Electron-phonon renormalization in small Fermi energy systems

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The puzzling features of recent photoemission data in cuprates have been the object of several analyses in order to identity the nature of the underlying electron-boson interaction. In this paper we point out that many basic assumptions of the conventional analysis are expected to fail in small Fermi energy systems, when, as in the cuprates, the Fermi energy E_F is comparable with the boson energy scale. We discuss in detail the features appearing in the self-energy of small Fermi energy systems and the possible implications for the angle-resolved photoemission spectroscopy data in cuprates.

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Renewed interest has recently arisen in the role of the electron-phonon (el-ph) coupling in cuprates. A powerful tool of investigation is represented by angle-resolved photoemission spectroscopy (ARPES), which, in two-dimensional systems like the copper oxides, is in principle able to extract the electronic self-energy directly from the momentum and energy distribution curves if the bare band structure is known.[1] The aim of this analysis is to determine the microscopic origin and properties of the electron scattering.[2–5] For example, in qualitative terms, the report of a remarkable kink in the electronic dispersion has been discussed as evidence of a retarded electron-boson interaction (most probably of phononic nature), where the energy at which the kink occurs sets the energy scale of the bosonic spectrum.[6] In the same framework, the ratio between the slope of the electronic dispersion at low energy (below the kink) and at high energy (above the kink) is expected to give a qualitative estimate of the strength of the electron-boson coupling.[2,4,6]

Some puzzling features cast doubt, however, on this conventional el-ph picture. On one hand, the low-energy electronic dispersion shows a quite weak dependence on the hole doping, in contrast with a significant dependence of the apparent el-ph coupling constant.[7] More interesting, the *high-energy* electronic dispersion turns out to be strongly dependent on the hole doping.[7] This is particularly astonishing because the high-energy part of the electronic dispersion is expected to represent the bare electronic structure and it should not be dependent on any electron-phonon properties.[8,9] In this situation, an attempt to fit this experimental scenario within a conventional el-ph framework by means of inversion techniques on the raw data would lead to unrealistic assumptions for the hypothetical underlying electron-boson spectrum.[10,11]

The reliability of the conventional analysis concerning the electron-phonon properties in cuprates has been questioned also on theoretical grounds. Due to the high degree of electronic correlation, the charge carriers in cuprates are characterized by a weakly dispersive effective band, with a Fermi energy $E_F \simeq 0.3-0.4$ eV.[12] Similar estimates of E_F are obtained by penetration depth measurements as reported in Uemura *et al.*'s plot.[13] This value should be compared with the highest phonon frequencies in cuprates, $\omega_{\mathrm{ph}}^{\mathrm{max}} \simeq 80-100$ meV, defining an adiabatic ratio $\omega_{\mathrm{ph}}^{\mathrm{max}}/E_F \sim 0.2-0.3$. In this situation, the adiabatic assumption ($\omega_{\mathrm{ph}} \ll E_F$), on which the conventional el-ph analysis relies, breaks down, and nonadiabatic interferences between the electronic and lattice degrees of freedom are expected to affect the normal and superconducting state phenomenology.[14] Among other features, the appearance of nonadiabatic effects has been shown to account in a natural way for the presence of a finite isotope effect on the effective electron mass and for the possibility of high-T_c superconductivity within an el-ph scenario.[15,16]

The aim of the present paper is to investigate in some detail how the presence of a small Fermi energy, of the same order as the phonon frequencies, affects the electron-phonon phenomenology. As a first step in this direction, we do not consider here the onset of nonadiabatic vertex diagrams which arise in the nonadiabatic regime,[14,15] but retain only the nonadiabatic effects related to the finite electronic bandwidth. Note, however, that, while vertex diagrams play a fundamental role in determining the effective enhancement of the superconducting pairing,[15] finite bandwidth effects alone have been shown to account in a qualitative way for the anomalous el-ph effects in different normal state properties (effective mass m^*, Pauli spin susceptibility, etc.).[16,17] We anticipate here, as our main results, that the conventional (adiabatic) el-ph analysis needs to be greatly revised in small Fermi energy systems. In particular, we show that the following fundamental el-ph properties[8,9] are *no longer valid* when $E_F \sim \omega_{\mathrm{ph}}$: (i) the el-ph self-energy $\Sigma(\omega)$ does not renormalize the electronic dispersion for ω much larger than the phonon energy scale ω_{ph}; (ii) impurity scattering affects only the imaginary part of the self-energy but not the real part, and hence not the electronic dispersion; and, (iii) different channels of electron scattering (phonons, impurities, etc.) just sum in the self-energy.

The working tools of our analysis will be the Marsiglio-Schossmann-Carbotte (MSC) equations[18] properly generalized to the case of finite bandwidth. The formal derivation of the MSC iterative procedure in the case of finite Fermi energy systems follows quite closely the steps outlined in Refs. 18 and 19. Here we report only the final equations. The pro-

cedure can be derived in full generality for any shape of the density of states (DOS) and any electron filling. For the sake of simplicity, and in order to disentangle finite bandwidth effects from the breaking of particle-hole symmetry, we consider a simple system at half filling with a constant DOS: $N(\epsilon)=N(0)$ for $|\epsilon|\leq E_F$, where the half bandwidth also represents the Fermi energy. We consider also impurity scattering in the weak coupling Born approximation. The MSC equations read thus:

$$\Sigma(i\omega_n)=-2iT\sum_m \lambda(i\omega_n-i\omega_m)\,\eta(\omega_m)-2i\gamma\eta(\omega_n), \tag{1}$$

$$\Sigma'(\omega)=2T\sum_m \lambda'(\omega,\omega_m)\,\eta(\omega_m)-\int_{-\infty}^{\infty}d\Omega\;\alpha^2F(\Omega) \times[N(\Omega)+f(\Omega-\omega)]\,\eta'(\omega-\Omega)-\gamma\eta'(\omega), \tag{2}$$

$$\Sigma''(\omega)=-\int_{-\infty}^{\infty}d\Omega\;\alpha^2F(\Omega)[N(\Omega)+f(\Omega-\omega)] \times\eta''(\omega-\Omega)-\gamma\eta''(\omega), \tag{3}$$

where $N(x)$ and $f(x)$ are, respectively, the Bose and Fermi distribution functions, $\alpha^2F(\Omega)$ is the el-ph Eliashberg function, and γ is the impurity scattering rate. Moreover, $\lambda(z)=\int_{-\infty}^{\infty}d\Omega\;\alpha^2F(\Omega)/[\Omega-z]$ (z a complex number), $\lambda'(\omega,\omega_m)=\mathrm{Im}\,\lambda(\omega-i\omega_m)$, and

$$\eta(\omega_m)=\arctan\left[\frac{F_F}{\omega_m Z(\omega_m)}\right],$$

$$\eta'(\omega)=\frac{1}{2}\ln\left[\frac{[E_F-\omega Z'(\omega)]^2+[\omega Z''(\omega)]^2}{[E_F+\omega Z'(\omega)]^2+[\omega Z''(\omega)]^2}\right],$$

$$\eta''(\omega)=\arctan\left[\frac{E_F-\omega Z'(\omega)}{\omega Z''(\omega)}\right]+\arctan\left[\frac{E_F+\omega Z'(\omega)}{\omega Z''(\omega)}\right],$$

where $Z(z)=1-\Sigma(z)/z$. As usual, the self-energy on the real axis is obtained by using the Matsubara solution [Eq. (1)] as input in Eqs. (2) and (3). Note that, in the normal state, this is necessary only as long as the Fermi energy E_F is finite. Note in addition that the self-consistency of Eqs. (2) and (3) is intrinsically related to the finiteness of E_F, so that the factors $\eta'(\omega)$ and $\eta''(\omega)$ are functions of the self-energy itself through the $Z(\omega)$ function.

In order to underline the small Fermi energy effects on the el-ph spectral properties, let us consider for the moment a simple Einstein phonon mode with phonon frequency ω_0 in the absence of impurities. In Fig. 1(a) we show the real and imaginary parts of the self-energy for an Einstein spectrum with $\lambda=\int_{-\infty}^{\infty}d\Omega\;\alpha^2F(\Omega)/\Omega=1$ and different Fermi energies. Throughout this paper we consider a temperature $T=0.02\omega_0$, which is much smaller than any other energy scale and can be considered as representative of the $T=0$ limit. Note that the highest temperatures employed in ARPES are $T^{\max}\sim 100\ \mathrm{K}\ll\omega_{\mathrm{ph}}\sim 700-800\ \mathrm{K}$, so that temperature smearing is negligible. The dashed lines represent the case of the conventional $E_F=\infty$ el-ph: the low-energy part of $\Sigma'(\omega)$ is just $\Sigma'(\omega)\sim\lambda\omega$, which gives the well-known renormalization of the electronic dispersion $E_{\mathbf{k}}=\epsilon_{\mathbf{k}}/(1+\lambda)$ close to the Fermi level.[8,9] Note that the real part of the self-energy is always negative, implying that the effective electronic band $E_{\mathbf{k}}$ is always less steep than the bare one $\epsilon_{\mathbf{k}}$: $E_{\mathbf{k}}\leq\epsilon_{\mathbf{k}}$ for any energy. Note also that the magnitude of $\Sigma''(\omega)$ is a monotonically increasing function with ω and saturates for $\omega\geq\omega_{\mathrm{ph}}^{\max}$.

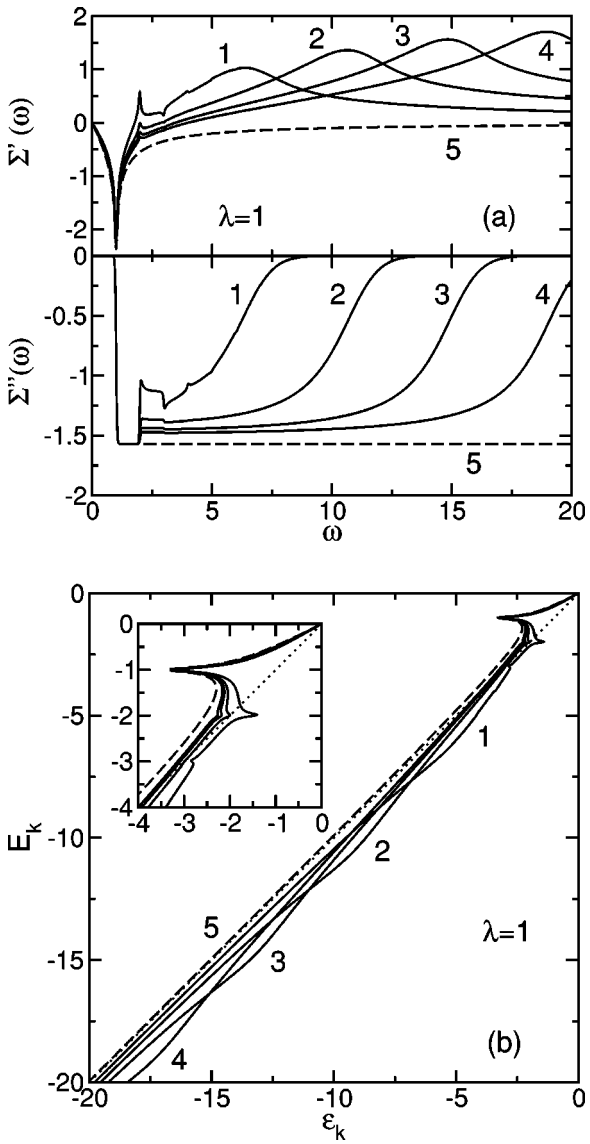

FIG. 1. (a) Real and imaginary parts of the self-energy for an Einstein phonon mode with $\lambda=1$ and different Fermi energies. Solid lines from 1 to 4: $E_F=4\omega_0, 8\omega_0, 12\omega_0, 16\omega_0$; dashed line 5: $E_F=\infty$. All quantities are in units of ω_0. (b) Corresponding renormalized electron dispersion $E_{\mathbf{k}}$ as function of the bare one $\epsilon_{\mathbf{k}}$ (dotted line). Inset: Enlargement of the low-energy part.

The presence of a Fermi energy of the same order of the phonon frequencies gives rise to a number of anomalous features. The most commonly known, although usually small, is the reduction of the low-energy el-ph renormaliza-

tion $E_{\mathbf{k}}=\epsilon_{\mathbf{k}}/(1+\lambda_{\text{eff}})$, where $\lambda_{\text{eff}}=-\lim_{\omega\to 0}\Sigma'(\omega)/\omega$ is already shown by a simple Matsubara analysis to be less than λ due to finite bandwidth effects, roughly $\lambda_{\text{eff}}=\lambda/(1+\omega_{\text{ph}}/E_F)$.[14] More interesting, we note two *qualitatively* different features that appear for $\omega_0/E_F\neq 0$. The first one is that $\Sigma''(\omega)$ is no longer a monotonic function of ω, but when ω becomes roughly $\omega\gtrsim E_F$ the imaginary part of the self-energy starts to decrease in modulus and it goes quite rapidly to zero. This is easily understandable in small Fermi energy systems if one considers that for $\omega\gg E_F$ there are no electronic states into which an electron with energy ω could decay within an energy window $\sim\omega_0$. On experimental grounds such a drop is expected to be hardly detectable since it falls out of the band. However, as we are going to see, its presence has important consequences on the real part, as one can see by using the Kramers-Kronig relations. Another interesting feature is indeed the large positive hump of the real part of the self-energy, which occurs in correspondence to the drop of the imaginary part, and scales with E_F. In particular, we note that, in contrast to the case $E_F=\infty$, for finite E_F the real part of the self-energy $\Sigma'(\omega)$ becomes positive in a large range of energy for $\omega\gtrsim 2\omega_0$. Similar results were found in Ref. 20. Our expression for the self-energy by using the MSC equations permits an understanding in simple terms of the physical origin of this effect, since the first term, written as a function of Matsubara frequencies, is always negative and is the only one surviving in the $E_F\to\infty$ limit, while the latter two terms, expressed as functions of real axis quantities, vanish for $E_F\to\infty$ and are always positive. Roughly speaking, we can relate the first term to the dynamical polarization of the *lattice* background, which leads to a net attraction between the electrons, while the latter two arise from the finite dynamics of the *electronic* background, which must be considered no longer instantaneous ($E_F=\infty$) but is now ruled by $E_F\neq\infty$. These terms survive even if the bosonic mediator does not have an intrinsic dynamics, as in the impurity scattering case depicted by the third term. The positiveness of $\Sigma'(\omega)$ has important consequences on the renormalized electronic dispersion obtained from $E_{\mathbf{k}}-\epsilon_{\mathbf{k}}-\Sigma'(E_{\mathbf{k}})=0$ which corresponds in ARPES measurements to the dispersion inferred by the momentum distribution curves. As shown in Fig. 1(b) the positive part of $\Sigma'(\omega)$ implies an ''antirenormalization'' of the electron band, namely, $E_{\mathbf{k}}>\epsilon_{\mathbf{k}}$. This feature extends up to an energy scale that does not depend on ω_0 but only on E_F, while its magnitude depends on el-ph parameters like λ or E_F itself. In such a situation the high-energy part $E_{\mathbf{k}}>\omega_{\text{ph}}$ of the experimental electronic dispersion[6,7] no longer represents the bare band $\epsilon_{\mathbf{k}}$ but is expected to show a *steeper* behavior than $\epsilon_{\mathbf{k}}$. As a last observation, note the kinks/jumps in the real and imaginary parts of the self-energy occurring at multiples of ω_0. These anomalies were already predicted in Ref. 9.

As we have just shown, in small Fermi energy systems particular care is needed in order to disentangle el-ph properties from a knowledge of the renormalized electronic dispersion such as one could get from ARPES. This issue is made more difficult by the fact that other actors can play an important role in the renormalization of the electron band. Most important is the presence of disorder and impurities. In conventional metals where E_F is much larger than any other energy scale, impurity scattering can be considered in good approximation as static: it provides a finite quasiparticle lifetime in the imaginary part of the self-energy, but it does not affect the real part of Σ, and consequently the electronic dispersion, which can be considered as determined by only the retarded (boson-mediated) scattering. As we are going to see, in small Fermi energy systems, the impurity self-energy acquires a finite real part which contributes to the renormalization of the electronic dispersion.

In Fig. 2(a) we plot the real and imaginary parts of the self-energy for an el-ph Einstein model with $E_F=4\omega_0$ and $\lambda=1$ in the presence of impurity scattering. In contrast with the $E_F=\infty$ case, we see that the impurity scattering has important effects on the real part of Σ. On one hand, it smooths the el-ph resonance at $\omega=\omega_0$ as well as the additional ones at $\omega=n\omega_0$. On the other hand, it significantly enhances the positive part of $\Sigma'(\omega)$ for $\omega\gg\omega_0$. The difficulty in extracting correctly information about the el-ph spectrum $\alpha^2F(\Omega)$ from the (ARPES-like) $E_{\mathbf{k}}$ vs $\epsilon_{\mathbf{k}}$ is thus even higher than in the absence of impurities, as we show in Fig. 2(b). In particular, one should take into account that neither the magnitude of the kink at $\omega=\omega_0$ nor its broadness are directly related anymore to properties of the el-ph spectrum $\alpha^2F(\Omega)$, like its total strength $\sim\lambda$ and its frequency shape. To be more specific, even the low- and high-energy parts of $E_{\mathbf{k}}$ are affected in a remarkable way by the impurity scattering. In the inset we plot the dependence of the ''effective'' $\lambda_{\text{eff}}=-\lim_{\omega\to 0}\Sigma'(\omega)/\omega$ as a function of the impurity scattering rate. We thus note that, if the slope of the low-energy part were used to extract the el-ph coupling, we would get a strong underestimation of λ. In addition, the discrepancy between $E_{\mathbf{k}}$ and the bare dispersion $\epsilon_{\mathbf{k}}$ at high energy is even larger in the presence of impurities, so that a steeper bare electron dispersion than the real one would be predicted if the high-energy part of $E_{\mathbf{k}}$ was used to estimate it. For instance, for $E_F=4\omega_0$, $\lambda=1$, $\gamma/\omega_0=1$ we would get $E_{\mathbf{k}}^{\text{high}}\sim 1.6\epsilon_{\mathbf{k}}$.

As a last point in this paper, we would like to stress the nonlinear and self-consistent nature of the normal-state MSC equations (2) and (3) in the presence of a finite Fermi energy. In fact, when $E_F\to\infty$, $\eta'(\omega)=0$, $\eta''(\omega)=\pi\,\text{sgn}(\omega)$, the right-hand side of Eqs. (2) and (3) no longer depend on the function $Z(\omega)$, and the different channels of interaction (el-ph, impurities, spin fluctuations etc.) just sum up linearly, so that $\Sigma(\omega)=\Sigma_{\text{el-ph}}(\omega)+\Sigma_{\text{imp}}(\omega)+\Sigma_{\text{spin}}(\omega)+\cdots$, where each term can be evaluated in the absence of the other interaction channels. Due to the self-consistent feedback of η' and η'', this is no longer true in small Fermi energy systems, and a simplistic analysis where the self-energy is fitted by the sum of independent different contributions is expected to fail. To illustrate this point explicitly, we show in Fig. 3 the total self-energy $\Sigma_{\text{el-ph+imp}}$ for an el-ph+impurities system with $\lambda=1$, $\gamma=\omega_0$, and $E_F=4\omega_0$, in comparison with the self-energy obtained as the sum of independent contributions $\Sigma_{\text{el-ph}}+\Sigma_{\text{imp}}\equiv\Sigma(\lambda=1,\gamma/\omega_0=0)+\Sigma(\lambda=0,\gamma/\omega_0=1)$. As we see, the discrepancies between the fully self-consistent

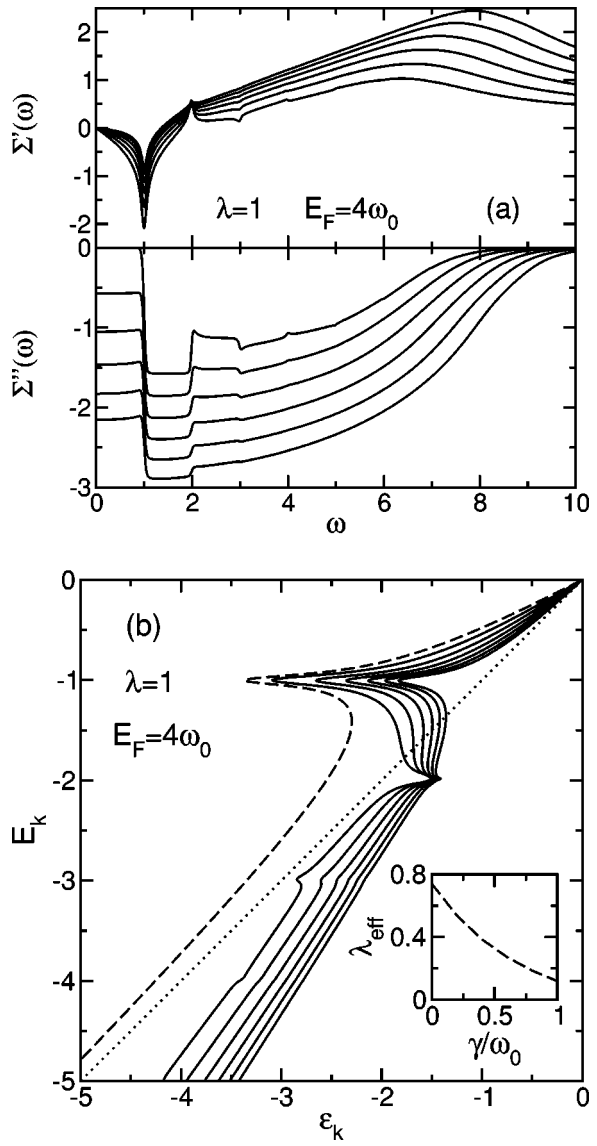

FIG. 2. (a) Real and imaginary parts of Σ for an Einstein phonon mode with $\lambda=1$ and $E_F=4\omega_0$ in the presence of impurity scattering. Solid lines correspond to (upper panel: from bottom to the top; lower panel: from top to the bottom) $\gamma/\omega_0=0,0.2,0.4,...,1.0$, where γ is the impurity scattering rate. Energy quantities are expressed in units of ω_0. (b) Renormalized electron dispersion corresponding (from left to the right) to (a). The dashed line represents the adiabatic limit. Inset: dependence of the effective parameter λ_{eff} on the impurity scattering rate.

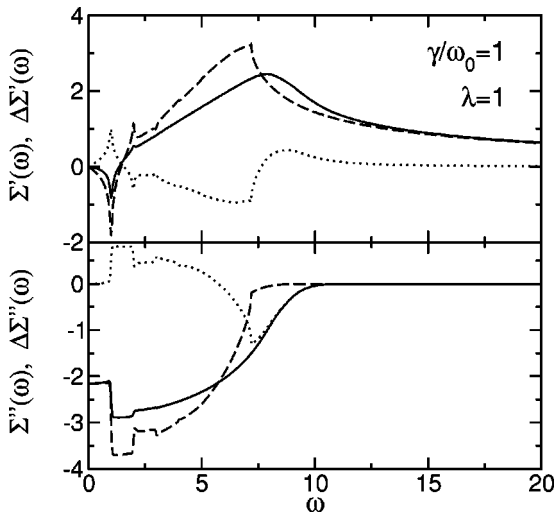

FIG. 3. Real and imaginary parts of the self-energy $\Sigma_{\text{el-ph+imp}}$ of an el-ph+impurities system with $\lambda=1$, $\gamma=\omega_0$, and $E_F=4\omega_0$ (solid line), as compared with the self-energy obtained by summing independent contributions $\Sigma_{\text{el-ph}}+\Sigma_{\text{imp}}$ (dashed line). The dotted line represents the difference $\Delta\Sigma=\Sigma_{\text{el-ph+imp}}-\Sigma_{\text{el-ph}}-\Sigma_{\text{imp}}$, which is related to the nonlinear feedback arising in small Fermi energy systems.

self-energy and its approximation as the sum of two independent contributions can be quite important in the whole range of energy ω. In particular, we note in the imaginary part that the jump at $\omega=\omega_0$ due to the onset of el-ph decay processes can be much smaller than is expected from a simple sum of independent el-ph and impurity contributions. This observation thus casts doubt on the possibility of estimating the el-ph coupling by the difference between $\Sigma_{\text{el-ph}}(\omega>\omega_{\text{ph}}^{\max})$ and $\Sigma_{\text{el-ph}}(\omega=0)$ if the other contributions could be disentangled, in contrast with the $E_F=\infty$ case, where this difference is simply related to $\lambda\langle\omega\rangle$. We also note, however, that, due to the vanishing of the el-ph processes, the limit $\omega\to 0$ of the self-energy is not affected by the interplay between the different channels of interaction but is mainly determined by only the impurity scattering. It can thus still be used in a safe way to estimate γ.

In conclusion, motivated by the puzzling features of recent ARPES measurements in cuprates, in this paper we have revised the el-ph properties in small Fermi energy systems with E_F of the same order as the phonon frequencies, and the interplay with other kinds of scattering, such as impuritylike scattering. We find that many basic assumptions which are valid in conventional metals where $E_F\gg\omega_{\text{ph}},\gamma$ need to be strongly reconsidered. In more detail, we have shown that at small Fermi energy the following effects occur.

(1) A positive part of the self-energy is predicted for $\omega\gtrsim\omega_{\text{ph}}$. This implies an ''antirenormalization'' of the electronic band for $\omega\gtrsim\omega_{\text{ph}}$. ARPES data are thus expected to measure in this regime an electronic dispersion steeper than the bare one.

(2) Impurity scattering can significantly affect the real part of the self-energy and hence the electronic dispersion. In particular, the effective renormalization of the low-energy part of the electronic dispersion is reduced by the impurity scattering which can also ''wash out'' the el-ph kink at $\omega\simeq\omega_{\text{ph}}$.

(3) Different scattering channels are not additive as in the case of conventional systems. Fitting data by using a sum of independent self-energy contribution is expected to fail.

Taking into account all these effects in a compelling way would make the analysis of ARPES data in cuprates more complex but also more interesting, and it could contribute to understand many puzzling features which are still open issues in these compounds. We would like to stress finally that the present analysis is not restricted to the el-ph case but

applies equally well for any retarded interaction independently of the specific origin of the bosonic mediator. We would also like to mention that the present analysis takes into account only the *dynamical* renormalization, while in real small Fermi energy systems the **k** dependence of the self-energy could also play a relevant role. These effects could be consistently included by means of fast-Fourier-transform techniques as in Ref. 21.

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