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Interplay between single-particle and collective features in the boson fermion model

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We study the interplay between the single-particle and fermion-pair features in the boson fermion model, both above and below the transition temperature T_c, using the flow equation method. Upon lowering the temperature the single-particle fermionic spectral function (a) gradually develops a depletion of the low-energy states (pseudogap) for $T^* > T > T_c$ and a true superconducting gap for $T < T_c$ and (b) exhibits a considerable transfer of spectral weight between the incoherent background and the narrow coherent peak(s) signifying long-lived quasiparticle features. The Cooperon spectral function consists of a δ-function peak, centered at the renormalized boson energy $\omega = \tilde{E}_{\mathbf{q}}$ and a surrounding incoherent background which is spread over a wide energy range. When the temperature approaches T_c from above, this peak for $\mathbf{q}=\mathbf{0}$ moves to $\omega=0$, so that the static pair susceptibility diverges (Thouless criterion for the broken symmetry phase transition). Upon decreasing the temperature below T_c the Cooperon peak becomes the collective (Goldstone) mode $E_{\mathbf{q}} \propto |\mathbf{q}|$ in the small-momentum region and simultaneously splits off from the incoherent background states which are expelled to the high-energy sector $|\omega| \geq 2\Delta_{sc}(T)$. We discuss the smooth evolution of these features upon approaching T_c from above and consider its feedback on the single-particle spectrum where a gradual formation of damped Bogoliubov modes (above T_c) is observed.

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I. INTRODUCTION

The boson fermion model (BFM) was initially invented for a description of the conduction-band electrons coupled to the lattice vibrations in the region of intermediate electron-phonon coupling.[1] The underlying physics emerges from the assumption that in the crossover region the electrons exist partly in the form of bound pairs (hard-core bosons) and partly as quasifree particles (fermions). Many-body correlations of such a two-component system are induced due to charge exchange processes converting the fermion pairs into the hard-core bosons and vice versa. The initially very heavy bosons effectively increase their mobility and, at the critical temperature T_c, undergo a Bose-Einstein (BE) condensation while the fermions are simultaneously driven to a superconducting state.

Upon approaching T_c from above there are several precursor features of superfluidity and superconductivity showing up in the system. In this paper we address these precursor effects by means of a renormalization group scheme which is outlined in some detail in Sec. II. We will show that, *in the pseudogap phase* $(T < T^*)$ *and in superconducting state* $(T < T_c)$, *the single- and two-particle properties become strongly interdependent*. In the pseudogap phase this is seen, for instance, through a gradual destruction of the single-particle states (near the Fermi surface) which is accompanied by a simultaneous emergence of fermion-pair features. Fermion pairs with total zero momentum show up in the normal state only as damped entities which propagate over a finite time and/or spatial scales. However, we find that there is a certain critical momentum $q_{crit}(T)$ above which fermion pairs become long-lived quasiparticles (they become separated from the incoherent background as discussed in Sec. III). At the phase transition $q_{crit}(T_c) \rightarrow 0$ and below T_c all the Cooperons become good quasiparticles. The appearance of fermion pairs above T_c affects the single-particle spectrum, leading to the emergence of the Bogoliubov shadow branches as has been recently discussed by us in Ref. 2.

Let us recall that the single-particle spectrum of classical superconductors is gapped only for temperatures $T < T_c$. BCS theory predicts the quasiparticle dispersion $E_{\mathbf{k}}^{BCS} = \text{sgn}(\varepsilon_k - \mu)\sqrt{(\varepsilon_k - \mu)^2 + |\Delta_{sc}|^2}$, where the excitation gap Δ_{sc} progressively increases for a lowering temperature. However, the total single-particle spectral function contains two contributions $u_{\mathbf{k}}^2 \delta(\omega - E_{\mathbf{k}}^{BCS}) + v_{\mathbf{k}}^2 \delta(\omega + E_{\mathbf{k}}^{BCS})$ with the BCS spectral weights $u_{\mathbf{k}}^2 = \frac{1}{2}[1 + |\varepsilon_k - \mu| / E_{\mathbf{k}}^{BCS}] = 1 - v_{\mathbf{k}}^2$. The existence of these two branches signifies that near the Fermi energy the true quasiparticles are mixtures of electron and hole excitations. One peak occurring at $\omega = E_{\mathbf{k}}^{BCS}$ corresponds to what is left of the single-particle state with initial energy $\varepsilon_{\mathbf{k}} - \mu$. The second branch, at $\omega = -E_{\mathbf{k}}^{BCS}$, is a kind of mirror reflection of the former and we will further call it the *Bogoliubov shadow* branch. The two-peak structure of the single-particle spectral function is a direct consequence of the BCS-type wave function[3] and indeed it has been experimentally confirmed for conventional and uncoventional superconductors.[4]

Besides this single-particle feature there are also other properties (showing up, e.g., in the Andreev reflection, Josephson tunneling, etc.) which unambiguously characterize the new type of quasiparticles (Cooperons). A detailed study of the pair propagation in superconductors has been investigated by many authors. For instance, Thouless indicated that the static pair susceptibility becomes divergent at T_c in the long-wavelength limit (this is now often used as a criterion for transition temperature itself). Anderson, on the other hand, explained that superconducting state breaks up the global U(1) symmetry and hence there should emerge a gapless

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sound-wave branch (Goldstone mode) in the pair spectrum which in the usual charged systems is pushed to the plasmon frequencies.[5] In this work we explore whether the spectral function of the fermion-pair propagator shows any *Cooperon peaks* (seen as narrow peaks which do not overlap with the incoherent background) already above T_c.

We expect that approaching T_c there should be a smooth evolution from the pseudogapped to the fully gapped single-particle spectrum where the Bogoliubov features (caused by the existence of the fermion pairs) are present below as well as above T_c. In the superconducting state, we moreover find that the interdependence between the single- and two-particle properties leads to the characteristic peak-dip-hump structure. Similar conclusions have recently been reached independently by Pieri *et al.*[6] although in a different theoretical approach.

As has been widely emphasized by Uemura,[7] there are a number of very convincing experimental indications for precursor phenomena in the underdoped high-temperature superconducting (HTS) cuprates. Whether the whole pseudogap phase can be exclusively attributed to such precursor effects is still under debate. Nevertheless, for temperatures sufficiently close to T_c (in the underdoped samples) the existence of fermion pairs, being correlated on a small spatial and temporal scale, was confirmed by measurements of the optical conductivity in the terahertz regime.[8] On the other hand, static experiments measuring the Nernst coefficient[9] gave indications for the existence of "moving pairs" with a certain phase slippage above T_c. These facts together with the peak-dip-hump structure found by angle-resolved photoemission spectroscopy[10] (ARPES) acquire here a natural explanation within precursor phenomena which are intrinsic to the BFM or similar scenarios, accounting for strong pair fluctuations.

On a more general basis, the BFM is often believed to capture essential aspects of the crossover physics between weakly coupled and strongly paired lattice electrons.[11,12] Various unconventional properties of the superconducting state have been investigated within this model by several groups.[13–16] Several authors concluded according to phenomenological considerations[17,18] that the BFM can serve as an effective model for the description of quasi-two-dimensional strongly correlated cuprate superconductors.[19]

The crossover issue and the BFM turned out to be of particular interest also in atomic physics,[20–22] where a resonant Feshbach scattering is induced between trapped alkali atoms, such as ^{40}K or ^{6}Li. By applying external magnetic fields the effective interaction between atoms can be varied from the weak (BCS) to the strong coupling (BE) limits. Under optimal conditions a *resonant superconductivity* is expected to arise at $T_c \sim 0.5 T_F$,[22] which is presently routinely observed in several research laboratories.[23] This very general scenario of the Feshbach resonance can be theoretically expressed via the BFM, as was recently shown by one of us.[24]

It has been frequently stressed in the literature[27–29] that a self-consistent and conserving treatment of single-particle and pair correlations has a crucial importance for the description of the HTS cuprates. In this paper we study the mutual interdependence between such single- and two-particle properties (paying special attention to the precursor features) by extending our previous work[25] based on the *flow equation* method.[26] Our former study focused on a diagonalization of the Hamiltonian and determination of the renormalized fermion and boson energies.[25] In the present paper we derive the Green's functions (dynamic quantities) which determine the propagation of single fermions, single bosons, and of fermion pairs. From these functions we obtain the corresponding excitation spectra. The methodological virtue of the flow equations method is that, besides treating the single- and two-particle entities on equal footing, it distinguishes between the contribution of long-lived and damped quasiparticles in the spectrum. The former are usually represented by δ-function peaks with a given spectral weight while the latter are given in form of a broad incoherent background.

For our study we use the Hamiltonian[1]

$$H = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} (\Delta_B - 2\mu) b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} + \frac{v}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} (b^{\dagger}_{\mathbf{q}} c_{\mathbf{q}-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \text{H.c.}), \tag{1}$$

where the operators $c^{\dagger}_{\mathbf{k}\sigma}$ ($c_{\mathbf{k}\sigma}$) refer to the creation (annihilation) of fermions with energy $\varepsilon_{\mathbf{k}}$ and $b^{\dagger}_{\mathbf{q}}$ ($b_{\mathbf{q}}$) correspondingly to bosons in localized states Δ_B. The boson-fermion coupling v will be taken here as isotropic, although for real HTS systems it should be used with a d-wave prefactor.[16–18] For simplicity we neglect here also the hard-core property of bosons, which is justified as long as the concentration of bosons is small.

II. METHOD

A. Generalities

We apply a canonical transformation $S(l)$ in order to eliminate the interaction between the boson and fermion subsystems. This transformation will be carried out in a continuous way (l denotes the continuous *flow parameter*) so that the transformed Hamiltonian $H(l) = e^{S(l)} H e^{-S(l)}$ reduces to a manageable form for further analysis. The more generally known classical single-step transformation projects out the terms which are linear with respect to a given perturbation. Here we demand much more stringent constraints on a transformed Hamiltonian going beyond such a standard perturbative scheme.

The evolution of the Hamiltonian $H(l)$ with respect to the varying flow parameter l is determined through the differential equation

$$dH(l)/dl = [\eta(l), H(l)], \tag{2}$$

subject to the initial condition $H(0) = H$. A generating operator is defined by $\eta(l) \equiv (de^{S(l)}/dl) e^{-S(l)}$.

In principle, one can transform the Hamiltonian in many different ways by choosing various operators $\eta(l)$ [or $S(l)$]. Some particularly efficient schemes have been proposed by Wegner[26] and independently by Wilson and Głazek[30] going back to the RG approach ideas.[31] Through a continuous transformation of the Hamiltonian one effectively renormalizes its *coupling constants* while keeping a given constrained structure. In other words, the parameters of the Hamiltonian such as the energies, the two-body potentials and so on are assumed to be l dependent.

In some distinction from the RG approach one does not integrate out the high-energy states, but instead they are renormalized in the initial part of the transformation until $l \sim (\Delta\varepsilon)^{-2}$.[32] Subsequently, states with small energy differences start to be renormalized and finally, for $l \to \infty$, the transformed Hamiltonian $H(\infty)$ eventually reduces to a (block-)diagonal structure.[33] In our previous work[25] we have derived such a continuous canonical transformation for the BFM. Some details which are important for the present work are summerized in Appendix A.

B. Dynamical quantities

In this work we focus on determining thermal equilibrium Green's functions of the form

$$\langle\langle O_1(\tau);O_2\rangle\rangle = -\langle \mathcal{T}_\tau O_1(\tau)O_2\rangle, \tag{3}$$

where the time evolution of the operators is given by $O(\tau) = e^{\tau H}Oe^{-\tau H}$, with $\tau \in \langle 0,\beta\rangle$ and $\beta = 1/k_BT$. As usual, $\mathcal{T}$ denotes ordering with respect to the imaginary time $\tau = it$.

The computation of the thermal averages $\langle\cdots\rangle = \mathrm{Tr}\{e^{-\beta H}\cdots\}/\mathrm{Tr}\{e^{-\beta H}\}$ is easiest to carry out using the transformed Hamiltonian $H(\infty)$ because of its (block-)diagonal structure. Due to the invariance of the trace under the unitary transformation, we can write

$$\mathrm{Tr}\{e^{-\beta H}O\} = \mathrm{Tr}\{e^{S(l)}e^{-\beta H}Oe^{-S(l)}\} = \mathrm{Tr}\{e^{-\beta H(l)}O(l)\}, \tag{4}$$

where $O(l) = e^{S(l)}Oe^{-S(l)}$. Hence, if we want to use the transformed Hamiltonian $H(l=\infty)$ in the Boltzmann factor $e^{-\beta H(l)}$, we ought to transform the observable O too. For the continuous transformation this is, however, a nontrivial problem because, in order to get $O(\infty)$, one must analyze the whole transformation process. The evolution of the arbitrary observable $O(l)$ with respect to l must be deduced on a basis of the differential equation

$$dO(l)/dl = [\eta(l),O(l)]. \tag{5}$$

For the Hamiltonian $O=H$ it thus is given by Eq. (2) which was already discussed previously by us[25] for this model.

In the next sections we study the l dependence of the individual boson and fermion operators and fermion-pair operators. By looking at the limit $l \to \infty$, we shall derive effective spectral functions

$$A^{F,B,pair}(\mathbf{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G^{F,B,pair}(\mathbf{k},\omega), \tag{6}$$

where $G(\mathbf{k},\omega) = \int_0^\beta d\tau e^{\tau\omega}G(\mathbf{k},\tau)$ with the single-particle Green's functions

$$G^B(\mathbf{q},\tau) = \langle\langle b_{\mathbf{q}}(\tau);b^\dagger_{\mathbf{q}}\rangle\rangle, \tag{7}$$

$$G^F_d(\mathbf{k},\tau) = \langle\langle c_{\mathbf{k}\uparrow}(\tau);c^\dagger_{\mathbf{k}\uparrow}\rangle\rangle, \tag{8}$$

$$G^F_{od}(\mathbf{k},\tau) = \langle\langle c_{\mathbf{k}\uparrow}(\tau);c_{-\mathbf{k}\downarrow}\rangle\rangle, \tag{9}$$

and the two-particle pair propagator given by

$$G^{pair}(\mathbf{q},\tau) = \frac{1}{N^2}\sum_{\mathbf{k},\mathbf{p}}\langle\langle c_{\mathbf{k}\downarrow}(\tau)c_{\mathbf{q}-\mathbf{k}\uparrow}(\tau);c^\dagger_{\mathbf{q}-\mathbf{p}\uparrow}c^\dagger_{\mathbf{p}\downarrow}\rangle\rangle. \tag{10}$$

We will next investigate the structure of these spectral functions and discuss their related physical properties.

III. BOSONS AND COOPERONS

A. Flow of the boson operators

In the course of such a continuous transformation, the initial boson operator $b_{\mathbf{q}}$ becomes convoluted for $l>0$ with the fermion-pair (Cooperon) operator. This can be seen from the $l=0$ derivative

$$\frac{db_{\mathbf{q}}}{dl} = [\eta(0),b_{\mathbf{q}}] = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\alpha_{\mathbf{k},\mathbf{q}-\mathbf{k}}(0)c_{\mathbf{k}\downarrow}c_{\mathbf{q}-\mathbf{k}\uparrow}. \tag{11}$$

Physically this means that while disentangling the boson from fermion subsystem we obtain some new quasiparticles made out of the initial bosons and cooperons (like in the BCS theory where the quasiparticles are composed of electrons and holes).

Guided by the structure of Eq. (11) it is judicious to choose the following superposition for the l-dependent boson operator:

$$b_{\mathbf{q}}(l) = \mathcal{A}_{\mathbf{q}}(l)b_{\mathbf{q}} + \frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\mathcal{B}_{\mathbf{q},\mathbf{k}}(l)c_{\mathbf{k}\downarrow}c_{\mathbf{q}-\mathbf{k}\uparrow}, \tag{12}$$

where $\mathcal{A}_{\mathbf{q}}(l)$ and $\mathcal{B}_{\mathbf{q},\mathbf{k}}(l)$ are some complex functions with the initial condition $\mathcal{A}_{\mathbf{q}}(0)=1$ and $\mathcal{B}_{\mathbf{q},\mathbf{k}}(0)=0$. Substituting Eq. (12) into the flow equation (5) we obtain

$$\frac{d\mathcal{A}_{\mathbf{q}}(l)}{dl} = -\frac{1}{N}\sum_{\mathbf{k}}\alpha_{\mathbf{k},\mathbf{q}-\mathbf{k}}(l)f_{\mathbf{k},\mathbf{q}-\mathbf{k}}\mathcal{B}_{\mathbf{q},\mathbf{k}}(l), \tag{13}$$

$$\frac{d\mathcal{B}_{\mathbf{q},\mathbf{k}}(l)}{dl} = \alpha_{\mathbf{k},\mathbf{q}-\mathbf{k}}(l)\mathcal{A}_{\mathbf{q}}(l), \tag{14}$$

where we introduced the shorthand notation

$$f_{\mathbf{k},\mathbf{p}} = 1 - n^F_{\mathbf{k}\downarrow} - n^F_{\mathbf{p}\uparrow}. \tag{15}$$

From Eqs. (13) and (14) we notice the invariance

$$|\mathcal{A}_{\mathbf{q}}(l)|^2 + \frac{1}{N}\sum_{\mathbf{k}}|B_{\mathbf{q},\mathbf{k}}(l)|^2 f_{\mathbf{k},\mathbf{q}-\mathbf{k}} = 1, \tag{16}$$

which guarantees that the commutation relations between the l-dependent boson operators $[b_{\mathbf{q}}(l),b^\dagger_{\mathbf{p}}(l)] = \delta_{\mathbf{q},\mathbf{p}}$ are correctly preserved.

The parametrization (12) which follows from the flow equation (5) for the operator $b_{\mathbf{q}}(l)$ yields the boson spectral function (6):

$$A^B(\mathbf{q},\omega) = |\mathcal{A}_{\mathbf{q}}(\infty)|^2\delta(\omega - \tilde{E}_{\mathbf{q}}) + \frac{1}{N}\sum_{\mathbf{k}} f_{\mathbf{k},\mathbf{q}-\mathbf{k}}|B_{\mathbf{q},\mathbf{k}}(\infty)|^2 \times \delta(\omega - \tilde{\varepsilon}_{\mathbf{k}} - \tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}). \tag{17}$$

The first term in Eq. (17) describes the coherent part of the

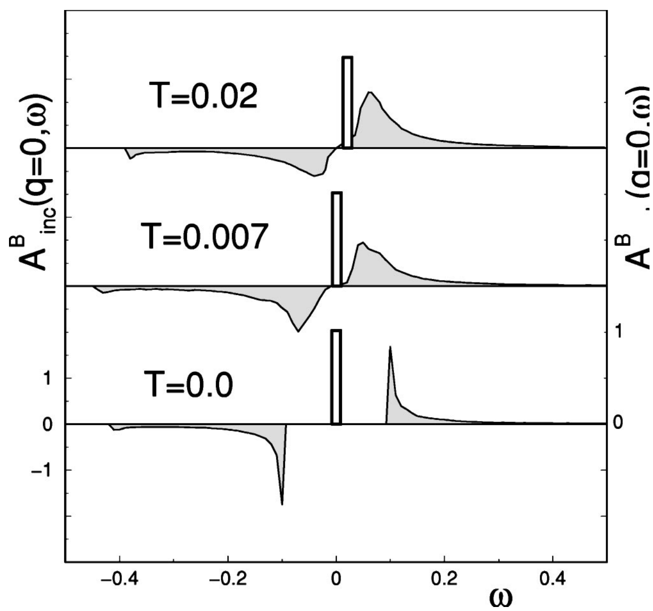

FIG. 1. The boson spectral function $A^B(\mathbf{q}=\mathbf{0},\omega)$ for three representative temperatures $T=0.02>T^*$ (top), $T=0.007<T^*$ (middle), and the ground-state superconducting phase $T=0$ (bottom). The BFM parameters are $n_{\mathrm{tot}}=1$, $v=0.1$, and $\Delta_B=-0.6$ (energies are expressed in units of the initial fermion bandwidth $D\equiv 1$).

boson spectral function corresponding to the long-lived quasiparticles with renormalized energy $\tilde{E}_{\mathbf{q}}$. The second contribution describes some incoherent background of the boson spectral function which represents the states of a relatively short lifetime.

We solve the flow equations (13) and (14) fully self-consistently, applying a numerical procedure based on the Runge-Kutta algorithm. For any value of l we discretized the coefficients $\mathcal{A}_{\mathbf{q}}(l)$ and $\mathcal{B}_{\mathbf{q},\mathbf{k}}(l)$ using a mesh of 4000 equidistant points for representing the vectors $\mathbf{k}$ and $\mathbf{q}$ in the Brillouin zone. Due to computational limitations, we restrict ourselves to a bare one-dimensional tight-binding dispersion $\varepsilon_{\mathbf{k}}(l=0)=-2t\cos(k_x a)$ and throughout this paper use the bandwidth $\mathcal{D}=4t$ as a unit for energies and for the temperature. Starting from the initial value $\mathcal{A}_{\mathbf{q}}(0)=1$ the l-dependent coefficients are calculated via the scheme $\mathcal{A}_{\mathbf{q}}(l+\delta l)=\mathcal{A}_{\mathbf{q}}(l)+\delta l\, d\mathcal{A}_{\mathbf{q}}(l)/dl$, where the derivative is given in Eq. (13). The coefficients $\mathcal{B}_{\mathbf{q},\mathbf{k}}(l)$ are determined in the same way. Since the renormalizations of both these coefficients [as well as other quantities such as energies $\varepsilon_{\mathbf{k}}(l)$, $E_{\mathbf{q}}(l)$ and boson-fermion coupling $v_{\mathbf{k},\mathbf{p}}(l)$] occur at the initial steps of the transformation procedure, we adjust the increment δl in the following way: $\delta l=0.01$ (for $l\leqslant 5$), $\delta l=0.1$ (for $5<l\leqslant 10^2$), $\delta l=1.0$ (for $10^2<l\leqslant 10^3$), and $\delta l=10$ (for $10^3<l\leqslant 10^4$), where both l and δl are expressed in units D^{-2}. The asymptotic (fixed) points are obtained already around $l\simeq 500$ but the transformation procedure is continued up to a good convergence—i.e., $l=10^4$.

Figure 1 shows the results obtained numerically for the single-particle boson spectral function $A^B(\mathbf{q},\omega)$ in the long-wavelength limit $\mathbf{q}=\mathbf{0}$. We illustrate three distinct situations corresponding to the normal phase above T^* (top panel), the normal phase with the pseudogap structure present in the single-particle fermion spectrum (middle panel), and the superconducting state at $T=0$ (bottom panel). In this paper we have chosen the same set of parameters as previously[25]—i.e., $\Delta_B=0.4$, $n_{tot}=1$, $v=0.1$—such that the temperature at which the pseudogap begins to open up is roughly $T^*\sim 0.1$.

Our study of the superconducting phase (following the previous work[25]) is based on a three-dimensional system with a BCS type of approach, as far as the fermionic subsystems is concerned, and a BE condensation approach for free bosons, as far as the bosonic subsystem is concerned. We notice that in this phase there is a perfect separation of the coherent part (describing the long-lived quasiparticles) from the incoherent part of the spectrum. Moreover, (a) the coherent peak is pinned at $\omega=0$, allowing for a macroscopic occupancy of the zero-momentum state by a certain fraction n^B_{cond} of the BE condensed bosons, and (b) the incoherent part $A^B_{inc}(\mathbf{q},\omega)$ exists only outside an energy window (equal to $2v\sqrt{n^B_{cond}}$ as will be explained in Sec. IV D). Owing to such behavior, the condensed bosons are not damped and they are able to establish a long-range order parameter in the boson subsystem. On the other hand, in the normal phase above T^* the coherent and incoherent parts overlap with each other and consequently the boson quasiparticles are damped. This damping is caused by some very reduced remanent interboson interaction of the order of v^4, which arises in this renormalization procedure.[25]

The pseudogap phase (middle panel of Fig. 1) represents some intermediate situation, where we notice that the incoherent background is partly pushed away from the coherent peak. Thus the zero-momentum bosons start to emerge as better and better quasiparticles upon approaching T_c from above. Yet the zero-momentum boson state is macroscopically occupied only below T_c.

In the BFM there is a strict relation between the single-particle boson and fermion-pair excitation spectra [see Eqs. (24) and (25) in the next section]. By inspecting Fig. 1 (and Fig. 3 presented below) we conclude that zero-momentum fermion pairs gradually emerge in the pseudogap phase ($T^*>T$). Upon lowering the temperature, the surrounding incoherent background fades away and thus effectively leads to increase of the lifetime of the zero-momentum bosons and fermion pairs. For $T<T_c$, these entities acquire an infinite lifetime. Experiments, sensitive to the short-lived Cooper pairs, should be able to detect their presence above T_c. This type of a precursor phenomenon was indeed observed for the HTS cuprates using the alternating magnetic fields in the terahertz frequencies regime.[8] A residual Meissner effect was seen there up to nearly 25 K above the transition temperature T_c and which is an indication that propagating fermion pairs exist there on a corresponding short-time scale.

In Fig. 2 we compare the boson spectral function $A^B(\mathbf{q},\omega)$ for several momenta $q=|\mathbf{q}|$ at two different temperatures: above (column on the left) and below T^* (column on the right). We notice that at finite momenta there is is a qualitative difference between these spectra. At temperatures $T>T^*$ the coherent peak is always covered by the incoherent background, signaling that these components are convoluted with each other. On the contrary, at temperatures below T^*, the coherent boson peak separates from the incoherent states.

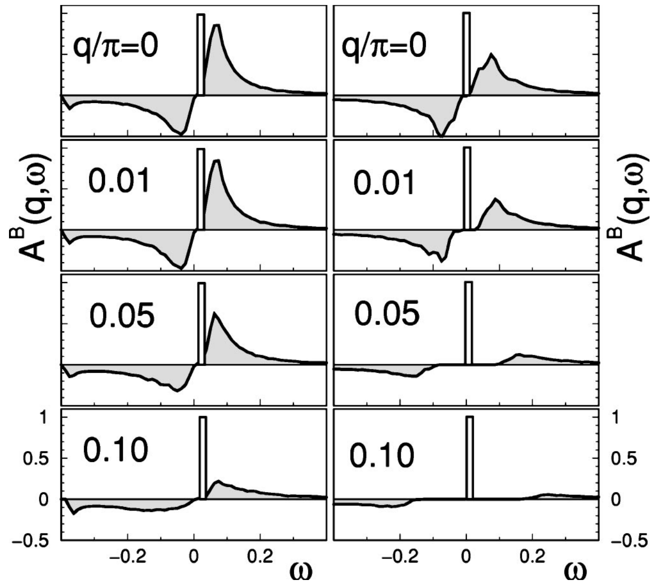

FIG. 2. Variation of the boson spectral function $A^B(\mathbf{q},\omega)$ with respect to changing momentum q at high temperature $T=0.02>T^*$ (panels on the left-hand side) and low temperature $T=0.004$ (panels on the right-hand side) corresponding to the pseudogap region $T^*>T>T_c$. The lattice constant is taken as a unit $a\equiv 1$.

Such a splitting off is very sensitive to moderate temperature changes and—for example, at $T=0.004$—occurs above a critical momentum $q_{crit}\simeq 0.01\times\pi/a$. This critical value decreases with decreasing temperature and finally $q_{crit}(T_c)\to 0$. We thus see that for momenta $q>q_{crit}(T)$ the coherent boson states, representing the long-lived propagating modes, are not scattered by the incoherent background.

Our finding that under certain conditions the boson peak becomes well separated from the background of incoherent states $A^B_{inc}(\mathbf{q},\omega)$ means that in the pseudogap regime $(T^*>T>T_c)$ the finite-momentum bosons are well-defined quasiparticles with infinite lifetime. Since bosons are closely related to the fermion Cooper pairs, we further conclude that for $q>q_{crit}(T)$ there exist infinite-lifetime Cooperons above the transition temperature T_c. According to the Heisenberg principle, experiments measuring the pair-pair correlations restricted to a spatial distance smaller than $\Delta x\sim 1/q_{crit}(T)$ (of the order of several lattice constants) should be able to detect such fermion pairs. And indeed, such long-lived "moving" fermion pairs were observed up to very high temperatures above T_c by applying a thermal gradient and measuring the Nernst coefficient in underdoped HTS materials.[9]

B. Flow of the Cooperon operators

We have seen in the previous section that the boson operators get mixed for $l>0$ with the fermion pair operators. Now we expect that, in turn, also the latter become convoluted with $b_{\mathbf{q}}$ during such a transformation. By calculating the initial $(l=0)$ derivative of the Cooperon operators $S^-_{\mathbf{q}}\equiv N^{-1}\Sigma_{\mathbf{k}}c_{\mathbf{k}\downarrow}c_{\mathbf{q}-\mathbf{k}\uparrow}$ we obtain

$$\frac{dS^-_{\mathbf{q}}}{dl}=-\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\alpha_{\mathbf{k},\mathbf{q}-\mathbf{k}}(0)f_{\mathbf{k},\mathbf{q}-\mathbf{k}}b_{\mathbf{q}}. \tag{18}$$

In accordance with the previous substitution (12) we propose the ansatz

$$S^-_{\mathbf{q}}(l)=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\mathcal{M}_{\mathbf{k},\mathbf{q}}(l)c_{\mathbf{k}\downarrow}c_{\mathbf{q}-\mathbf{k}\uparrow}+\mathcal{N}_{\mathbf{q}}(l)b_{\mathbf{q}}, \tag{19}$$

with the initial conditions $\mathcal{M}_{\mathbf{q},\mathbf{k}}(0)=1$ and $\mathcal{N}_{\mathbf{q}}(0)=0$. After substituting the expression (19) into Eq. (5) we get

$$\frac{d\mathcal{M}_{\mathbf{q},\mathbf{k}}(l)}{dl}=\alpha_{\mathbf{k},\mathbf{q}-\mathbf{k}}(l)\mathcal{N}_{\mathbf{q}}(l), \tag{20}$$

$$\frac{d\mathcal{N}_{\mathbf{q}}(l)}{dl}=-\frac{1}{N}\sum_{\mathbf{k}}\alpha_{\mathbf{k},\mathbf{q}-\mathbf{k}}(l)f_{\mathbf{k},\mathbf{q}-\mathbf{k}}\mathcal{M}_{\mathbf{q},\mathbf{k}}(l). \tag{21}$$

We recognize that the flow equations (20) and (21) for the unknown coefficients $M_{\mathbf{q},\mathbf{k}}(l)$ and $N_{\mathbf{q}}(l)$ have a structure identical to that given by Eqs. (13) and (14). There is only a difference in the initial conditions which in this case lead to the invariance

$$|\mathcal{N}_{\mathbf{q}}(l)|^2+\frac{1}{N}\sum_{\mathbf{k}}f_{\mathbf{k},\mathbf{q}-\mathbf{k}}|\mathcal{M}_{\mathbf{q},\mathbf{k}}(l)|^2=1-n_F. \tag{22}$$

On the right-hand side (RHS) of Eq. (22) we made use of the property that $N^{-1}\Sigma_{\mathbf{k}}f_{\mathbf{k},\mathbf{q}-\mathbf{k}}=1-n_F$, where $n_F=N^{-1}\Sigma_{\mathbf{k},\sigma}n^F_{\mathbf{k}\sigma}$ denotes the total concentration of fermions. Equation (22) assures the proper statistical relation between the Cooperon operators $[S^-_{\mathbf{q}}(l),S^+_{\mathbf{q}}(l)]=N^{-1}\Sigma_{\mathbf{k}}(1-c^\dagger_{\mathbf{q}-\mathbf{k}\uparrow}c_{\mathbf{q}-\mathbf{k}\uparrow}-c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}\downarrow})$, which can be approximated by the c number $\simeq 1-n_F$.

With the ansatz (19) and using its Hermitian conjugate $S^+_{\mathbf{q}}(l)$ we can now determine the two-particle fermion Green's function $G^{pair}(\mathbf{k},\tau)$ defined in Eq. (10). The corresponding spectral function (6) becomes

$$A^{pair}(\mathbf{q},\omega)=|\mathcal{N}_{\mathbf{q}}(\infty)|^2\delta(\omega-\tilde{E}_{\mathbf{q}})+\frac{1}{N}\sum_{\mathbf{k}}f_{\mathbf{k},\mathbf{q}-\mathbf{k}}|M_{\mathbf{q},\mathbf{k}}(\infty)|^2 \times\delta(\omega-\tilde{\varepsilon}_{\mathbf{k}}-\tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}). \tag{23}$$

The Cooperon spectral function turns out to have a structure similar to $A^B(\mathbf{q},\omega)$, expressed in Eq. (17). This is a general feature of the BFM which, in particular, implies, that bosons condense simultaneously with the fermion pairs driven to superconductivity.[35]

We limit our quantitative discussion of the Cooperon spectral function (23) by only presenting in Fig. 3 a distribution of the occupied coherent and incoherent states in the long-wavelength limit $\mathbf{q}=\mathbf{0}$. Above T^* almost all the Cooperons exist as incoherent objects. Upon decreasing the temperature more and more incoherent pairs are converted into coherent ones. Yet because of their overlap with the incoherent background, the Cooper pairs can propagate only on a short-time scale.

The fact that the overall structure of the Cooperon spectral function $A^{pair}(\mathbf{q},\omega)$ is to great extent similar to the single-particle boson function $A^B(\mathbf{q},\omega)$ is not surprising. Us-

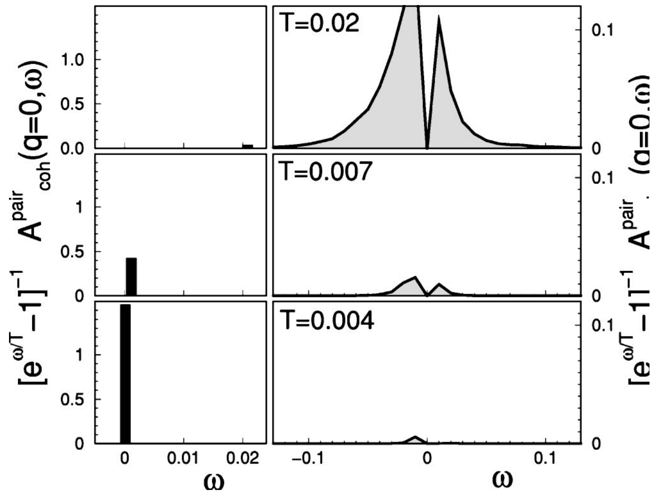

FIG. 3. The Cooperon occupancy $[\exp(\omega/k_BT)-1]^{-1}A^{pair}(\mathbf{q},\omega)$ of the zero-momentum coherent (LHS panel) and incoherent (RHS panel) states for three representative temperatures $T=0.02$ (above T^*) and $T=0.007$, 0.004 (below T^*). With lowering temperature the incoherent fermion pairs are converted into the coherent quasiparticles.

ing, for instance, the equation-of-motion technique for the Green's functions one can prove the important identity[35]

$$G^B(\mathbf{q},\omega) = G_0^B(\mathbf{q},\omega) + v^2 G_0^B(\mathbf{q},\omega)G^{pair}(\mathbf{q},\omega)G_0^B(\mathbf{q},\omega), \tag{24}$$

where $G_0^B(\mathbf{q},\omega)=[\omega-\Delta_B+2\mu]^{-1}$ denotes the single-particle boson Green's function of the noninteracting system. Both Green's functions $G^{pair}(\mathbf{q},\omega)$ and $G^B(\mathbf{q},\omega)$ have thus common poles and their spectral functions are correspondingly related via

$$A^{pair}(\mathbf{q},\omega) = \frac{(\omega-\Delta_B+2\mu)^2}{v^2}A^B(\mathbf{q},\omega). \tag{25}$$

For $\mathbf{q}=\mathbf{0}$, when the single-particle boson Green's function develops a pole at $\omega=0$, the two-particle Cooperon propagator is characterized by the same pole—although with a different weight. This automatically causes a divergence of the static pair susceptibility and via the Thouless criterion leads to the phase transition into a superconducting state.

We want to stress that all our conclusions concerning the evolution of the boson spectral function $A^B(\mathbf{q},\omega)$ are also valid for $A^{pair}(\mathbf{q},\omega)$. In particular, we emphasize that in the pseudogap region $T^*>T>T_c$ there exist fermion Cooper pairs. Fermion pairs with total zero momentum are convoluted with incoherent background states and therefore their lifetime is finite. They can be detected experimentally only via some short-time impulses. On the other hand, long-lived fermion pairs can safely exist if their total momentum exceeds the critical value $q>q_{crit}(T)$. In this case correlations between the fermion pairs can possibly extend over the spatial distance up to $\Delta x\sim 1/q_{crit}$. A possibility to observe correlations between the fermion pairs above T_c over a short spatial and temporal scale had been previously suggested by Tchernyshyov.[27]

IV. FERMIONS

A. Flow of the single-particle fermion operators

Some aspects of the effective single-particle fermion excitations were already discussed in our recent Letter.[2] We focused our discussion there on the single-particle fermion spectrum for a narrow region around the Fermi surface $\mathbf{k}\sim\mathbf{k}_F$. We have shown that the pseudogap is accompanied by the appearance of Bogoliubov-like branches. The shadow part of these Bogoliubov modes is visible above T_c as a broad structure which narrows upon approaching T_c. Below T_c both branches become infinitely narrow, signaling that Bogoliubons become then the true, long-lived quasiparticles. This result is herewith confirmed from our present direct study of the boson and fermion pair spectra, illustrated in Figs. 1–3

In this section we would like to present a detailed derivation of the diagonal and off-diagonal parts (in a Nambu spinor representation) of the single-particle fermion Green's function. We will discuss the diagonal and off-diagonal parts studying their structure over the whole Brillouin zone above and below T_c.

Let us briefly recapitulate the main properties of the fermion operators $c^\dagger_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}\sigma}$ resulting from the continuous canonical transformation. At the initial step (i.e., for $l=0$) their derivatives read

$$\mp\frac{dc_{\mathbf{k}\sigma}}{dl} = \alpha_{-\mathbf{k},\mathbf{k}}(0)\frac{b_0}{\sqrt{N}}c^\dagger_{-\mathbf{k},-\sigma} + \frac{1}{\sqrt{N}}\sum_{\mathbf{q}\neq\mathbf{0}}\alpha_{\mathbf{q}-\mathbf{k},\mathbf{k}}(0)b_{\mathbf{q}}c^\dagger_{\mathbf{q}-\mathbf{k},-\sigma}, \tag{26}$$

where the negative sign corresponds to $\sigma=\uparrow$ and the positive sign to $\sigma=\downarrow$. The first term on the RHS of Eq. (26) shows that the fermion particles get mixed with the fermion holes. The last term in Eq. (26) corresponds to *scattering* of fermions on bosons with finite momentum.

As a consequence of Eq. (26) we imposed the following parametrization of the l-dependent fermion operators:

$$c_{\mathbf{k}\uparrow}(l) = \mathcal{P}_{\mathbf{k}}(l)c_{\mathbf{k}\uparrow} + \mathcal{R}_{\mathbf{k}}(l)c^\dagger_{-\mathbf{k}\downarrow} + \frac{1}{\sqrt{N}}\sum_{\mathbf{q}\neq\mathbf{0}}[p_{\mathbf{k},\mathbf{q}}(l)b^\dagger_{\mathbf{q}}c_{\mathbf{q}+\mathbf{k}\uparrow} + r_{\mathbf{k},\mathbf{q}}(l)b_{\mathbf{q}}c^\dagger_{\mathbf{q}-\mathbf{k}\downarrow}], \tag{27}$$

$$c^\dagger_{-\mathbf{k}\downarrow}(l) = -\mathcal{R}^*_{\mathbf{k}}(l)c_{\mathbf{k}\uparrow} + \mathcal{P}^*_{\mathbf{k}}(l)c^\dagger_{-\mathbf{k}\downarrow} - \frac{1}{\sqrt{N}}\sum_{\mathbf{q}\neq\mathbf{0}}[r^*_{\mathbf{k},\mathbf{q}}(l)b^\dagger_{\mathbf{q}}c_{\mathbf{q}+\mathbf{k}\uparrow} - p^*_{\mathbf{k},\mathbf{q}}(l)b_{\mathbf{q}}c^\dagger_{\mathbf{q}-\mathbf{k}\downarrow}]. \tag{28}$$

In this case, the initial conditions read $\mathcal{P}_{\mathbf{k}}(0)=1$, $\mathcal{R}_{\mathbf{k}}(0)=0$ and $p_{\mathbf{k},\mathbf{q}}(0)=0$, $r_{\mathbf{k},\mathbf{q}}(0)=0$. As we have stated previously,[2] Eqs. (27) and (28) generalize the standard Bogoliubov-Valatin transformation[36] in a twofold way: (a) the initial particle and hole operators are transformed into Cooperons (Bogoliubons) through a continuous transformation and (b) the scattering of finite-momentum Cooper pairs is additionally taken into account via terms containing the coefficients $p_{\mathbf{k},\mathbf{q}}(l)$ and $r_{\mathbf{k},\mathbf{q}}(l)$.

From Eq. (5) one can derive the set of differential equations for a determination of the l-dependent coefficients appearing in Eqs. (27) and (28). Because of their importance, for our further discussion we repeat them here again[2]:

$$\frac{d\mathcal{P}_{\mathbf{k}}(l)}{dl} = \sqrt{n^B_{cond}}\alpha_{-\mathbf{k},\mathbf{k}}(l)\mathcal{R}_{\mathbf{k}}(l) + \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} \alpha_{\mathbf{q}-\mathbf{k},\mathbf{k}}(l) \times (n^B_{\mathbf{q}} + n^F_{\mathbf{q}-\mathbf{k}\downarrow})r_{\mathbf{k},\mathbf{q}}(l), \tag{29}$$

$$\frac{d\mathcal{R}_{\mathbf{k}}(l)}{dl} = -\sqrt{n^B_{cond}}\alpha_{\mathbf{k},-\mathbf{k}}(l)\mathcal{P}_{\mathbf{k}}(l) - \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} \alpha_{-\mathbf{k},\mathbf{q}+\mathbf{k}}(l) \times (n^B_{\mathbf{q}} + n^F_{\mathbf{q}+\mathbf{k}\uparrow})p_{\mathbf{k},\mathbf{q}}(l), \tag{30}$$

$$\frac{dp_{\mathbf{k},\mathbf{q}}(l)}{dl} = \alpha_{-\mathbf{k},\mathbf{q}+\mathbf{k}}(l)\mathcal{R}_{\mathbf{k}}(l), \tag{31}$$

$$\frac{dr_{\mathbf{k},\mathbf{q}}(l)}{dl} = -\alpha_{\mathbf{k},\mathbf{q}-\mathbf{k}}(l)\mathcal{P}_{\mathbf{k}}(l). \tag{32}$$

n^B_{cond} denotes the concentration of the BE condensed bosons and $n^B_{\mathbf{q}} \equiv \langle b^\dagger_{\mathbf{q}} b_{\mathbf{q}}\rangle$ is the distribution of finite-momentum $\mathbf{q} \neq \mathbf{0}$ bosons. Equations (29)–(32) properly preserve the fermionic anticommutation relations $\{c_{\mathbf{k}\uparrow}(l), c_{\mathbf{p}\uparrow}(l)^\dagger\} = \delta_{\mathbf{k},\mathbf{p}}$ and $\{c_{\mathbf{k}\sigma}(l), c_{\mathbf{p}\sigma'}(l)\} = 0$.

The single-particle fermion Green's function can be easily obtained in the limit $l \to \infty$ when the fermions are no longer coupled to the boson subsystem $v_{\mathbf{k},\mathbf{p}}(\infty) = 0$. We have shown previously[2] that the diagonal part reads

$$A^F_d(\mathbf{k},\omega) = |\mathcal{P}_{\mathbf{k}}(\infty)|^2\delta(\omega - \tilde{\varepsilon}_{\mathbf{k}}) + |\mathcal{R}_{\mathbf{k}}(\infty)|^2\delta(\omega + \tilde{\varepsilon}_{-\mathbf{k}}) + \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} (n^B_{\mathbf{q}} + n^F_{\mathbf{q}+\mathbf{k}\uparrow})|p_{\mathbf{k},\mathbf{q}}(\infty)|^2\delta(\omega + \tilde{E}_{\mathbf{q}} - \tilde{\varepsilon}_{\mathbf{q}+\mathbf{k}}) + \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} (n^B_{\mathbf{q}} + n^F_{\mathbf{q}-\mathbf{k}\downarrow})|r_{\mathbf{k},\mathbf{q}}(\infty)|^2\delta(\omega - \tilde{E}_{\mathbf{q}} + \tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}) \tag{33}$$

and that it correctly satisfies the sum rule $\int d\omega A^F_d(\mathbf{k},\omega) = 1$. The spectral function Eq. (33) consists of the δ-function peaks which represent the long-lived quasiparticles and a remaining incoherent background $A^F_{d,inc}(\mathbf{k},\omega)$ of the damped fermion states. It should be mentioned that a similar result was obtained by Lannert, Fisher, and Senthil[37] for the two-dimensional Hubbard model with a fractionalized structure. Those authors considered the spinon and chargon degrees of freedom coupled to a Z_2 gauge field. At low temperatures the spinons and chargons are confined. Their deconfinement becomes possible at finite temperatures by overcoming the gap of "vison" excitations. From an analysis of the low-energy excitations those authors derived the effective spectral function for physical electrons which took exactly the same form as our result (33). Apart from a common structure of the spectral functions, the remaining discussion and interpretation for both models are different.

The spectral function for the off-diagonal part of the fermion Green's function $\langle\langle c_{\mathbf{k}\uparrow}(\tau); c_{-\mathbf{k}\downarrow}\rangle\rangle$ becomes

$$A^F_{od}(\mathbf{k},\omega) = \mathcal{P}_{\mathbf{k}}(\infty)\mathcal{R}_{\mathbf{k}}(\infty)[\delta(\omega + \tilde{\varepsilon}_{\mathbf{k}}) - \delta(\omega - \tilde{\varepsilon}_{\mathbf{k}})] + \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} p_{\mathbf{k},\mathbf{q}}(\infty)r_{\mathbf{k},\mathbf{q}}(\infty)\{\delta(\omega + \tilde{E}_{\mathbf{q}} - \tilde{\varepsilon}_{\mathbf{q}+\mathbf{k}}) \times [n^B_{\mathbf{q}} + n^F_{\mathbf{q}+\mathbf{k}\uparrow}] - \delta(\omega - \tilde{E}_{\mathbf{q}} + \tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}})[n^B_{\mathbf{q}} + n^F_{\mathbf{q}-\mathbf{k}\downarrow}]\}, \tag{34}$$

which conserves the sum rule $\int d\omega A^F_{od}(\mathbf{k},\omega) = 0$. This function consists also of the δ peaks and some fraction distributed over a wide energy region. In what follows below we shall study the properties of the diagonal and off-diagonal spectral functions in various temperature regions.

B. Normal phase spectrum

Above the critical temperature T_c there is no boson condensate $n^B_{cond} = 0$ and in such a case the flow equations (29) and (32) become decoupled from Eqs. (30) and (31). Consequently the coefficients $\mathcal{R}_{\mathbf{k}}(l)$ and $p_{\mathbf{k},\mathbf{q}}(l)$ do not change their initial zero values—i.e.,

$$\mathcal{R}_{\mathbf{k}}(l) = 0, \quad p_{\mathbf{k},\mathbf{q}}(l) = 0. \tag{35}$$

This property (35) has a strong influence on both fermion spectral functions. The off-diagonal part identically vanishes $A^F_{od}(\mathbf{k},\omega) = 0$, which implies that above T_c there exists no long-range order parameter in the fermion system.

The spectral function of the diagonal part is described by

$$A^F_d(\mathbf{k},\omega) = |\mathcal{P}_{\mathbf{k}}(\infty)|^2\delta(\omega - \tilde{\varepsilon}_{\mathbf{k}}) + \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} (n^B_{\mathbf{q}} + n^F_{\mathbf{q}-\mathbf{k}\downarrow}) \times |r_{\mathbf{k},\mathbf{q}}(\infty)|^2\delta(\omega - \tilde{E}_{\mathbf{q}} + \tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}). \tag{36}$$

We thus have just one branch of long-lived fermion states described by the dispersion $\tilde{\varepsilon}_{\mathbf{k}}$ and which can be obtained from the renormalization scheme discussed by us in Ref. 25 For a clear understanding of the resulting low-energy physics we show the temperature evolution of this quantity in Fig. 4 together with the corresponding spectral weight $|\mathcal{P}_{\mathbf{k}}(\infty)|^2$. Below a certain characteristic temperature T^* (in this case $T^* \sim 0.1$) we observe a tendency to form the pseudogap. Simultaneously there occurs a partial transfer of the spectral weight from the quasiparticle peak to the incoherent background states (see the bottom panel of Fig. 4).

Such a transfer of the spectral weight is responsible for the appearance of the Bogoliubov shadow band, as shown from the self-consistent numerical calculations in Ref. 2. We will prove this result here analytically. When the temperature approaches T_c from above, bosons tend to occupy macroscopically the lowest-lying states of energies $\tilde{E}_{\mathbf{q}} \simeq 0$. These states are spread over the momentum region $|\mathbf{q}| \leqslant \Lambda$ with the cutoff Λ being a fraction of the inverse lattice spacing a^{-1}. Since the boson occupancy of low momenta is much larger than the fermion population $n^F_{\mathbf{q}-\mathbf{k}}$, we can simplify Eq. (36) to the form

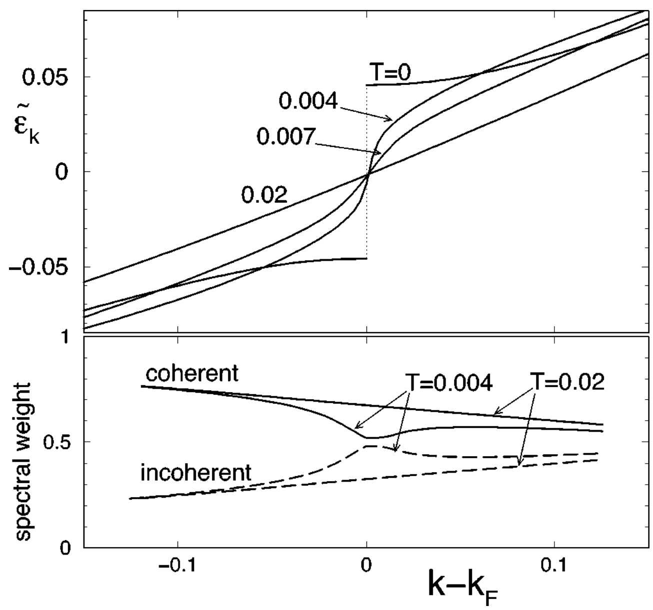

FIG. 4. Dispersion of the effective single-particle fermion energy $\tilde{\varepsilon}_{\mathbf{k}}$ for several temperatures (upper panel) and spectral weights of the coherent and incoherent parts for $T=0.02$ and 0.004 (bottom panel). Momentum is expressed in units $1/a$.

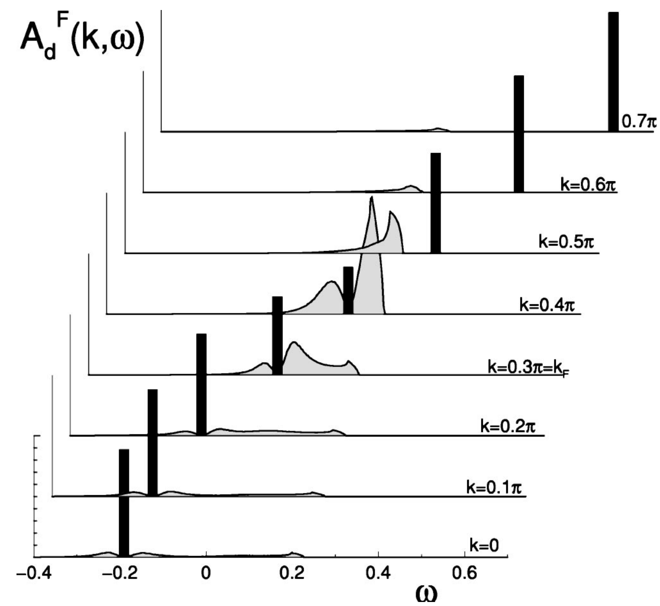

FIG. 5. Diagonal part of the single-particle fermion spectral function (36) for a large part of the Brillouin zone at $T=0.007$. Vertical bars represent the coherent part $A^F_{d,coh}(\mathbf{k},\omega)$ while the shaded area corresponds to $A^F_{d,inc}(\mathbf{k},\omega)$. Besides only a close vicinity of the Fermi surface [consult Eq. (38) or see Fig. 1 in Ref. 2] this spectral function is rather weakly affected by temperature.

$$A^F_d(\mathbf{k},\omega) \simeq |\mathcal{P}_{\mathbf{k}}(\infty)|^2\delta(\omega-\tilde{\varepsilon}_{\mathbf{k}}) + |r_{\mathbf{k},\mathbf{q}\simeq 0}(\infty)|^2 \times \sum_{|\mathbf{q}|\leqslant\Lambda}\frac{n^B_{\mathbf{q}}}{N}\delta(\omega+\tilde{\varepsilon}_{-\mathbf{k}}-\tilde{E}_{\mathbf{q}}) + A^F_{d,rigid}(\mathbf{k},\omega), \tag{37}$$

where $A^F_{d,rigid}(\mathbf{k},\omega)=N^{-1}\Sigma_{|\mathbf{q}|>\Lambda}n^F_{\mathbf{q}-\mathbf{k}\downarrow}|r_{\mathbf{k},\mathbf{q}}(\infty)|^2\delta(\omega+\tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}-\tilde{E}_{\mathbf{q}})$ represents a rigid background which is weakly sensitive to varying temperature. Integrating over the small-momentum boson states (whose energies are negligible $\tilde{E}_{\mathbf{q}}\simeq 0$) we obtain a partly broadened peak with its maximum occurring at $\omega=-\tilde{\varepsilon}_{\mathbf{k}}$. This additional branch of fermion excitations can well be fitted by the Lorentzian shape

$$\sum_{|\mathbf{q}|\leqslant\Lambda}\frac{n^B_{\mathbf{q}}}{N}\delta(\omega+\tilde{\varepsilon}_{-\mathbf{k}}-\tilde{E}_{\mathbf{q}}) \simeq \frac{n^B}{\pi}\frac{\Gamma_{\mathbf{k}}}{(\omega+\tilde{\varepsilon}_{-\mathbf{k}})^2+\Gamma^2_{\mathbf{k}}}, \tag{38}$$

with n^B being the concentration of bosons. For $T<T_c$, Eq. (38) shrinks to $\Gamma\to 0$. Similar Bogoliubov shadow bands were also indicated for the normal phase of the $U<0$ Hubbard model using the quantum Monte Carlo studies[38] and the conserving diagrammatic treatment of Vilk and Tremblay.[39] In our case the Bogoliubov-like branches are characterized by the pseudogap dispersion $\pm\tilde{\varepsilon}_{\mathbf{k}}$ shown here in Fig. 4. Above T_c the shadow branch (corresponding to the–sign) is broad as discussed in our Letter.[2]

Far away from the Fermi surface the renormalized energies are nearly equal to the bare values $\tilde{\varepsilon}_{\mathbf{k}}=\varepsilon_{\mathbf{k}}-\mu$. The long-lived quasiparticle contains, however, only part of the spectral weight—i.e., $|\mathcal{P}_{\mathbf{k}}(\infty)|^2<1$. In Fig. 5 we illustrate the coherent and incoherent contributions of the single-particle fermion spectral function (36) in a large part of the Brillouin zone. The damped fermion states are spread over the large energy regime ω; they exist even for momenta quite distant from k_F. This result agrees well with previous studies based on self-consistent perturbative theory (see the third reference of Ref. 15). The presence of the substantial incoherent background states might possibly be related to the experimental signal observed in the ARPES measurements for the HTS compounds.[10]

C. Long-lived quasiparticles below T_c

Below the critical temperature T_c there exists a finite amount of the BE condensed bosons $n^B_{cond}\neq\mathbf{0}$. This has important effects on the fermionic spectrum. Using the flow equation method we have shown analytically[25] that $\tilde{\varepsilon}_{\mathbf{k}}=\mathrm{sgn}(\varepsilon_{\mathbf{k}}-\mu)\sqrt{(\varepsilon_{\mathbf{k}}-\mu)^2+v^2n^B_{cond}}$. In the superconducting phase the effective dispersion is thus characterized by the true gap $\Delta_{sc}(T)=v\sqrt{n^B_{cond}(T)}$.

For a finite condensate fraction n^B_{cond}, we can see from Eqs. (30) and (31) that the coefficients $\mathcal{R}_{\mathbf{k}}$ and $p_{\mathbf{k},\mathbf{q}}$ become finite too. The long-lived fermion excitations are then represented by the two sharp Bogoliubov branches

$$A^F_{d,coh}(\mathbf{k},\omega) = |\mathcal{P}_{\mathbf{k}}(\infty)|^2\delta(\omega-\tilde{\varepsilon}_{\mathbf{k}}) + |\mathcal{R}_{\mathbf{k}}(\infty)|^2\delta(\omega+\tilde{\varepsilon}_{\mathbf{k}}). \tag{39}$$

Similarly, the coherent part of the off-diagonal spectral function (34) reads

$$A^F_{od,coh}(\mathbf{k},\omega) = \mathcal{P}_{\mathbf{k}}(\infty)\mathcal{R}_{\mathbf{k}}(\infty)\times[\delta(\omega+\tilde{\varepsilon}_{\mathbf{k}})-\delta(\omega-\tilde{\varepsilon}_{\mathbf{k}})]. \tag{40}$$

Equations (39) and (40) resemble the BCS-type results which usually appear in mean-field studies of this model.[13–15] Let us stress that in distinction to these we obtain here the total spectral weight engaged in the coherent parts to be[2]

$$|\mathcal{P}_{\mathbf{k}}(\infty)|^2 + |\mathcal{R}_{\mathbf{k}}(\infty)|^2 < 1. \tag{41}$$

The rest of the weight is redistributed over the damped fermionic states. This will be discussed separately in the next section.

In order to show the correspondence of our present analysis to the previous results for this BF model we prove in Appendix B that upon neglecting the incoherent background states of Eqs. (33) and (34) one obtains exactly the usual BCS coherence factors

$$|\mathcal{P}_{\mathbf{k}}(\infty)|^2 = \frac{1}{2}\left(1 + \frac{|\varepsilon_{\mathbf{k}} - \mu|}{\xi_{\mathbf{k}}^{MF}}\right) = 1 - |\mathcal{R}_{\mathbf{k}}(\infty)|^2, \tag{42}$$

$$\mathcal{P}_{\mathbf{k}}(\infty)\mathcal{R}_{\mathbf{k}}(\infty) = -\frac{v\sqrt{n_{cond}^B}}{2\xi_{\mathbf{k}}^{MF}}, \tag{43}$$

where $\xi_{\mathbf{k}}^{MF} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_{sc}^2}$. By neglecting the incoherent parts, the flow equation procedure reproduces exactly the standard mean-field equations[13–15]

$$\langle c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} \rangle = \frac{1}{2}\left[1 - \frac{\varepsilon_{\mathbf{k}} - \mu}{\xi_{\mathbf{k}}^{MF}} \tanh\left(\frac{\xi_{\mathbf{k}}^{MF}}{2k_B T}\right)\right], \tag{44}$$

$$\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = -\frac{v n_{cond}^B}{2\xi_{\mathbf{k}}^{MF}} \tanh\left(\frac{\xi_{\mathbf{k}}^{MF}}{2k_B T}\right). \tag{45}$$

We shall generalize these equations (44) and (45) in the next section, taking into account the contribution from the damped fermion states.

D. Damped quasiparticles below T_c

The finite-lifetime (damped) states do participate in the fermionic excitation spectrum both above T_c as well as below it. Nevertheless, their presence does not spoil a long-range coherent behavior between the fermion pairs which is necessary for superconductivity to occur. In Sec. III we saw that boson as well as the fermion pair spectra are characterized below T_c by long-lived collective modes with $\tilde{E}_{\mathbf{q}} \propto |\mathbf{q}|$,[25] which becomes separated from the surrounding background of incoherent states by the gap $2\Delta_{sc}$. We show below that in the single-particle excitation spectrum the incoherent states can exist only outside the gap Δ_{sc} around the Fermi energy.

The contribution from the damped fermionic states is described by the following part of the spectral function (33):

$$\begin{aligned} A_{d,inc}^F(\mathbf{k},\omega) &= A_d^F(\mathbf{k},\omega) - A_{d,\cancel{coh}}^F(\mathbf{k},\omega) \\ &= \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} [(n_{\mathbf{q}}^B + n_{\mathbf{q}+\mathbf{k}\uparrow}^F) \\ &\quad \times |p_{\mathbf{k},\mathbf{q}}(\infty)|^2 \delta(\omega + \tilde{E}_{\mathbf{q}} - \tilde{\varepsilon}_{\mathbf{q}+\mathbf{k}}) + (n_{\mathbf{q}}^B + n_{\mathbf{q}-\mathbf{k}\downarrow}^F) \\ &\quad \times |r_{\mathbf{k},\mathbf{q}}(\infty)|^2 \delta(\omega - \tilde{E}_{\mathbf{q}} + \tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}})] \end{aligned} \tag{46}$$

and, similarly in case of the off-diagonal function (34),

$$\begin{aligned} A_{od,inc}^F(\mathbf{k},\omega) &= -\frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} p_{\mathbf{k},\mathbf{q}}(\infty) r_{\mathbf{k},\mathbf{q}}(\infty) \\ &\quad \times [(n_{\mathbf{q}}^B + n_{\mathbf{q}+\mathbf{k}\uparrow}^F)\delta(\omega + \tilde{E}_{\mathbf{q}} - \tilde{\varepsilon}_{\mathbf{q}+\mathbf{k}}) \\ &\quad - (n_{\mathbf{q}}^B + n_{\mathbf{q}-\mathbf{k}\downarrow}^F)\delta(\omega - \tilde{E}_{\mathbf{q}} + \tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}})]. \end{aligned} \tag{47}$$

It is instructive to consider first the incoherent spectral functions (46) and (47) for the ground state $T=0$. Finite-momentum bosons have $\tilde{E}_{\mathbf{q}\neq\mathbf{0}} > 0$, such that all bosons are condensed at $T=0$ and we can put $n_{\mathbf{q}}^B=0$ for any $\mathbf{q}\neq\mathbf{0}$. On the other hand, fermions occupy only the states below the Fermi surface—i.e., $n_{\mathbf{k}\sigma}^F = \theta(-\tilde{\varepsilon}_{\mathbf{k}}) n_{\mathbf{k}\sigma}^F$. Therefore, the first term on the RHS of Eq. (46) gives rise to the appearance of incoherent fermion states at negative energies. It can be written as

$$A_{d,inc}^F(\mathbf{k},\omega<0) = \frac{1}{N}\sum_{\tilde{\varepsilon}_{\mathbf{q}+\mathbf{k}}<0} n_{\mathbf{q}+\mathbf{k}\uparrow}^F |p_{\mathbf{k},\mathbf{q}}(\infty)|^2 \delta[\omega + (\tilde{E}_{\mathbf{q}} + |\tilde{\varepsilon}_{\mathbf{q}+\mathbf{k}}|)]. \tag{48}$$

Similarly, the last term in Eq. (46), which corresponds to incoherent states at positive energies, becomes

$$A_{d,inc}^F(\mathbf{k},\omega>0) = \frac{1}{N}\sum_{\tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}<0} n_{\mathbf{q}-\mathbf{k}\downarrow}^F |r_{\mathbf{k},\mathbf{q}}(\infty)|^2 \delta[\omega - (\tilde{E}_{\mathbf{q}} + |\tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}|)]. \tag{49}$$

The off-diagonal spectral function (47) can be derived in the same manner. From inspecting their structure we notice that (i) no damped fermion states are allowed to occur within the superconducting energy gap window $|\omega| \leqslant \Delta_{sc}$ because $|\tilde{\varepsilon}_{\mathbf{q}\pm\mathbf{k}}| \geqslant \Delta_{sc}$ and (ii) even outside the superconducting gap, in a close vicinity of the coherence peaks (39), there is a partial suppression of the damped fermion states due to finite $\tilde{E}_{\mathbf{q}}$ in Eqs. (48) and (49). As shown in our earlier studies[15,25] the width of such a boson band is rather small and of the order v^2/D.

The incoherent fermion states can thus be formed only outside the superconducting gap $|\omega| > \Delta_{sc}$ and yet they are strongly suppressed over some small energy region (of the order v^2/D from the coherence peaks).

To summarize our results of the last two sections, we conclude that the single-particle fermion spectral function (33) is characterized in the superconducting phase by (a) the presence of narrow quasiparticle *peaks* at $\omega = \pm\sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_{sc}^2}$, (b) the partial suppression of the fermionic states very close to the coherence peaks, giving rise to the appearance of the *dip*-like structure, and (c) the existence of a broad incoherent background spectrum with its flat maximum (*hump*) situated fairly away from the Fermi energy. Upon increasing the temperature we expect the *dip*-like structure to be gradually filled in via absorbing part of the spectral weight from the coherent Bogoliubov peaks. Our expectation is motivated here by the fact that the spectral weights $|\mathcal{P}_{\mathbf{k}}(\infty)|^2$, $|\mathcal{R}_{\mathbf{k}}(\infty)|^2$ of the coherent peaks are very sensitive to temperature because of $n_{cond}^B(T)$ appearing in their flow equations (29) and (30).

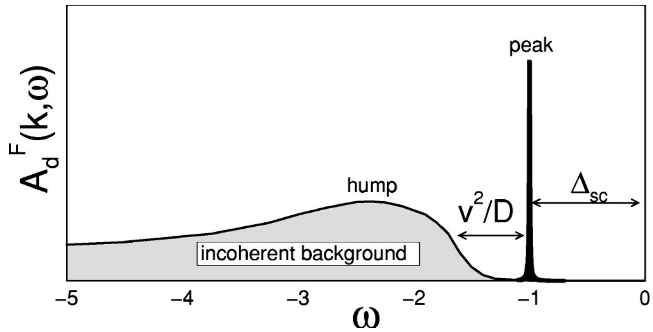

FIG. 6. Schematic view of the single-particle fermion spectral function $A_d^F(\mathbf{k}_F,\omega<0)$ in the ground state of the boson fermion model. Energy ω is expressed in units of the superconducting gap which is roughly scaled via $\Delta_{sc}\simeq v\sqrt{n_{cond}^B}$.

Our theoretical prediction concerning the single-particle spectrum of the superconducting phase is in qualitative agreement with the experimental data known for the high-T_c underdoped cuprates (see Fig. 6). The direct photoemission spectroscopy probes the occupied spectrum $A^F(\mathbf{k},\omega)[1+\exp(\omega/k_BT)]^{-1}$. Photoemission measurements indeed revealed the appearance of such a *peak-dip-hump* structure.[10] This issue has been so far interpreted in terms of the boson resonant mode to which the single-particle excitations are coupled. Several candidates have been proposed in the literature for such boson modes.[40–42] The BF model (1) is an alternative scenario, where bosons represent nearly localized electron pairs.

Concluding this discussion on the coherent and incoherent single-particle spectra, let us stress that the expectation values for the particle distribution $n_{\mathbf{k}\sigma}^F$ at arbitrary temperature can be obtained by integrating over the expression (33) after having been multiplied by the Fermi Dirac function $f(x)=(1+e^{x/k_BT})^{-1}$—i.e.,

$$n_{\mathbf{k}\sigma}^F=\int_{-\infty}^{\infty}d\omega A_d^F(\mathbf{k},\omega)f(\omega). \tag{50}$$

Similarly, the order parameter determined via Eq. (34) is given by

$$\begin{aligned}\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle &= \mathcal{P}_{\mathbf{k}}(\infty)\mathcal{R}_{\mathbf{k}}(\infty)[1-2f(\tilde{\varepsilon}_{\mathbf{k}})]+\frac{1}{N}\sum_{\mathbf{q}\neq 0}p_{\mathbf{k},\mathbf{q}}(\infty)r_{\mathbf{k},\mathbf{q}}(\infty)\\ &\times[(n_{\mathbf{q}}^B+n_{\mathbf{q}+\mathbf{k}\uparrow}^F)f(\tilde{\varepsilon}_{\mathbf{q}+\mathbf{k}}-\tilde{E}_{\mathbf{q}})-(n_{\mathbf{q}}^B+n_{\mathbf{q}-\mathbf{k}\downarrow}^F)\\ &\times f(-\tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}+\tilde{E}_{\mathbf{q}})].\end{aligned} \tag{51}$$

which generalizes the mean-field equation (45). Unfortunately, at the present stage we are not able to solve numerically these equations (50) and (51) for some realistic $d>2$ system when $T_c>0$. We will try to address this problem in the future by applying some approximate treatment.

V. CONCLUSIONS

In the present paper we studied the mutual relations between the single-particle and the pair excitation spectra within the BF model (1). We investigated their interdependence occurring in the superconducting phase below the critical temperature and in the pseudogap region above T_c. Many-body effects were treated by means of the continuous canonical transformation[26] originating from a general framework of the renormalization group technique.[31]

We have earlier reported[25] that, upon approaching T_c from above, there is a partial suppression of the single-particle fermion states near the Fermi energy (pseudogap). Here, we supplement this picture by showing that the pseudogap feature is accompanied by a subsequent emergence of the fermion-pair properties. Such pairs can show up in the pseudogap region as long-lived entities provided that their total momentum is finite and larger than a certain $q_{crit}(T)$. For $T\to T_c$ the critical momentum is $q_{crit}=0$; therefore, all the fermion pairs become good quasiparticles. The zero-momentum fermion pairs exist above T_c only as the damped objects because of their overlap with the incoherent background. However, upon lowering the temperature such an overlap gradually diminishes which effectively leads to an increase in their lifetime.

Although above T_c there exists no off-diagonal long-range order (ODLRO) we predict nevertheless the possibility to observe some ordering on a restricted spatial and temporal scale. Experiments using terahertz frequencies[8] did indeed confirm the existence of preformed pairs in underdoped HTS materials up to 25° above T_c. We moreover suspect that "moving" fermion pairs (on the basis of our study expected to have the infinite lifetime) have been observed in measurements of the Nernst coefficient.[9]

As far as the single-particle excitations are concerned we provided here the analytical arguments for the appearance of Bogoliubov-type bands in the pseudogap phase. Upon approaching T_c from above the shadow branch absorbs more and more spectral weight and simultaneously narrows as was previously indicated by us from the self-consistent numerical study.[2] Below T_c, the shadow branch shrinks to the usual δ-function peak and marks the appearance of infinite-lifetime Cooperons. In distinction to the conventional BCS superconductors we find that the quasiparticle peaks occurring at $\omega=\pm\sqrt{(\varepsilon_{\mathbf{k}}-\mu)^2+\Delta_{sc}^2}$ become slightly separated from the rest of the spectrum which is present in the form of a incoherent background. This effectively leads to the formation of the intriguing *peak-dip-hump* structure which has been well documented experimentally by ARPES measurements. In our scenario such a structure is a consequence of the pair correlations (see also the similar conclusion in Ref. 6).

In a future study we plan take into consideration an anisotropic two-dimensional version of this model which is more realistic for describing the HTS cuprates. The boson-fermion coupling v should then be appropriately factorized by the d-wave form factor. Another important aspect which has not been fully explored so far concerns the doping dependence of the pseudogap and other related precursor features discussed above. Such a study requires a proper treatment of the hard-core nature of the local electron pairs, which is an issue which is rather nontrivial. Preliminary results were so far obtained using a perturbative approach[43] and from exact-diagonalization studies.[44] As we realized, the crossover between the BCS type superconductivity and BE condensation of preformed pairs was addressed by Eagles in Ref. 45.

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APPENDIX A

In our previous work[25] we have derived the continuous canonical transformation for block diagonalization of the BFM. The transformed Hamiltonian was constrained to the structure $H(l)=H_0(l)+H_{int}(l)$, where

$$H_0(l) = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}}(l) - \mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} (E_{\mathbf{q}}(l) - 2\mu)b^\dagger_{\mathbf{q}}b_{\mathbf{q}} + \frac{1}{N}\sum_{\mathbf{k},\mathbf{p},\mathbf{q}} U_{\mathbf{k},\mathbf{p},\mathbf{q}}(l)c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{p}\downarrow}c_{\mathbf{q}\downarrow}c_{\mathbf{k}+\mathbf{p}-\mathbf{q}\uparrow}, \tag{A1}$$

$$H_{int}(l) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{p}} v_{\mathbf{k},\mathbf{p}}(l)(b^\dagger_{\mathbf{p}+\mathbf{k}}c_{\mathbf{k}\downarrow}c_{\mathbf{p}\uparrow} + \text{H.c.}). \tag{A2}$$

For eliminating $H_{int}(l)$ we follow an idea proposed by Wegner[26] who showed that, upon using $\eta(l) =[H_0(l),H_{int}(l)]$, one obtains $\lim_{l\to\infty}H_{int}(l)=0$. In this case,

$$\eta(l) = -\frac{1}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{p}} \alpha_{\mathbf{k},\mathbf{p}}(l)(b^\dagger_{\mathbf{p}+\mathbf{k}}c_{\mathbf{k}\downarrow}c_{\mathbf{p}\uparrow} - \text{H.c.}), \tag{A3}$$

where $\alpha_{\mathbf{k},\mathbf{p}}(l)=[\varepsilon_{\mathbf{k}}(l)+\varepsilon_{\mathbf{p}}(l)-E_{\mathbf{k}+\mathbf{p}}(l)]v_{\mathbf{k},\mathbf{p}}(l)$. All l-dependent parameters of the Hamiltonian (A1) and (A2) are determined via a set of the flow equations (16)–(21) given in Ref. 25. They are obtained from the operator equation (2) by reducing the higher-order interactions through normal ordering (linearization).

Since at $l=\infty$ the bosons are no longer hybridized with fermions, we essentially obtain the (semi)free subsystems with renormalized effective spectra. Only the fermion part contains the long-range Coulomb interaction $U_{\mathbf{k},\mathbf{p},\mathbf{q}}$ which in some cases can play an important role. For instance, in the $\mathbf{q}=\mathbf{p}$ channel one obtains[24] a resonant-type amplitude of the potential $U_{\mathbf{k},\mathbf{p},\mathbf{p}}(\infty)$ for $\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{p}}=E_{\mathbf{p}+\mathbf{k}}$. This corresponds to the resonant (Feshbach) scattering between electrons when their total energy is equal to energy of the bound pair (hard-core boson).[20] In the context of HTS such unusual scattering is also important, leading to the particle-hole asymmetry of the low-energy spectrum both, in the pseudogap and superconducting phases.[34]

One should remember that the amplitude of the induced Coulomb potential $U_{\mathbf{k},\mathbf{p},\mathbf{q}}(\infty)$ is finite for any channel. It was estimated to be residual, of the order v^2.[25] In the following we will thus treat the transformed Hamiltonian

$$H(\infty) = H^F(\infty) + H^B(\infty) \tag{A4}$$

as composed of two contributions from bosons $H^B(\infty) =\Sigma_{\mathbf{q}}\tilde{E}_{\mathbf{q}}b^\dagger_{\mathbf{q}}b_{\mathbf{q}}$ with their effective energy $\tilde{E}_{\mathbf{q}}\equiv E_{\mathbf{q}}(\infty)-2\mu$ and fermions approximated by $H^F(\infty)\simeq\Sigma_{\mathbf{k}\sigma}\tilde{\varepsilon}_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$ with effective energy

$$\tilde{\varepsilon}_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}}(\infty) - \mu + \frac{1}{N}\sum_{\mathbf{p}} U_{\mathbf{k},\mathbf{p},\mathbf{p}}(\infty)n^F_{\mathbf{p},-\sigma}. \tag{A5}$$

Here $n^F_{\mathbf{p},\sigma}=\langle c^\dagger_{\mathbf{p},\sigma}c_{\mathbf{p},\sigma}\rangle$, where the spin is a dummy index which will be kept throughout the remainder of this paper in order to indicate the origin of such terms.

APPENDIX B

Neglecting the incoherent background states of the single-particle functions $A^F_d(\mathbf{k},\omega)$ and $A^F_{od}(\mathbf{k},\omega)$ is equivalent to the assumption that $p_{\mathbf{k},\mathbf{q}}(l)=0$ and $r_{\mathbf{k},\mathbf{q}}(l)=0$. In such a case the flow equations (29) and (30) simplify to

$$\frac{d\mathcal{P}_{\mathbf{k}}(l)}{dl} = \sqrt{n^B_{cond}}\alpha_{-\mathbf{k},\mathbf{k}}(l)\mathcal{R}_{\mathbf{k}}(l), \tag{B1}$$

$$\frac{d\mathcal{R}_{\mathbf{k}}(l)}{dl} = -\sqrt{n^B_{cond}}\alpha_{\mathbf{k},-\mathbf{k}}(l)\mathcal{P}_{\mathbf{k}}(l). \tag{B2}$$

We will now assume that both functions $\mathcal{P}_{\mathbf{k}}(l)$ and $\mathcal{R}_{\mathbf{k}}(l)$ are real (this requirement does not restrict the generality of our considerations). We rewrite Eq. (B1) as

$$\frac{d\mathcal{P}_{\mathbf{k}}(l)}{\mathcal{R}_{\mathbf{k}}(l)} = \sqrt{n^B_{cond}}\alpha_{-\mathbf{k},\mathbf{k}}(l)dl \tag{B3}$$

and integrate both sides of Eq. (B3) in the limits $\int_{l=0}^{l=\infty}$. Using the sum rule 10 of Ref. 2 we can substitute $\mathcal{R}_{\mathbf{k}}(l) =\sqrt{1-\mathcal{P}^2_{\mathbf{k}}(l)}$. Upon integration we get, for the LHS,

$$\int_{l=0}^{l=\infty} \frac{d\mathcal{P}_{\mathbf{k}}(l)}{\sqrt{1-[\mathcal{P}_{\mathbf{k}}(l)]^2}} = -\operatorname{arcos}[\mathcal{P}_{\mathbf{k}}(\infty)] \tag{B4}$$

because $\operatorname{arcos}[\mathcal{P}_{\mathbf{k}}(0)]=0$.

Integration of the RHS of Eq. (B3) requires knowledge of $\alpha_{-\mathbf{k},\mathbf{k}}(l)$ for the superconducting phase. First, let us notice that from the general definition of this parameter we have $\alpha_{-\mathbf{k},\mathbf{k}}(l)=2[\varepsilon_{\mathbf{k}}(l)-\mu]v_{-\mathbf{k},\mathbf{k}}(l)$. Using Eq. (43) of Ref. 25 we can further write

$$v_{-\mathbf{k},\mathbf{k}}(l)dl = -\frac{dv_{-\mathbf{k},\mathbf{k}}(l)}{4[\varepsilon_{\mathbf{k}}(l)-\mu]}. \tag{B5}$$

In the superconducting phase we can additionally make use of the invariance shown in Eq. (51) of Ref. 25:

$$\varepsilon_{\mathbf{k}}(l) - \mu = \pm\sqrt{(\xi^{MF}_{\mathbf{k}})^2 - n^B_{cond}v^2_{-\mathbf{k},\mathbf{k}}(l)}, \tag{B6}$$

where $\pm=\text{sgn}(\varepsilon_{\mathbf{k}}-\mu)$. By substituting Eqs. (B5) and (B6) into the RHS of Eq. (B4) we obtain

$$\sqrt{n_{cond}^B}\int_0^\infty dl\,\alpha_{-\mathbf{k},\mathbf{k}}(l) = -\frac{\sqrt{n_{cond}^B}}{2}\int_{l=0}^{l=\infty}\frac{dv_{-\mathbf{k},\mathbf{k}}(l)}{\varepsilon_{\mathbf{k}}(l)-\mu}$$
$$= \frac{\mp 1}{2}\sqrt{n_{cond}^B}\int_v^0 \frac{dv_{-\mathbf{k},\mathbf{k}}}{\sqrt{(\xi_{\mathbf{k}}^{MF})^2 - n_{cond}^B v_{-\mathbf{k},\mathbf{k}}^2}}$$
$$= \pm\frac{1}{2}\left[\frac{\pi}{2} - \arccos\left(\frac{v\sqrt{n_{cond}^B}}{\xi_{\mathbf{k}}^{MF}}\right)\right]. \qquad (B7)$$

In the second line of Eq. (B7) we applied the initial condition $v_{-\mathbf{k},\mathbf{k}}(0)=v$ and also the final result $v_{-\mathbf{k},\mathbf{k}}(\infty)=0$ when changing the integration variable from dl to $dv_{-\mathbf{k},\mathbf{k}}(l)$.

By comparing the results (B4) and (B7) we obtain

$$\mp 2\arccos[\mathcal{P}_{\mathbf{k}}(\infty)] = \frac{\pi}{2} - \arccos\left(\frac{v\sqrt{n_{cond}^B}}{\xi_{\mathbf{k}}^{MF}}\right), \qquad (B8)$$

and by taking the cosine function on both sides, we get $2\mathcal{P}_{\mathbf{k}}^2(\infty)-1=|\varepsilon_{\mathbf{k}}-\mu|/\xi_{\mathbf{k}}^{MF}$, which leads to the usual BCS coherence factors

$$\mathcal{P}_{\mathbf{k}}^2(\infty) = \frac{1}{2}\left[1 + \frac{|\varepsilon_{\mathbf{k}}-\mu|}{\xi_{\mathbf{k}}^{MF}}\right] = 1 - \mathcal{R}_{\mathbf{k}}^2(\infty). \qquad (B9)$$

In this way we also know that the magnitude of the product is $|\mathcal{P}_{\mathbf{k}}(\infty)\mathcal{R}_{\mathbf{k}}(\infty)|=v\sqrt{n_{cond}^B}/2\xi_{\mathbf{k}}^{MF}$. Hence, assuming that $\mathcal{P}_{\mathbf{k}}(l)$ is positive (in particular also for $l=\infty$), then on a basis of the flow equation (B2) we conclude that $\mathcal{R}_{\mathbf{k}}(l)=-\text{sgn}(\varepsilon_{\mathbf{k}}-\mu)|\mathcal{R}_{\mathbf{k}}(l)|$ and thus finally

$$\mathcal{P}_{\mathbf{k}}(\infty)\mathcal{R}_{\mathbf{k}}(\infty) = -\frac{v\sqrt{n_{cond}^B}}{2\xi_{\mathbf{k}}^{MF}}. \qquad (B10)$$

This product (B10) enters the off-diagonal Green's function and in consequence yields Eq. (45) for the order parameter.

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