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General analysis of the angle-resolved photoemission line shape for strongly correlated electron systems

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In many cases the standard perturbation approach appears to be too simple to describe precisely the angle-resolved photoemission spectrum of a strongly correlated electron system. In particular, to describe the momentum asymmetry observed in the photoemission spectra of high-T_c cuprates, a phenomenological approach based on an extremely correlated Fermi-liquid model has been recently introduced. Here we analyze the general structure of the Green's function of quasiparticles in strongly correlated electron systems and stress that it is defined not only by the self-energy of Hubbard quasiparticles but also by a strength operator. The latter leads to an additional odd momentum contribution to the spectral function and alone can explain the observed asymmetry. So, the asymmetry of the angle-resolved photoemission spectra can be a measure of the strength of electron correlations in materials.

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I. INTRODUCTION

Angle-resolved photoemission spectroscopy (ARPES) is a very powerful method to study the electronic structure of solids, especially for anisotropic layered materials such as high-T_c cuprates where the quasiparticle dispersion law $\epsilon(k_x,k_y)$ may be obtained [1]. It is particularly important for strongly correlated electron systems where the conventional *ab initio* local density approximation to the density functional theory (LDA-DFT) fails to get the correct quasiparticle electronic structure.

While the conventional description of electrons is based on "bare electron" parameters renormalized by interactions, it is difficult to understand what the "bare electron" is in the strongly correlated system. The modern understanding of strong or extreme correlations is still primitive. The exact solution for the basic model in the theory of correlated materials, the Hubbard model, is available only for one-dimensional cases. It results in unconventional physics of holons and spinons with a Luttinger liquid instead of a Fermi liquid. In the absence of exact results for two- and higher-dimensional strongly correlated electronic systems it is instructive to discuss some alternative approaches to the theory of multielectron systems with strong interactions. In this situation the role of angle-resolved photoemission spectroscopy is extremely important because it provides the experimental data on the electronic dispersion and spectral weight. Nevertheless, a theoretical analysis is required to get these fundamental electronic properties from experimental data. That is why a general analysis of the ARPES line shape for strongly correlated systems should be done.

Within the usually applied three-step model of photoemission and using the sudden approximation [2], the photoelectron counts $I(\mathbf{k},\omega)$ as a function of energy ω and momentum $\mathbf{k}$ are given by $I(\mathbf{k},\omega) = |M_{ij}|^2 f(\omega) A(\mathbf{k},\omega)$, where M_{ij} is the dipole matrix element for the photoexcitation, $f(\omega)$ is the Fermi-Dirac distribution, and $A(\mathbf{k},\omega) = (-1/\pi)\mathrm{Im}\, G(\mathbf{k},\omega)$ is the spectral function for the single-electron retarded Green's function $G(\mathbf{k},\omega)$. If one disregards the effect of the energy and momentum resolutions as well as the matrix element effect [3] and the extrinsic background [4], the photoelectron intensity is proportional to the spectral function multiplied by the Fermi function.

Usually the standard perturbation representation of the Green's function $G(\mathbf{k},\omega)$ in terms of Fermi-type operators is used for the analysis [1,5] of ARPES data. Introducing the real and imaginary parts of the quasiparticle self-energy $\Sigma_{\mathbf{k}}(\omega) = \Sigma'_{\mathbf{k}}(\omega) + i\,\Sigma''_{\mathbf{k}}(\omega)$, one can write the spectral function as

$$A\,(\mathbf{k},\omega) = \frac{1}{\pi}\frac{\Sigma''_{\mathbf{k}}\,(\omega)}{[\omega - \varepsilon_{\mathbf{k}} - \Sigma'_{\mathbf{k}}\,(\omega)]^2 + \Sigma''_{\mathbf{k}}(\omega)^2}. \tag{1}$$

This is the central formula for the ARPES analysis. It provides the Lorentzian line shape for the momentum distribution curve (MDC) defined as $I(\mathbf{k},\omega = \text{const})$ [6] as long as the self-energy $\Sigma_{\mathbf{k}}(\omega)$ can be considered as momentum independent and the bare dispersion $\varepsilon_{\mathbf{k}}$ is linearized in the vicinity to the Fermi level. (A more general assumption [7] is that $\frac{\partial \Sigma'_{\mathbf{k}}(\omega)}{\partial k}$ can only be a constant independent of ω.)

This approach works well for metals where the Fermi-liquid picture is adequate and for many high-T_c cuprates [1,5,8]. Nevertheless, from a theoretical point of view, the standard perturbation approach seems to be inappropriate for strongly correlated electron systems such as underdoped and optimally doped hole cuprates where non-Fermi-liquid effects have been found in the pseudogap state. Various approaches towards clarifying the quasiparticle properties in the regime of strong electron correlations have been attempted: a phenomenological marginal Fermi-liquid approach [9], an asymptotic solution to the Gutzwiller projected ground state of the t-J model [10], and low-dimensional non-Fermi-liquid theory [11]. Recently the extremely correlated Fermi-liquid model has been suggested [12]. Its improved phenomenological version [13] successfully describes the dichotomy of the spectral functions of momentum and energy. One important result obtained in Ref. [13] is the MDC asymmetry that has been observed

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for under- and optimally doped $La_{2-x}Sr_xCuO_4$ (as discussed in Ref. [13] with a link to the data of Ref. [14]) and $Ca_{2-x}Na_xCuO_2Cl_2$ [15].

In this Rapid Communication we have demonstrated that the MDC asymmetry is not a particular model [12,13] property. It is a general property of the spectral function in strongly correlated electron systems, where the Coulomb interaction U is much larger than the quasiparticle kinetic energy and the perturbation over $\varepsilon_{\mathbf{k}}/U \ll 1$ seems to be more appropriate. We have also shown that the odd-in-energy term in the spectral function can be used to measure the strength of electron correlations in materials.

This Rapid Communication is organized as follows: The idea of a quasiparticle description of electrons in strongly correlated systems is described in Sec. II. Section III provides the equation for the exact single-electron Green's function, which is a linear combination of the Green's functions of these quasiparticles. The general structure of the corresponding spectral function is analyzed in Sec. IV. Section V is dedicated to a comparison between that approach and the phenomenological theory from Ref. [13]. Section VI presents the conclusion.

II. QUASIPARTICLE DESCRIPTION OF ELECTRONS IN STRONGLY CORRELATED SYSTEMS

When the Coulomb energy is much higher than the kinetic energy, the idea of a bare electron as a zero approximation of a theory does not work. On the contrary, the localized multielectron $d^n(f^n)$ configurations for a separate ion in the crystal field can be easily determined. The appropriate number of localized electrons is clear from local electroneutrality. There are many possible terms for the given configuration $d^n(f^n)$, so let us denote these terms as $E_q(n)$. One of them is the ground term $E_0(n)$ that is occupied at zero temperature. An excitation from the ground to any term with the energy $\Delta E_{q0} = E_q(n) - E_0(n)$ is the local Bose-type quasiparticle (exciton, magnon, etc.). If the external electron comes to the given ion, the latter changes its configuration to $d^{n+1}(f^{n+1})$ with its own energy spectra $E_p(n+1)$. The electron addition energy $\Omega_{pq} = E_p(n+1) - E_q(n)$ may be considered as the single particle excitation between two multielectron configurations, with the initial state $E_q(n)$ and the final state $E_p(n+1)$. Due to the large number of initial- and final-state terms, there are different quasiparticles with all possible pairs of (p,q).

Thus we arrive at the idea that an electron in a strongly correlated system is the linear combination of different quasiparticles. Of course, the contribution of a particular $|q,n\rangle \to |p,n+1\rangle$ excitation is determined by the matrix element $\langle p,n+1|c^{\dagger}|q,n\rangle$ of the electron creation operator $c^{\dagger}$. For example, it is not possible to change the spin $\Delta S > \frac{1}{2}$ with a single particle excitation. Also, it is evident that excitation from empty $|q,n\rangle$ to empty $|p,n\rangle$ has zero spectral weight while its energy Ω_{pq} is defined. Total or partial occupation of the participating multielectron terms results in a nonzero spectral weight of the quasiparticle.

This definition of the local quasiparticles results from the exact Lehmann representation for the single-electron Green's function [16]. It is a straightforward generalization of the original Hubbard idea of the perturbation theory from the atomic limit. In the Hubbard model there are two Fermi-type local quasiparticles corresponding to the low Hubbard band and upper Hubbard band. The interatomic hoppings of the electron result in a quasiparticle dispersion, and the local excitation energy Ω_{pq} transforms into the quasiparticle band $\Omega_{pq}(\mathbf{k})$.

III. EXACT SINGLE-ELECTRON GREEN'S FUNCTION IN THE GENERALIZED TIGHT-BINDING METHOD

The natural and proper mathematical tool in the atomic limit $\varepsilon_{\mathbf{k}}/U \ll 1$ is given by the Hubbard X operators [17]. Their algebra automatically fulfills the constraint condition that forbids some sectors of the Hilbert space due to strong electron correlations. Formerly, Hubbard's ideas about the X operators have been developed in a cluster perturbation theory within the generalized tight-binding (GTB) method [18,19]. This approach has been proposed to calculate the electronic structure of correlated materials such as underdoped cuprates, manganites, and cobaltites [20]. Its *ab initio* LDA+GTB version [21] is a hybrid scheme using the local density approximation to construct the Wannier functions and obtain the single-electron and Coulomb parameters of the multiband Hubbard-like Hamiltonian. At the next step this method combines the exact diagonalization of the intracell part of the Hamiltonian, the construction of the Hubbard operators on the basis of exact intracell multielectron eigenstates, and the perturbation treatment of the intercell hoppings and interactions.

This is essentially a multielectron approach which does not use the idea of a bare electron. An electron in a generalized tight-binding method is a linear combination of quasiparticle excitations between the multielectron initial d^n and final $d^{n\pm1}$ configurations. Each excitation from the initial state $|q\rangle$ to final state $|p\rangle$ is described by the Hubbard operator $X_f^{pq} = |p\rangle\langle q|$. Thereby, any local operator can be represented as a linear combination of X operators. So, the operator of removing of an electron with spin σ at a lattice site f takes the form

$$\begin{aligned} a_{f,\sigma} &= \sum_{p,q} |p\rangle \langle p|a_{f,\sigma}|q\rangle \langle q| \\ &= \sum_{p,q} \gamma_\sigma(p,q)\, X_f^{pq} = \sum_m \gamma_\sigma(m)\, X_f^m. \end{aligned} \tag{2}$$

To simplify the notations we introduce the quasiparticle band index m corresponding to the pair (p,q). Equation (2) clearly shows the difference between the description of Fermi-type quasiparticles in the single-electron language and the multielectron one. The operator $a_{f,\sigma}$ simultaneously decreases the number of electrons by one for all sectors of the Hilbert space, while the X_f^m operator describes the partial process of removing the electron from the (n)-electron configuration $|q\rangle$, with the final $(n-1)$-electron configuration $|p\rangle$. The matrix element $\gamma_\sigma(m)$ gives the probability of such a process. It should be noted that splitting of an electron onto different Hubbard fermions as stated by Eq. (2) and the following spectral weight redistribution over these quasiparticles are the underlying effects of the band structure formation in correlated systems.

According to Eq. (2), the single-electron retarded Green's function $G(\mathbf{k},\omega) = \langle\langle a_{\mathbf{k},\sigma} | a^{\dagger}_{\mathbf{k},\sigma}\rangle\rangle_{\omega}$ is given by a linear combination of the Green's functions of Hubbard quasiparticles $D^{mn}_{\mathbf{k},\omega} = \langle\langle X^{m}_{\mathbf{k}} | X^{n\dagger}_{\mathbf{k}}\rangle\rangle_{\omega}$,

$$G(\mathbf{k},\omega) = \sum_{m,n} \gamma_{\sigma}(m)\gamma^{*}_{\sigma}(n) D^{mn}_{\mathbf{k},\omega}, \tag{3}$$

and here the notation of Zubarev [22] for Green's functions is used. Due to complicated commutation rules there is no conventional Wicks theorem and conventional diagram technique for Hubbard operators. Nevertheless, the generalized Wicks theorem has been proved [23] and then the diagram technique for X operators was developed [24,25]. The Dyson equation [26] for the matrix Green's function $\hat{D}(\mathbf{k},\omega) = \{D^{mn}_{\mathbf{k},\omega}\}$ has also been modified,

$$\hat{D}(\mathbf{k},\omega) = \hat{\mathcal{G}}_{\mathbf{k}}(\omega)\hat{P}_{\mathbf{k}}(\omega), \tag{4a}$$

with propagator $\hat{\mathcal{G}}_{\mathbf{k}}(\omega)$ as

$$\hat{\mathcal{G}}_{\mathbf{k}}(\omega) = \left[\hat{\mathcal{G}}^{-1}_{0}(\omega) - \hat{P}_{\mathbf{k}}(\omega)\hat{t}_{\mathbf{k}} - \hat{\Sigma}_{\mathbf{k}}(\omega)\right]^{-1}. \tag{4b}$$

Here $\hat{\mathcal{G}}^{-1}_{0}(\omega)$ is a local propagator determined by the multielectron eigenstates $|p\rangle$ and $|q\rangle$, and $\hat{t}_{\mathbf{k}}$ is the interaction matrix with elements $t^{mn}_{\mathbf{k}} = \gamma_{\sigma}(m)\gamma^{*}_{\sigma}(n)\varepsilon_{\mathbf{k}}$, where $\varepsilon_{\mathbf{k}}$ is the bare band dispersion. It should be stressed that the function $\hat{\Sigma}_{\mathbf{k}}(\omega)$ in Eq. (4b) is the self-energy for the Hubbard fermions and therefore it is different from the single-electron one in Eq. (1).

Besides the self-energy $\hat{\Sigma}_{\mathbf{k}}(\omega)$ of Hubbard quasiparticles, the unusual strength operator $\hat{P}_{\mathbf{k}}(\omega)$ appears in Eq. (4). It results in both the redistribution of the quasiparticle spectral weight and in the renormalization of quasiparticle dispersion which becomes dependent on doping and temperature. Initially the strength operator has been introduced in the diagram technique for spin operators [27]. It is important that in order to use the generalized Dyson equation in the perturbation expansion, it is necessary to calculate both functions $\hat{\Sigma}_{\mathbf{k}}(\omega)$ and $\hat{P}_{\mathbf{k}}(\omega)$ in the same order of perturbation [28].

IV. SPECTRAL FUNCTION

The dimension of the $\hat{D}(\mathbf{k},\omega)$ matrix depends on the energy interval under consideration. For example, in cuprates only one kind of quasiparticle is involved in the low excitation energy limit of ARPES. To demonstrate that the general structure of the quasiparticle Green's functions in perturbation theory for strongly correlated electron systems results in an additional odd contribution to the spectral function $A(\mathbf{k},\omega)$, we proceed with the above case. This involves no loss of generality. For hole-doped cuprates the quasiparticle index m is given by the terms $(-\sigma,2)$, where the doublet $|\sigma\rangle$ and singlet $|2\rangle$ are the ground terms of the $\mathrm{CuO_4}$ unit cell with one and two holes per site, respectively. In this low-energy limit the exact single-electron Green's function reads

$$G(\mathbf{k},\omega) = |\gamma_{\bar{\sigma},2}|^{2}\frac{P_{\mathbf{k},\omega}}{\omega - \varepsilon - t_{\mathbf{k}}P_{\mathbf{k},\omega} - \Sigma_{\mathbf{k},\omega}}, \tag{5}$$

where $\varepsilon = \varepsilon_0 - \mu$ is the eigenvalue of the local state $|\sigma\rangle$ and μ is the chemical potential. Generally, both the self-energy and strength operator can be presented as a sum of real $P'_{\mathbf{k},\omega}, \Sigma'_{\mathbf{k},\omega}$ and imaginary $P''_{\mathbf{k},\omega}, \Sigma''_{\mathbf{k},\omega}$ parts, respectively. Therefore, the electron spectral function takes the form

$$A(\mathbf{k},\omega) = \frac{|\gamma_{\bar{\sigma}2}|^{2}}{\pi} \times \left(\frac{P'_{\mathbf{k},\omega}\Gamma_{\mathbf{k},\omega}}{(\omega - \epsilon_{\mathbf{k},\omega})^{2} + \Gamma^{2}_{\mathbf{k},\omega}} + \frac{P''_{\mathbf{k},\omega}(\omega - \epsilon_{\mathbf{k},\omega})}{(\omega - \epsilon_{\mathbf{k},\omega})^{2} + \Gamma^{2}_{\mathbf{k},\omega}}\right), \tag{6}$$

where $\epsilon_{\mathbf{k},\omega} = \varepsilon + t_{\mathbf{k}}P'_{\mathbf{k},\omega} + \Sigma'_{\mathbf{k},\omega}$ is the renormalized quasiparticle dispersion and $\Gamma_{\mathbf{k},\omega} = t_{\mathbf{k}}P''_{\mathbf{k},\omega} + \Sigma''_{\mathbf{k},\omega}$ is the inverse lifetime of the quasiparticles. It should be emphasized that Eqs. (4)–(6) are exact. Below we have used some general assumptions on the properties $P_{\mathbf{k},\omega}$ and $\Sigma_{\mathbf{k},\omega}$ in the vicinity of the Fermi level that are similar to the Fermi-liquid theory.

Since we are interested in analyzing the MDC line shape determined by Eq. (6), we fix the energy $\omega = \omega_0$ and assume a **k** independence of the quasiparticle inverse lifetime $\Gamma_{\mathbf{k},\omega}$ and strength operator $P_{\mathbf{k},\omega}$ in a small vicinity to the Fermi level. In such a case the spectral function $A(\mathbf{k},\omega_0)$ appears to be a sum of even $A^{\mathrm{even}}(\mathbf{k},\omega_{\mathbf{0}})$ and odd $A^{\mathrm{odd}}(\mathbf{k},\omega_{\mathbf{0}})$ contributions. In the limit $\Gamma_{\omega_0} \to 0$ the even part tends to a δ function with a renormalized spectral weight $|\gamma_{\bar{\sigma}2}|^{2}P'_{\omega_0}$. For the finite quasiparticle inverse lifetime Γ_{ω_0} and linearized quasiparticle dispersion $\epsilon^{\mathrm{lin}}_{\mathbf{k},\omega_{\mathbf{0}}}$ the even part has a Lorentzian line shape that is similar to the case of a noncorrelated Fermi liquid,

$$A^{\mathrm{even}}(\mathbf{k},\omega_{\mathbf{0}}) = \frac{|\gamma_{\bar{\sigma}2}|^{2}}{\pi}\frac{P'_{\omega_0}\Gamma_{\omega_0}}{\left(\omega_0 - \epsilon^{\mathrm{lin}}_{\mathbf{k},\omega_{\mathbf{0}}}\right)^{2} + \Gamma^{2}_{\omega_0}}. \tag{7}$$

Essentially the different feature of the spectral function in strongly correlated electron systems is the odd contribution that appears in Eq. (6) due to the imaginary part $P''_{\mathbf{k},\omega}$ of the strength operator,

$$A^{\mathrm{odd}}(\mathbf{k},\omega_{\mathbf{0}}) = \frac{|\gamma_{\bar{\sigma}2}|^{2}}{\pi}\frac{P''_{\omega_0}\left(\omega - \epsilon^{\mathrm{lin}}_{\mathbf{k},\omega_{\mathbf{0}}}\right)}{\left(\omega - \epsilon^{\mathrm{lin}}_{\mathbf{k},\omega_{\mathbf{0}}}\right)^{2} + \Gamma^{2}_{\omega_0}}. \tag{8}$$

The strength operator in Eq. (4) results from the non-Fermi commutation rules of the Hubbard X operators in the same way as in the spin Green's function it results from the non-Bose commutation rules of the spin operators [27]. In the limit of weak correlations the anticommutator (commutator) of the Fermi (Bose)-like operators of Hubbard's quasiparticles is equal to the c number. Formally in this limit the strength operator tends to unity $P_{\mathbf{k},\omega} \to 1$ and the odd contribution to the spectral function disappears. Thus the odd contribution to the spectral function close to the Fermi level is a measure of strong correlations.

To briefly discuss the problem in the superconducting state we write down the matrix Green's function $\hat{D}(\mathbf{k},\omega) = \langle\langle \Psi_{\mathbf{k}\sigma} | \Psi^{\dagger}_{\mathbf{k}\sigma}\rangle\rangle_{\omega}$ in terms of the Nambu operators $\Psi^{\dagger}_{\mathbf{k}\sigma} = (X^{\sigma 0}_{\mathbf{k}}, X^{0,-\sigma}_{-\mathbf{k}})$ and then denote the components of all relevant matrices via the corresponding superscript. According to Eq. (4a), the normal-state function $D^{(11)}_{\mathbf{k},\omega} = \langle\langle X^{0\sigma}_{\mathbf{k}} | X^{\sigma 0}_{\mathbf{k}}\rangle\rangle_{\omega}$ is given by the expression

$$D^{(11)}_{\mathbf{k},\omega} = \mathcal{G}^{(11)}_{\mathbf{k},\omega}P^{(11)}_{\mathbf{k},\omega} + \mathcal{G}^{(12)}_{\mathbf{k},\omega}P^{(21)}_{\mathbf{k},\omega}, \tag{9a}$$

TABLE I. The key features of the spectral functions in the different approaches of the ECFL model [12,13] and in the present work.

Model	Numerator of the spectral function	The model describes successfully/cannot describe
sECFL	$Q_n \Phi''_\omega - \frac{Q_n}{\gamma_{n0}}(\omega - \varepsilon_{\mathbf{k}})\Phi''_\omega$	EDCs/conventional and asymmetrical MDCs
MI pECFL	$Q_n \Phi''_\omega - \frac{Q_n}{\gamma_{n0}}\omega\Phi''_\omega$	EDCs and conventional MDCs/asymmetrical MDCs
MD pECFL	$Q_n \Phi''_\omega - \frac{Q_n}{\gamma_{n\mathbf{k}}}(\omega - \varepsilon_{\mathbf{k}})\Phi''_\omega$	EDCs, conventional and asymmetrical MDCs/–
Present work	$P'_{\mathbf{k},\omega}\Gamma_{\mathbf{k},\omega} + (\omega - \epsilon_{\mathbf{k},\omega})P''_{\mathbf{k},\omega}$	

where the propagator functions $\mathcal{G}^{(11)}_{\mathbf{k},\omega}$ and $\mathcal{G}^{(12)}_{\mathbf{k},\omega}$ are solutions of Eq. (4b),

$$\mathcal{G}^{(11)}_{\mathbf{k},\omega} = \frac{1}{\det \hat{\mathcal{G}}_{\mathbf{k},\omega}}\left(\omega + \varepsilon - t^{(22)}_{\mathbf{k}} P^{(22)}_{\mathbf{k},\omega} - \Sigma^{(22)}_{\mathbf{k},\omega}\right), \tag{9b}$$

$$\mathcal{G}^{(12)}_{\mathbf{k},\omega} = \frac{1}{\det \hat{\mathcal{G}}_{\mathbf{k},\omega}}\left(t^{(11)}_{\mathbf{k}} P^{(21)}_{\mathbf{k},\omega} + \Sigma^{(12)}_{\mathbf{k},\omega}\right), \tag{9c}$$

and the denominator reads

$$\begin{aligned}\det \hat{\mathcal{G}}_{\mathbf{k},\omega} = {} & \left(\omega + \varepsilon - t^{(22)}_{\mathbf{k}} P^{(22)}_{\mathbf{k},\omega} - \Sigma^{(22)}_{\mathbf{k},\omega}\right) \\ & \times \left(\omega - \varepsilon - t^{(11)}_{\mathbf{k}} P^{(11)}_{\mathbf{k},\omega} - \Sigma^{(11)}_{\mathbf{k},\omega}\right) \\ & + \left(\Sigma^{(12)}_{\mathbf{k},\omega} + t^{(22)}_{\mathbf{k}} P^{(12)}_{\mathbf{k},\omega}\right)\left(\Sigma^{(21)}_{\mathbf{k},\omega} + t^{(11)}_{\mathbf{k}} P^{(21)}_{\mathbf{k},\omega}\right).\end{aligned} \tag{9d}$$

In the superconducting state the off-diagonal components of the strength operator, just as the off-diagonal self-energy components, differ from zero [28,29]. That is why the normal-state function $D^{(11)}_{\mathbf{k},\omega}$ has such a complicated structure. We do not give the cumbersome expression for the spectral function $A^{(11)}(\mathbf{k},\omega) = (-1/\pi)\mathrm{Im}\ D^{(11)}_{\mathbf{k},\omega}$ in the superconducting state since a general analysis of its symmetry is beyond the scope of this Rapid Communication. Nevertheless, it is easy to show that in the nodal direction ($k_x = k_y$) the spectral function $A^{(11)}(\mathbf{k},\omega)$ of superconductors with a $d_{x^2-y^2}$-gap symmetry has the same structure as the function given by Eq. (6), to wit, the additional odd contribution to the ARPES line shape should be present.

V. DISCUSSIONS

The odd contribution to the spectral function demonstrated above results from the general structure [Eqs. (3) and (4)] of the Green's function of quasiparticles in strongly correlated systems. The particular form of Eq. (6) determining the line shape of ARPES data depends on the expressions for the self-energy $\hat{\Sigma}_{\mathbf{k}}(\omega)$ and the strength $\hat{P}_{\mathbf{k}}(\omega)$ operators. The way to obtain these expressions is given by a diagram technique [24–26] for Hubbard operators, and examples for different systems can be found elsewhere [28,29]. A discussion of the experimental data in the context of the present analysis is a subject for future research. Nevertheless, we believe that the general structure of the Green's function and of the spectral function of quasiparticles in correlated systems should be a reference point in experimental data analyses.

Below we compare the proposed approach and the theory that suitably describes the ARPES data of high-T_c compounds. As it has been shown recently, the phenomenologically improved [13] version of the extremely correlated Fermi-liquid (ECFL) model [12] successfully reproduces the normal-state data, both EDCs and MDCs, obtained in different experimental conditions and for different materials, with the same intrinsic parameters. In various modifications of the ECFL model the spectral function can be written as

$$A(\mathbf{k},\omega) = \mathcal{C}_n(\mathbf{k},\omega)\, A_{\mathrm{FL}}(\mathbf{k},\omega), \tag{10}$$

where $\mathcal{C}_n(\mathbf{k},\omega)$ is the "caparison factor" [12,13,30] playing the role of k- and ω-dependent adaptive spectral weights and $A_{\mathrm{FL}}(\mathbf{k},\omega)$ is the spectral function for the "auxiliary Fermi-liquid" Green's function $A_{\mathrm{FL}}(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}[\omega - \varepsilon_{\mathbf{k}} - \Phi_\omega]^{-1}$. Here the notations of the authors [13] have been kept so that Φ_ω is an ordinary Fermi-liquid self-energy and $\varepsilon_{\mathbf{k}}$ is the one-electron dispersion relation. According to Eq. (10) the spectral function has the form

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\frac{\mathcal{C}_n(\mathbf{k},\omega)\,\Phi''_\omega}{(\omega - \varepsilon_{\mathbf{k}} - \Phi'_\omega)^2 + \Phi''^2_\omega}. \tag{11}$$

There is an apparent difference between this expression and the general one (6) which consists of the definition of the self-energy operators Φ_ω and $\Sigma_{\mathbf{k},\omega}$. However, we have also found a significant correlation between the two approaches.

To demonstrate it, we list in Table I the ECFL spectral function numerator given by a product of the "caparison factor" $\mathcal{C}_n(\mathbf{k},\omega)$ and of the imaginary part Φ''_ω of the single-electron self-energy value in various approximations of Refs. [12,13]: (i) the not modified or so-called simplified ECFL (sECFL) model and phenomenologically improved (ii) momentum independent (MI p) or phenomenologically improved (iii) momentum dependent (MD p) ECFL models. The numerator of the general spectral function (6) is also presented in Table I. Each expression in this table consists of two contributions. In the modified ECFL models the first terms are even and correspond to the ordinary Fermi-liquid theory with a renormalized spectral weight. The coefficient Q_n reducing the spectral weight at high energies is given by the expression $(1 - \frac{n}{2})$, where n is the number of electrons (holes) per unit cell. The same expression has the real part of the strength operator $P'_{\mathbf{k},\omega}$ in the Hubbard-I approximation. In addition, the first terms are formally equivalent in all approaches if the general theory is taken in a small vicinity to the Fermi level when $\Gamma_{\mathbf{k},\omega} \to \Gamma_\omega$.

The second contribution to the spectral functions differs in the two theories even formally since the imaginary part of the different strength operator appears in our approach instead of the imaginary part of self-energy in the modified ECFL models. At the same time we should point out the fact of nonuniversal modification of the k dependence of the "caparison factor" within the ECFL models. Namely, in the expressions of Table I the "caparison factor" $\mathcal{C}_n(\mathbf{k},\omega)$ is the constant independent of k and ω for the sECFL and MI pECFL models and is the function of k in the MD pECFL model. Moreover, in the MI pECFL model there is no k dependence of the "caparison factor" at all. However, comparing the expression in our approach with the ones in the modified ECFL theory, we find that the structures of the spectral functions turn out to be similar in both theories under several conditions. In the sECFL model the structure of the spectral function is equivalent to the one in the general approach if (i) a small vicinity to the Fermi level is considered and (ii) corrections to the quasiparticle dispersion $\epsilon_{\mathbf{k},\omega}$ from the real part of the self-energy operator $\Sigma^{'}_{\mathbf{k},\omega}$ can be neglected. In such a case, the expression $[(\omega - \epsilon_{\mathbf{k},\omega})P''_{\mathbf{k},\omega}]$ tends to $[(\omega - \varepsilon_{\mathbf{k}})P''_{\omega}]$, where $\varepsilon_{\mathbf{k}} = \varepsilon + t_{\mathbf{k}} P'_{\mathbf{k}}$. Keeping the assumption regarding the quasiparticle spectra, we immediately find similarities between the spectral functions in our approach and in MD pECFL. The similarity in spectral functions in our and MI pECFL approaches can be found under different conditions, for example, if we assume that $(\varepsilon_{\mathbf{k}} + \Sigma'_{\mathbf{k},\omega})$ tends to zero and $P''_{\mathbf{k},\omega} \to P''_{\omega}$. The same conclusion may result from a more complicated structure of the imaginary part of the strength operator.

Therefore, we reveal strong correlations between the structures of the phenomenologically designed spectral function and the function (6) derived from the general consideration. We believe that all modifications of the ECFL model, each of which has its own strong features as indicated in Table I, can be combined into a more general one.

VI. CONCLUSION

We argue that the asymmetrical structure of the spectral function in strongly correlated electron systems has, among other things, the fundamental reason considered above and can reflect the strength of the correlations. The odd contribution to MDC may be found experimentally in the underdoped samples of cuprates that are close to the doped Mott-Hubbard insulator and in optimally doped ones where correlation effects are still strong enough. In overdoped cuprates as well as in Fe pnictides, the electron correlations are not so strong, hence an odd contribution is not expected.

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