}$ being the direction in which the conductivity is measured) weighted with the momentum distribution n_k,[18,19]

$$E_K=(2/a^2N)\sum_k \frac{\partial^2\epsilon_k}{\partial k_x^2}n_k, \quad (3)$$

with N being the number of k points. This quantity depends upon the bare single-particle band structure ϵ_k being proportional to minus the kinetic energy $E_K=-E_{kin}$ for a (nearest-neighbor) tight-binding (TB) model, while for free electrons it is a constant given by the electron density divided by the effective mass.

II. PHASE-FLUCTUATION SCENARIO FOR KINETIC-ENERGY REDUCTION

In this paper, we propose phase fluctuations as a mechanism for a kinetic-energy reduction. That is, in order to have condensation into the superconducting state one needs, in addition to the binding of charge carriers into Cooper pairs, long-range phase coherence among the pairs. Since superconductors with low superconducting carrier density (such as the organic and underdoped high-T_c superconductors) are characterized by a relatively small phase *stiffness*, this implies a significantly larger role for phase fluctuations than in conventional superconductors.[1,20,21] As a consequence, in these materials the transition to the superconducting state does not display a typical mean-field (BCS) behavior, and phase fluctuations, both classical and quantum, may have a significant influence on low-temperature properties. When coherence is lost due to thermal fluctuations of the phase at and above the transition temperature T_c, pairing remains, together with short-range phase correlations. These phase fluctuations can cause the pseudogap phenomena observed, e.g., in tunneling experiments[7,8,22,23] in the underdoped HTSC.

We show here that, indeed, phase fluctuations contribute to a significant reduction of the in-plane kinetic energy upon entering into the superconducting phase below T_c, with a magnitude comparable to recent experimental results. The physical reason for this kinetic-energy lowering is that due to phase fluctuations and the associated incoherent motion of Cooper pairs (cf. Fig. 1), the pseudogap region has a higher kinetic energy than the simple BCS mean-field state. When long-ranged phase coherence finally develops at T_c, the Cooper-pair motion becomes phase *coherent* and the kinetic energy decreases. The onset of the coherent motion can be seen, for example, from the development of coherence peaks in the tunneling spectrum of BiSrCaCuO compounds (see, e.g. Refs. 7,8 and Fig. 3). The initial *cost* of kinetic energy, which is needed for pairing, is paid at a mean-field temperature T_c^{MF} considerably higher than T_c. Therefore, the reduction of kinetic energy observed experimentally[13,14] can be attributed to a transition from a phase-disordered pseudogap to a phase-ordered superconducting state. We stress that this effect is independent of the particular mechanism leading to pair formation, as long as the superconductor considered is characterized by a small phase stiffness.[24]

Our starting Hamiltonian is of a simple BCS form given by

$$H=K-\frac{1}{4}\sum_{i\delta}(\Delta_{i\delta}\langle\Delta_{i\delta}^\dagger\rangle+\Delta_{i\delta}^\dagger\langle\Delta_{i\delta}\rangle), \quad (4)$$

with the nearest-neighbor hopping term

$$K=-t\sum_{\langle ij\rangle,\sigma}(c_{i\sigma}^\dagger c_{j\sigma}+c_{j\sigma}^\dagger c_{i\sigma}), \quad (5)$$

where $c_{i\sigma}^\dagger$ creates an electron of spin σ on the ith site and t denotes an effective nearest-neighbor hopping. The $\langle i\,j\rangle$ sum is over nearest-neighbor sites of a 2D square lattice and, in the pairing term, δ connects i to its nearest-neighbor sites. The local d-wave gap

$$\langle\Delta_{i\delta}^\dagger\rangle=\frac{1}{\sqrt{2}}\langle c_{i\uparrow}^\dagger c_{i+\delta\downarrow}^\dagger-c_{i\downarrow}^\dagger c_{i+\delta\uparrow}^\dagger\rangle=\Delta\, e^{i\Phi_{i\delta}} \quad (6)$$

is characterized by the *fluctuating* phases

$$\Phi_{i\delta}=\begin{cases}(\varphi_i+\varphi_{i+\delta})/2 & \text{for}\quad \delta \text{ in } x\text{-direction}\\ (\varphi_i+\varphi_{i+\delta})/2+\pi & \text{for}\quad \delta \text{ in } y\text{-direction}\end{cases} \quad (7)$$

and by a spatially constant amplitude Δ. We neglect the relative bond phase fluctuations between $\delta=\hat{x}$ and $\hat{y}$ as well as amplitude fluctuations. Thus, we consider only *center-of-mass* pair phase fluctuations, which are the relevant low-energy degrees of freedom, in a situation in which the superfluid density is small, like in the underdoped cuprates. In our 2D model T_c corresponds to the Kosterlitz-Thouless (KT) transition temperature T_{KT}, where the phase correlation length ξ diverges.

With this Hamiltonian it is straightforward to show that the optical-sum rule yields,[19,25,26]

$$\int_0^\infty \mathrm{Re}\,\tilde{\sigma}_{xx}(\omega)d\omega=-e^2\pi\langle k_x\rangle/2 \quad (8)$$

in units where $\hbar=c=1$, with $\langle k_x\rangle$ being the expectation value of the nearest-neighbor hopping[27] in the x-direction, i.e.,

$$\langle k_x\rangle=-t\sum_\sigma\langle c_{i\sigma}^\dagger c_{i+x\,\sigma}+c_{i+x\,\sigma}^\dagger c_{i\sigma}\rangle. \quad (9)$$

Since we are only interested in the temperature region $T\gtrsim T_c$, one can safely assume that the fluctuations of the phase φ_i are predominantly determined by a classical XY free energy,[1,20]

$$F[\varphi_i]=-J\sum_{\langle ij\rangle}\cos(\varphi_i-\varphi_j). \quad (10)$$

Our physical picture here is that the XY action arises from integrating out the shorter wavelength fermion degrees of freedom, including those responsible for the formation of the local pair amplitude and internal $d_{x^2-y^2}$ structure of the pair. Thus, the *scale* of the XY-lattice spacing is actually set by the pair coherence length ξ_0. In our work, we have chosen Δ so that $\xi_0 \sim v_F/\pi\Delta \sim 1$. In this case, the calculation of the phase configurations φ_i can be carried out on the same $L\times L$ ($L=32$) lattice that is used for the diagonalization of the Hamiltonian. This allows the Kosterlitz-Thouless phase correlation length ξ to grow over a sufficient range as T approaches T_{KT} and minimizes finite-size effects. Thus, we are always in the limit where the phase correlation length ξ is larger than the Cooper-pair size ξ_0, when the temperature T is below the mean-field critical temperature T_c^{MF}.

In principle, the coupling energy J can also be considered as arising from integrating out the high-energy degrees of freedom of the underlying microscopic system. Here, we will proceed phenomenologically, neglecting the temperature dependence of J and simply use it to set the Kosterlitz-Thouless transition temperature T_{KT} equal to some fraction of T_c^{MF}. Specifically, for the present calculations we will set $T_{KT}\simeq\frac{1}{4}T_c^{MF}$. This choice is motivated by the recent scanning-tunneling results in $Bi_2Sr_2CuO_{6+\delta}$, where $T_c \simeq 10K$ and the pseudogap regime extends to about 50 K, which we take as T_c^{MF}.

In a previous paper[7] we have presented a detailed numerical solution of the 2D BCS-like Hamiltonian of Eq. (4) with a d-wave gap and phase fluctuations. This is a minimal model but, nevertheless, contains the key ideas of the cuprate phase-fluctuation scenario: that is, a d-wave BCS gap amplitude forms below a mean-field temperature T_c^{MF}, but phase fluctuations suppress the actual transition to a considerably lower temperature T_c. In the intermediate temperature regime between T_c^{MF} and T_c, the phase fluctuations of the gap give rise to pseudogap phenomena. Comparison of these results with recent scanning-tunneling spectra of Bi-based high-T_c cuprates supports the idea that the pseudogap behavior observed in these experiments can be understood as arising from phase fluctuations.[7]

In the present calculations, where we assume a BCS temperature dependence of the pairing gap $\Delta(T)$, we have, therefore, set $\Delta(T=0)=1.0t$ corresponding to $T_c^{MF}\simeq 0.42t$ and selected J so that $T_{KT}=0.1t$.[28] The condition $\xi>\xi_0$ is thus always fulfilled if we are not too close to T_c^{MF}. The calculation of the kinetic energy for a $L\times L$ ($L=32$) periodic lattice now proceeds as follows[29,30]: a set of phases $\{\varphi_i\}$ is generated by a Monte Carlo importance sampling procedure, in which the probability of a given configuration is proportional to $\exp(-F[\varphi_i]/T)$ with F given by Eq. (10). With $\{\varphi_i\}$ given, the Hamiltonian of Eq. (4) is diagonalized and the kinetic energy $E_{kin}(T,\{\varphi_i\})=\langle k_x\rangle_{\{\varphi_i\}}$ is extracted. Further Monte Carlo $\{\varphi_i\}$ configurations are generated and an average kinetic energy $E_{kin}(T)=\langle k_x\rangle$, at a given temperature, is determined.

Figure 1 displays the kinetic energy $\langle k_x\rangle$ as a function of temperature for noninteracting tight-binding electrons, for BCS electrons, and for our phase-fluctuation model. We can clearly see that pairing, as expected, produces an overall increase of kinetic energy (indicated as vertical arrows) with respect to the free-electron case. We observe that in the phase-fluctuation model the kinetic energy is further increased (small vertical arrows) due to the incoherent motion of the paired electrons. The kinetic energy is a smoothly decreasing function of temperature for $T\rightarrow 0$. This is expected from the fact that at high temperature, more electrons are transferred to higher kinetic energies, and is in agreement with the experimental results.[13,14] What we are especially interested in is the rather pronounced change (magnified in Fig. 2 by using a different scale for the kinetic energy) near $T_c\equiv T_{KT}$, where the kinetic energy of our phase-fluctuation model rather suddenly reduces to the BCS value. This sudden deviation from the $T\gtrsim T_c$ behavior is also obtained in experiments, which show a kink in the temperature dependence of the low-frequency spectral weight $W_{low}+W_D$ at T_c.[13]

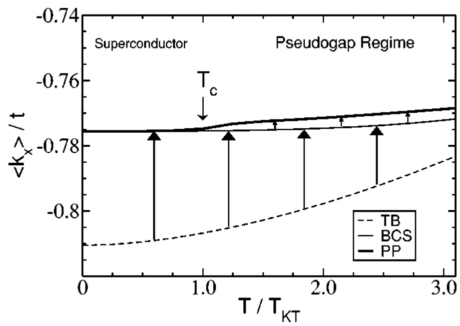

FIG. 1. Kinetic energy per bond, $\langle k_x\rangle$, as a function of temperature for the noninteracting tight-binding electrons (TB), the BCS solution (BCS), and our phase-fluctuation (PP) model for $\mu=0$ ($\langle n\rangle=1$). The large vertical arrows indicate the increase in kinetic energy upon pairing, relative to the free tight-binding model, and the small arrows indicate the additional increase due to phase fluctuations. This additional *phase-fluctuation energy* rapidly vanishes near $T_c\equiv T_{KT}$, which causes the significant change in the optical integral upon entering the superconducting state at $T_{KT}=0.1t$. Note that the thick line follows the actual kinetic energy encountered in our model, when going from the pseudogap to the superconducting regime.

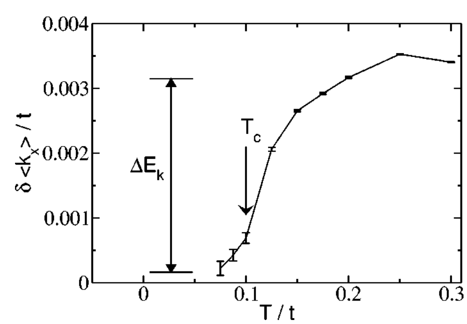

FIG. 2. Kinetic-energy contribution from phase fluctuations $\delta\langle k_x\rangle=\langle k_x\rangle_{PP}-\langle k_x\rangle_{BCS}$. One can clearly see the sharp decrease of the kinetic energy near the Kosterlitz-Thouless transition at $T=0.1t\equiv T_c$. ΔE_k gives an estimate of the kinetic condensation energy.

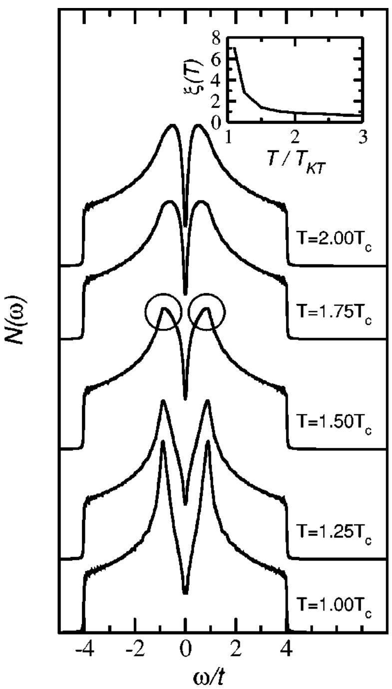

FIG. 3. Single particle density of states, $N(\omega)$, for different temperatures T for a 32×32 lattice. Coherence peaks develop (marked with circles for $T=1.5T_c$) as T approaches $T_c\equiv T_{KT}$ in exactly the same temperature regime ($T_c<T<1.5T_c$) where in Fig. 1 the kinetic-energy reduction occurs. The inset shows the corresponding temperature dependence of the phase correlation length $\xi(T)$.

This pronounced change of in-plane kinetic energy can be better observed in Fig. 2, where we plot the difference between the BCS kinetic energy and the kinetic anergy of our phase-fluctuation model, $\delta\langle k_x\rangle=\langle k_x\rangle_{PP}-\langle k_x\rangle_{BCS}$. As discussed above, this reduction is due to the onset of phase coherence of the Cooper pairs below the superconducting transition temperature $T_c\equiv T_{KT}$. This is signaled by the appearance of sharp coherence peaks in the single-particle spectral function upon developing long-range phase coherence.[7] The corresponding result for the density of states, $N(\omega)$, displaying these coherence peaks is shown in Fig. 3.

Notice that this argument for the reduction of kinetic energy at T_c due to a phase ordering transition is quite robust. For example, we expect it to be valid (and actually stronger) in a true three-dimensional system. As a matter of fact, it has been argued[1,20] that even small interplane couplings play an important role due to the infinite-order nature of the the KT transition.

In order to get a rough estimate of the kinetic condensation energy, we calculate the reduction in kinetic energy near T_c, i.e.,

$$\Delta E_k=-\frac{2}{e^2\pi}\int_0^\infty[\mathrm{Re}\,\tilde{\sigma}_{xx}^{sc}(\omega)-\mathrm{Re}\,\tilde{\sigma}_{xx}^{n}(\omega)]d\omega, \qquad (11)$$

as indicated by the energy change ΔE_k in Fig. 2. Assuming that $t\simeq250$ meV, we get a condensation energy estimate of 1.5 meV per Copper site, which is in order of magnitude agreement with the experimental results (again assuming a one-band TB analysis).

Up to now, to refrain from further approximations, we have set the chemical potential μ equal to zero and have only considered nearest-neighbor hopping. We have checked, to some extent, how robust these results are, with respect to finite doping ($\langle n\rangle\approx0.9$) and the inclusion of a next-nearest neighbor-hopping term t' in our Hamiltonian Eq. 4. Notice that in this case E_k is no longer proportional to the kinetic energy. For $t'\lesssim0.3t$, our results for the sum rule violation are reduced only by about 20%–30%.

III. SUMMARY

In conclusion, we have shown that the recently observed violation of the low-frequency optical-sum rule in the superconducting state, associated with a reduction of kinetic energy, can be related to the role of phase fluctuations. The decrease in kinetic energy is due to the sharpening of the quasiparticle peaks close to the superconducting transition at $T_c\equiv T_{KT}$, where the phase correlation length ξ diverges. We suggest that this sum rule violation should also appear in other superconductors with low charge carrier density (phase stiffness) such as the organic superconductors.

ACKNOWLEDGMENTS

We would like to acknowledge useful discussions and comments by S. A. Kivelson and D. J. Scalapino. This work was supported by the DFG under Grant Nos. Ha 1537/16-2 and AR 324/3-1 (Heisenberg), by the Bavaria California Technology Center (BaCaTeC), and the KONWHIR projects OOPCV and CUHE. The calculations were carried out at the high-performance computing centers HLRS (Stuttgart) and LRZ (München).

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