

Anomalous S-like dispersion of in-gap single-particle excitations in the pseudogap state of cuprate superconductors

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The single-particle excitations which control the opening of the pseudogap in the cuprate superconductors at some temperature T^* are considered to derive their specific local spectral features from resonant pairing, whereby charge carriers get momentarily trapped on dynamically deformable molecular Cu-O-Cu clusters. We show how such local excitations evolve into overdamped modes with a characteristic “S”-like dispersion around the Fermi energy, as one passes below T^* . This feature should be detectable in a “momentum distribution curve” angle-resolved photoemission spectroscopy analysis and help to elucidate the kind of pairing in the cuprates. Our study is based on a generic boson-fermion model for resonant pairing and is an extension of our previous dynamical mean-field theory study [A. Romano and J. Ranninger, *Phys. Rev. B* **62**, 4066 (2000)] of the spectral properties of the pseudogap state.

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I. INTRODUCTION

Pairing in classical low-temperature BCS superconductors occurs exclusively because of a collective phenomenon: below a certain temperature T_c , the ensemble of pairs of charge carriers with momenta and spin $[\mathbf{k}\uparrow, -\mathbf{k}\downarrow]$ in a thin layer around the Fermi surface, spontaneously lock up into a globally phase coherent state,¹ $\Pi_{\mathbf{k}}(u_{\mathbf{k}}e^{i\phi/2} + v_{\mathbf{k}}e^{-i\phi/2}c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger)|0\rangle$ with a \mathbf{k} -independent phase ϕ . It is the onset of this phase locking which binds those pairs into Cooper pairs, whose binding energy determines the size of the superconducting gap. Going above T_c , the ensemble of charge carriers returns to a normal Fermi-liquid state with a well-defined Fermi surface—apart from a very narrow temperature regime above T_c governed by superconducting phase fluctuations. The order parameter describing this superconducting state is controlled by the finite amplitude of the Cooper pairs. The phase rigidity between those pairs being big, phase fluctuations play a minor role in the destruction of the BCS superconducting state. The Uemura experiment,² measuring the superfluid density, early on told us that in the cuprate superconductors the inverse is the case. They exhibit weak phase rigidity but strong local pairing correlations,³ as manifest in the variation in T_c , which scales with the density of superfluid charge carriers. This situation favors an insulating state composed of phase uncorrelated pairs out of which a superconducting state evolves upon doping beyond a certain concentration of $x_{sc}=5-10\%$ holes per Cu ion. Alternatively, configurations of globally phase uncorrelated pairs exist above T_c for $x \geq x_{sc}$, which manifest themselves by the superconducting gap having been turned into a pseudogap upon increasing the temperature to above T_c . Phase locking on a long-range level then breaks down but continues to exist on a finite space-time scale, which gets shorter and shorter as one approaches a temperature T_M . Going beyond T_M , interpair phase correlations, even on a short space-time scale, disappear, while the finite amplitude of those pairs continues to resist up to T^* . Above T^* these pairs break up and we have

a liquid of fermionic charge carriers, albeit not being a true Fermi liquid. Understanding the microscopic origin of pairing for the cuprate superconductivity rests with understanding the mechanism driving the onset of the pseudogap phase at T^* , which is *unrelated* to any superconducting phase correlations. This is the region which we are going to explore in this study with the aim to propose an experimental test to either validate or invalidate the resonant pairing scenario for the cuprates. In this way we hope to contribute to pin down the pairing mechanism which ultimately controls the superconducting properties of the cuprates.

The opening of the pseudogap arises from the appearance of *locally* fluctuating diamagnetic pairs. That this is unrelated to any superconducting precursor pairing was shown in a variety of experiments (see Ref. 4 and citations therein), suggesting a picture where the preponderant charge carriers are diffusively propagating bosonic pairs in interaction with single-particle fermionic excitations.⁵ The effect of the superconducting phase correlation-driven pairing sets in below T_M and acquires its maximal effect upon approaching T_c . It manifests itself in transient Meissner screening,⁶ Nernst effect in thermal transport,⁷ torque magnetization measurements,⁸ and zero-bias conductance of pseudogap/superconducting junctions.⁹ $T_M(x)$ closely follows the doping dependence of T_c , which, in the low doped and overdoped regime is only slightly above T_c , while growing substantially above it in the region in between. The microscopic mechanism driving the onset of local pairing below T^* is still a matter of dispute. A possible explanation for it could be that it describes systems of Fermions in a self-created fluctuating environment, which momentarily traps them in form of bosonic diamagnetic singlet pairs. This leads to a resonant pairing scenario, which has been analyzed in detail over the past years by Ranninger and collaborators in terms of a generic boson-fermion model (BFM). The microscopic mechanism behind it could be either of polaronic origin, for which it was originally conjectured, or due to strong electronic correlations such as deriving from the Hubbard model^{10,11} and

the “resonating valence bond” (RVB) scenario of Anderson.¹²

II. RESONANT PAIRING SCENARIO

The intrinsic metastability of the cuprate crystal structure¹³ involves dynamically fluctuating molecular Cu-O-Cu clusters,^{14–16} which, on a finite space-time scale either capture charge carriers in form of bound singlet pairs or accommodate them as itinerant particles while passing through them. This breaks crystalline symmetry on a local level¹⁷ and causes the fermionic charge carriers to be simultaneously itinerant and localized, as observed in scanning tunneling microscope imaging studies (see Ref. 18 and references therein). Such a duplicitous feature of fermionic charge carriers,¹⁹ coexisting in localized as well as delocalized states, had been known for some time to occur in dilute polaronic systems, in the crossover region separating the antiadiabatic and adiabatic regimes.²⁰ It was this feature which led one of us (J.R.) to conjecture in the early eighties that in a many-body polaronic system it should result in the intrinsic metastability of such compounds. It represented a natural extension of the concept of bipolaronic superconductivity,²¹ an extremely fragile state of matter, most likely unrealizable in real materials, which prefer to localize their charge carriers under similar conditions. In an attempt to realize a superconducting state in strongly coupled electron-lattice systems, it appeared judicious to consider the possibility of fluctuating bipolaronic states rather than truly bound states, which led to the proposition of the phenomenological BFM. Its salient features are a local charge exchange coupling between bound pair states and states of pairs of uncorrelated itinerant charge carriers. Such a scenario preserves the fermionic character of the system (albeit with a generally fractionated Fermi surface^{17,22}), yet, at the same time, exhibits a critical temperature T_c , which is controlled by the phase of the bosonic diamagnetic pairs, as exemplified by the disappearance of the density of superfluid carriers rather than of amplitude fluctuations.

The fact that the pairing which emerges at T^* is strictly unrelated to any superconducting phase fluctuations has motivated us in the past to examine the single-particle spectral features which are involved in such pairing process, for a single isolated dynamically fluctuating molecular cluster (see Ref. 14 and references therein). Its basic physical features are strong local phase correlations between (i) states where two charge carriers are correlated in bosonic bonding and antibonding states and (ii) states where they are uncorrelated in nonbonding states while passing through such clusters. This results in a characteristic three-pole structured single-particle local spectral function, arising from transitions between the two distinct configurations.^{23,24} Incorporating the local physics of such individual clusters in a study of an ensemble of them, coupled with each other via the intercluster hopping of fermionic charge carriers, we have shown²⁵ how a globally phase correlated superconducting state evolves, via a quantum phase transition, out of a Mott correlation-driven insulator of hardcore bosonic pairs, as the boson-fermion exchange coupling decreases with increasing

hole doping. This is an analog of the classical Mott insulating state, deriving from purely fermionic correlations. The driving mechanism behind it is the competition between the local phase correlations on individual clusters, mentioned above, and the spatial phase correlations, which arise from Josephson tunneling between those clusters. With increasing temperature, those latter lose their efficiency and, as one approaches T^* , we are left with exclusively local phase correlations. The individual clusters form a regular lattice with electrons fluctuating in and out of them, forming a liquid of fermionic charge carriers with which the local excitations interact.

The aim of the present study is to demonstrate how the characteristic three-pole structure of such isolated individual clusters evolves into dispersive branches when those clusters are put together in a crystalline arrangement with single-particle hopping between them. Since the crossover at T^* is unrelated to the presence of any superconducting phase fluctuations, we must assure that they are explicitly excluded in our theoretical approach. A suitable tool for that is the dynamical mean-field theory (DMFT),²⁶ here supplemented by the noncrossing approximation (NCA) (Ref. 27) as impurity solver, where the effect of long as well as short-range phase correlations between the bosonic transient pairs can be controlled. The present work is a natural extension of our previous studies^{28,29} of the spectral properties of the pseudogap state. The features that we put to the reader’s attention are fingerprints of the local spectral features that could be tested experimentally looking at the “momentum distribution curves” in angle-resolved photoemission spectroscopy (ARPES) studies.

III. MODEL

Let us consider for that purpose a lattice of effective sites, acting as trapping centers which momentarily transform delocalized fermionic charge carriers into bound pairs and vice-versa. This, as we shall see below, makes them lose any Fermi-liquid properties near the chemical potential. The Hamiltonian which captures that physics is that of the generic boson-fermion model

$$H = \varepsilon_0 \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + E_0 \sum_i \rho_i^+ \rho_i^- + g \sum_i [\rho_i^+ c_{i\downarrow} c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rho_i^-]. \quad (1)$$

Here $c_{i\sigma}^{(\dagger)}$ denotes the annihilation (creation) operators for fermions with spin σ at some effective sites i and ρ_i^+ and ρ_i^- are pseudospin 1/2 operators, describing creation and annihilation operators of tightly bound fermion pairs which behave as hardcore bosons. The symbols t , g , $\varepsilon_0 = zt - \mu$, $E_0 = \Delta_B - 2\mu$ denote, respectively: the hopping integral for the fermions, the boson-fermion pair-exchange coupling, the local fermion and boson energy levels measured with respect to the chemical potential μ , which has to be common to fermions and bosons, up to a factor 2 for the latter which are made out of two fermions. This assures that at any given moment such a mixture of locally fluctuating bosonic pairs and itinerant

unpaired fermionic charge carriers are in chemical equilibrium with each other. A transition from a phase correlated superconducting state into a phase uncorrelated insulating one has been established to take place for a boson concentration close to $n_B=0.5$, when g is increased beyond a certain critical g_{SIT} .²⁵ We shall restrict ourselves here to the case $n_{\text{tot}}=n_F+2n_B=2$, our effective sites being constituted by two adjacent O-Cu-O molecular bonds. This is appropriate for the parent compound and the not too heavily overdoped cuprates since the doping rate hardly ever is beyond 20% and it can be monitored by a doping dependent boson-fermion exchange coupling $g(x)$, given the hardcore nature of the bosonic diamagnetic pairs (see Ref. 25). It permits us for a fixed $n_{\text{tot}}=2$ to track qualitatively, upon varying g , the cross-over at finite temperatures from a metallic paramagnetic state, characterizing the overdoped region, into the diamagnetic pairing fluctuation-driven pseudogap state and eventually into a correlation-driven insulating state of globally phase uncorrelated pairs. This is one of the main issues in our present study of the spectral features of the cuprates in the pseudogap state. Our approach for that will follow closely that employed in Ref. 29.

The molecular clusters which contain the vital physics of the cuprates are square plaquettes, consisting of four Cu ions surrounded by the oxygen ligands. This is the case for polaronic scenarios as well as for electronic ones where those clusters are the basic building stones of the RVB physics.¹⁰ In a polaronic scenario, such plaquettes represent clusters involving stereochemical $\text{C}^{\text{II}}\text{-O-C}^{\text{II}}$ configurations housing two electrons, which upon hole doping change into $\text{C}^{\text{III}}\text{-O-C}^{\text{III}}$ bonds.¹⁴⁻¹⁶

The essential physics of resonant pairing is manifest on the level of individual molecular clusters at effective lattice sites i , encoded in the spectral properties of the atomic limit of Eq. (1), $H_{\text{at}}=\lim_{t\rightarrow 0} H$. In order to keep the algebra as simple as possible, we shall restrict ourselves here to the case where the bosonic level coincides with the center of the fermionic band, i.e., $\Delta_B=2\varepsilon_0$. This dictates the position of the chemical potential $\mu\simeq\Delta_B/2$ and implies a half-filled fermionic band ($n_F\simeq 1$). Putting $\varepsilon_0=0$ then leads to $\Delta_B=\mu=0$. The Hilbert space of this local problem consists of eight configurations made out of four fermionic states $|2\rangle=|c_\uparrow^\dagger\rangle$, $|3\rangle=|c_\downarrow^\dagger\rangle$, $|6\rangle=|c_\uparrow^\dagger\rho^+\rangle$, and $|7\rangle=|c_\downarrow^\dagger\rho^+\rangle$ with energies $E_2=E_3=E_6=E_7=0$ and four bosonic states $|1\rangle=|0\rangle$, $|4\rangle\equiv|B\rangle=(1/\sqrt{2})[|c_\uparrow^\dagger c_\downarrow^\dagger\rangle-|\rho^+\rangle]$, $|5\rangle\equiv|AB\rangle=(1/\sqrt{2})[|c_\uparrow^\dagger c_\downarrow^\dagger\rangle+|\rho^+\rangle]$, and $|8\rangle=|c_\uparrow^\dagger c_\downarrow^\dagger\rho^+\rangle$ with energies $E_1=0$, $E_4=-g$, $E_5=+g$, and $E_8=0$. The single-particle Green's function for this atomic limit has been derived previously^{23,24} and is

$$G_{\text{at}}(i\omega_n) = - \int_0^\beta d\tau e^{i\omega_n\tau} \langle T [c_\sigma(\tau) c_\sigma^\dagger] \rangle$$

$$= \frac{Z^F}{i\omega_n - \varepsilon_0} + \frac{1 - Z^F}{i\omega_n - \varepsilon_0 - g^2/(i\omega_n + \varepsilon_0 - E_0)} \quad (2)$$

with $Z^F=2/(3+\cosh\beta g)$. The local single-particle spectral function $A_{\text{at}}(\omega)=-\frac{1}{\pi}\text{Im} G_{\text{at}}(i\omega_n=\omega+i0)$ is then composed of two contributions: the first one arises from uncorrelated charge carriers in states $|2\rangle, |3\rangle, |6\rangle, |7\rangle$ while the sec-

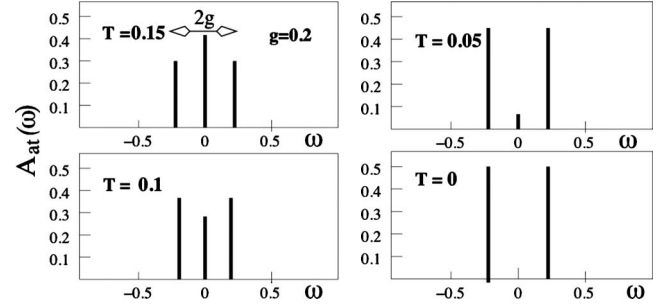


FIG. 1. The single-particle spectral function in the atomic limit as a function of frequency for different temperatures T .

ond one, which is reminiscent of the single-particle spectral function for BCS superconductivity, with g playing the role of the gap, describes the contributions coming from bonding and antibonding states $|4\rangle$, $|5\rangle$, respectively. The significant difference between resonant pairing and Cooper pairing in this single-particle spectral function is the simultaneous appearance of contributions coming from uncorrelated charge carriers and contributions coming from charge carriers being momentarily bound into pairs, controlled by the temperature-dependent spectral weights Z_F and $1-Z_F$, respectively. As one reduces the temperature below a characteristic value $T\simeq g$, the spectral intensity of the single-particle nonbonding excitations Z^F at $\omega=0$ shows a significant drop and goes to zero for $T\rightarrow 0$ while that of the bonding and antibonding states at $\omega=\mp g$ increases correspondingly. Simultaneously, the local exchange correlations, given by $\langle c_\uparrow c_\uparrow \rho^+ \rangle = (1/2)\tanh(\beta g/2)$, show a marked increase upon decreasing T below g and saturate at 0.5 for $T\rightarrow 0$ (see Fig. 4 in Ref. 24). We illustrate in Fig. 1 the variation with temperature of $A_{\text{at}}(\omega)$. We see that below $T\simeq g$ the local density of states at the chemical potential ($\omega=0$) rapidly drops to zero. For a finite system, this local physics foreshadows the opening of a gaplike structure at the Fermi surface, which is independent of any global symmetry breaking. We now explore how this local physics, described by $A_{\text{at}}(\omega)$, evolves into dispersive modes when putting such effective sites into a lattice with charge exchange between adjacent sites.

IV. SINGLE-PARTICLE SPECTRAL FEATURES

In order to evaluate the single particle spectral function for a macroscopic system composed of the local clusters considered in the previous section, we have to solve this problem in a way where the full physics of the local problem (H_{at}) is taken into account exactly. We refer to the DMFT approach, using as solver of the impurity problem the so-called NCA, based on the Keiter-Kimball perturbation expansion, further developed by Kuramoto and Grewe and reviewed by Bickers.²⁷ As in Refs. 28 and 29, we have reformulated the Hamiltonian, Eq. (1), for the D_∞ problem in the standard way, by coupling the local variables contained in H_{at} to a Weiss field which mimics the itinerancy of the original fermions $c_{i\sigma}^{(\dagger)}$ on a Bethe lattice. The effective Hamiltonian for that is

$$\begin{aligned}
 H = & g[c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}\rho^{-} + \rho^{+}c_{\downarrow}c_{\uparrow}] - t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger}c_{j\sigma} + \sum_{k, \sigma} w_k d_{k, \sigma}^{\dagger} d_{k, \sigma} \\
 & + \sum_{k, \sigma} v_k [d_{k, \sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} d_{k, \sigma}]. \quad (3)
 \end{aligned}$$

Here $d_{k, \sigma}^{(\dagger)}$ denote the operators of the auxiliary fermionic excitations of the Weiss field, having energies w_k and which are coupled to the original fermionic excitations on an ‘‘Anderson impurity’’ site by a hybridization term of strength v_k . Following our previous work on such a procedure,^{28,29} the Hamiltonian, Eq. (3) is re-expressed in terms of Hubbard operators corresponding to H_{at} of the isolated local problem. One then calculates the local Green’s function $G_{\text{imp}}(i\omega_n) = [i\omega_n - \varepsilon_0 - \Sigma_W(i\omega_n) - \tilde{\Sigma}_{\text{int}}^g(i\omega_n)]^{-1}$, where $\Sigma_W(i\omega_n)$ and $\tilde{\Sigma}_{\text{int}}^g(i\omega_n)$ denote, respectively, the self-energies of the original fermions due to their interaction with the Weiss field, and their proper self-energy due to their mutual interaction with each other. Imposing the condition that $G_{\text{imp}}(i\omega_n)$ should be identical to the local part of the lattice Green’s function, $G_{\text{lat}}(i\omega_n) = \int d\varepsilon \rho(\varepsilon) G_{\text{lat}}(i\omega_n, \varepsilon) \equiv \int d\varepsilon \rho(\varepsilon) [i\omega_n - \varepsilon - \tilde{\Sigma}_{\text{int}}^g(i\omega_n)]^{-1}$, one obtains $\Sigma_W(i\omega_n) = t^2 G_{\text{imp}}(i\omega_n)$, which determines the spectral distribution of the Weiss field energies $\{w_k\}$ in a self-consistent way. In the above equation $\rho(\varepsilon) = (1/2\pi t^2) \sqrt{\varepsilon(4t - \varepsilon)}$ denotes the bare fermionic density of states of the lattice problem in D_{∞} , characterized by a bandwidth $D=4t$ which serves as the energy unit in our study. Once $\Sigma_W(i\omega_n)$ is obtained, one deduces the self-energy for the lattice problem via $\tilde{\Sigma}_{\text{int}}^g(i\omega_n) = i\omega_n - \Sigma_W(i\omega_n) - [G_{\text{imp}}(i\omega_n)]^{-1}$. In determining $G_{\text{imp}}(i\omega_n)$, we have introduced in the past a modification²⁹ of the original NCA-DMFT scheme. This modification consists of introducing $\tilde{\Sigma}_{\text{int}}^g(i\omega_n) \equiv \Sigma_{\text{int}}^g(i\omega_n) - \Sigma_{\text{int}}^{g=0}(i\omega_n)$, which had permitted us to subtract out the effect of kinematic interactions arising in such a NCA formalism, and enabled us to describe in a qualitatively correct way the redistribution of spectral weight of the fermionic excitations over the entire frequency regime of the fermionic excitations.

The spectral properties deduced from the lattice Green’s function are now used to describe the evolution from the paramagnetic metallic phase ($0.05 < g < 0.1$) to the pseudogap phase with locally fluctuating pairs embedded in a liquid of fermionic itinerant charge carriers, merging into a correlation-driven insulator ($0.1 < g < 0.15$). The onset of the pseudogap phase is manifest in the single-particle excitations by the abrupt appearance above $g=0.1$ of a three-pole structure of the lattice Green’s function with the peak positions given by the solutions of the equation $\omega^* - \varepsilon - \text{Re} \tilde{\Sigma}_{\text{int}}^g(\omega^*) = 0$. In Fig. 2, we plot the solutions ω^* of this equation together with the imaginary parts of the self energy $\text{Im} \tilde{\Sigma}_{\text{int}}^g(\omega^*)$ at these poles. Upon approaching $g=0.1$ from below, ω^* as a function of the bare fermionic spectrum $\varepsilon_{\mathbf{k}} = -2t \cos \mathbf{k}$ (represented here by its corresponding energy ε) develops a sharp upturn around the hidden Fermi surface because of the presence of the pseudogap at $\varepsilon=0$. This initially rather smooth upturn finishes up in a vertical slope upon approaching $g=0.1$ for $T=0.05$. Upon further increasing g , we find three simultaneously nonvanishing dispersing modes in a re-

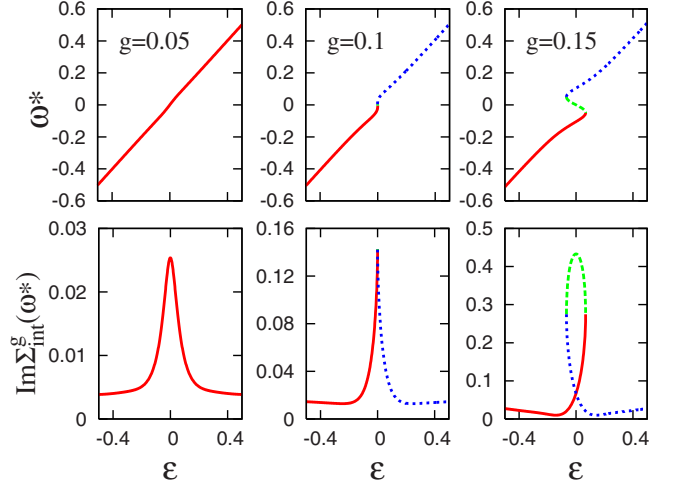


FIG. 2. (Color online) Poles ω^* of the single-particle Green’s functions (upper row), and imaginary part of the self-energy evaluated at ω^* (lower row), as functions of the bare energies ε of the fermionic particles, measured from the chemical potential, for a given temperature $T=0.05$ and different values of g in units of D .

stricted region of momentum (alias ε) around $\varepsilon=0$. Two of those modes, corresponding in Fig. 2 to the red continuous line and the blue dotted line, lie outside the pseudogap and follow qualitatively the unrenormalized bare dispersion $\varepsilon_{\mathbf{k}} \equiv \varepsilon$. Inside the pseudogap, however, the renormalization turns the nonbonding states into a characteristic ‘‘S’’-like shape (the green dashed line) in accordance with the three-pole structure of the atomic limit of the local spectral function of an isolated single cluster, $A_{\text{at}}(\omega)$, given by Eq. (2). This ‘‘S’’-like dispersing single-particle feature is a fingerprint of resonant pairing, which differently from what happens in the so-called crossover scenarios,³⁰ results not simply in bound pairs but in strongly locally phase-correlated intra-cluster localized and delocalized states having nonbonding, bonding, and antibonding character. Following the so-called Fermi arcs in the Brillouin zone of the cuprate CuO_2 planes, going from the nodal toward the antinodal point, whereupon the effective g increases,¹⁶ the single-particle in-gap excitations deriving from the first term in the atomic limit Green’s function, Eq. (2), lose any coherent quasiparticle features once those clusters are embedded in a crystalline structure with charge exchange between each other. We illustrate in Fig. 3 how this gradually happens as we increase g , plotting this spectral function for wave vectors at the Fermi surface ($\varepsilon=0$), or whatever remains of it, for a variety of different boson-fermion exchange couplings g . We notice that for low values of g ($=0.05$) the contributions to $A(\omega, \varepsilon=0)$, deriving from the nonbonding state, which are the representatives of itinerant single-particle excitations, are still very pronounced. As g is increased, we see a gradual transfer of the corresponding spectral weight toward the wings in the spectral functions, which represent localized fermionic excitations trapped in bosonic bonding and antibonding diamagnetic singlet states. In this way a pseudogap in the single-particle density of states $N(\omega) \equiv \int d\varepsilon A(\omega, \varepsilon)$ (see Fig. 3) gradually develops around the chemical potential ($\omega=0$), as g is increased. These features illustrate that the intrinsically

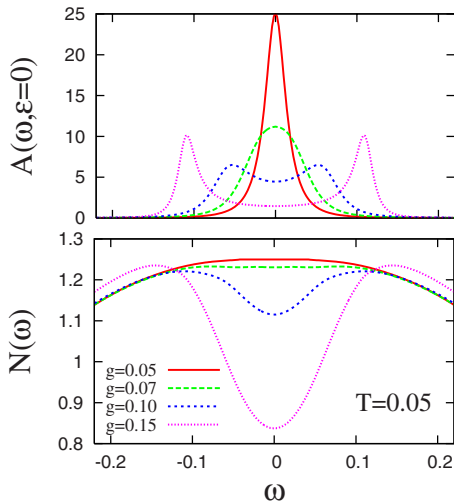


FIG. 3. (Color online) The single-particle spectral function $A(\omega, \varepsilon=0)$ together with the density of states $N(\omega)$ as a function of ω at $T=0.05$ and various values of g .

itinerant single-particle excitations observed above T^* do not become simply overdamped modes as we enter the pseudogap regime but rather lose their spectral weight by filling in the energy interval of that pseudogap in a fairly homogeneous fashion. Those in-gap states can no longer be described by poles in the single-particle Green's function for wave vectors close to the hidden Fermi surface. A first indication for that came from a self-consistent perturbative approach,³¹ where the analytic properties of such a spectral function were obtained in the complex frequency plane, upon analytical continuation from the Matsubara to the real frequency axis. Using N -point Padé approximants,³² unusual spectral features for the excitations, lying inside the pseudogap, were found in form of a dense cloud of complex poles, which had also complex residues. Approximating a function which has a cut by such Padé approximants, is known to require complex residues. This therefore signals that such in-gap single-particle states have spectral properties which derive from cut singularities and are not simply complex poles. The present finding which confirms our old conjecture for that is similar to the conjecture of Anderson. Within his “strange-metal hidden Fermi-liquid” scenario,³³ the single-particle Green's function exhibits such cutlike features in form of $G(k, \omega) \propto [v_F k - \omega]^{-1+p}$ with v_F denoting the Fermi velocity. The numerical constant p was introduced to account for the intrinsic wave-function incoherence in highly correlated systems and this Ansatz could reproduce rather well certain transport coefficients as well as spectral features seen in ARPES energy distribution curves.

Our present analysis of the frequency variation in the spectral function for wave vectors near the hidden Fermi surface ($\varepsilon=0$) does not show any clearly visible sign of a dispersing behavior as we vary the momentum, alias ε (not shown here). As a consequence, we do not expect to see a dispersion of these modes in standard energy distribution curve ARPES analysis. One should however be able to detect such an S-like dispersion when using a “momentum distribution curve” ARPES analysis, as can be clearly seen from

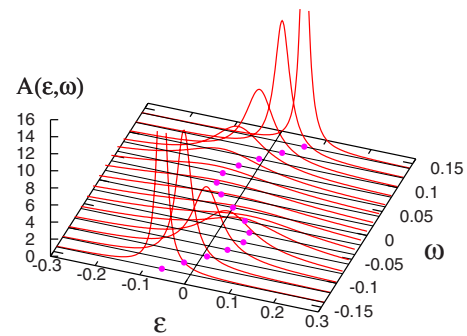


FIG. 4. (Color online) The single-particle spectral function $A(\varepsilon, \omega)$ as a function of the bare electron dispersion ε , scanning the various energies inside the pseudogap.

the plot in Fig. 4. There we present the single-particle spectral function $A(\varepsilon, \omega)$ for a set of equidistant energies ω in the pseudogap energy region $[-g \leq \omega \leq +g]$. Identifying the peak positions of the various curves, corresponding to different ω 's, with the corresponding values of ε , we can deduce the dispersion of those in-gap excitations, which, as it should be, coincide with the dispersion of $\omega^*(\varepsilon)$, shown in Fig. 2.

V. DISCUSSION

We have considered a general scenario of fermionic charge carriers in a self-created fluctuating environment, which captures them momentarily in form of diamagnetic locally bound singlet pairs. This gives rise to a resonant pairing mechanism, which bares no connection to any static attractive interaction. Its microscopic origin may be diverse. It can derive from either a polaronic mechanism in strongly coupled electron-lattice systems showing intrinsic dynamical lattice instabilities,¹⁴ or alternatively from strong electronic correlations leading to RVB physics.¹² In this case singlet pairs on plaquette clusters get exchanged with pairs of uncorrelated holes in their immediate neighborhood,¹⁰ forming bound states whereby a hole accompanies itinerant singlet electron pairs.¹¹

The main purpose of our study was to show how the local physics of individual clusters transpires as we embed them into a lattice and to propose an ARPES experiment to test this local physics. Since single isolated clusters, such as those examined in Ref. 14, show very specific spectral features, with a three-pole structure representing a fingerprint of resonant pairing, we wanted to see to what extent this can be visualized in an experiment testing the spectral features of the cuprates in the pseudogap state, where according to our scenario the resonant pairing should first come into action. In order to study the effect of the charge exchange of a cluster with its environment, the most suitable approach is the DMFT,²⁶ where the fluctuating cluster plays the role of the Anderson impurity site. It results in the S-like-shaped dispersion around the hidden Fermi surface and is distinctly different from any BCS-type physics.³⁴ Our results strongly suggest that those in-gap excitations correspond to cut singularities rather than poles. While the S-like dispersive feature in the single-particle spectral function cannot be ex-

pected to be easily detectable in “energy distribution curve” ARPES analysis, we have shown that an ARPES study focusing on “momentum distribution curves” should be able to verify this feature. If indeed it is, it would represent a strong

indication that resonant pairing might play a fundamental role in the opening of the pseudogap and in the subsequent establishment of the superconducting state, as the temperature is lowered.

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