Poor screening and nonadiabatic superconductivity in correlated systems

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In this paper we investigate the role of the electronic correlation on the hole doping dependence of electron-phonon and superconducting properties of cuprates. We introduce a simple analytical expression for the one-particle Green’s function in the presence of electronic correlation and we evaluate the reduction of the screening properties as the electronic correlation increases by approaching half-filling. The poor screening properties play an important role within the context of the nonadiabatic theory of superconductivity. We show that a consistent inclusion of the reduced screening properties in the nonadiabatic theory can account in a natural way for the $T_c$-$\delta$ phase diagram of cuprates. Experimental evidences are also discussed.

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I. INTRODUCTION

The role of the electron-phonon (el-ph) interaction in the high-$T_c$ superconducting cuprates has been a matter of debate for a long time. In early times the report of a negligible isotope effect on $T_c$ at optimal doping, the almost linear behaviour of the resistivity on temperature, also at optimal doping, and other exotic features of the copper oxides led to the common belief that electron-phonon coupling was a marginal ingredient to understand the phenomenology of these materials. However, over the years, there has been a revamping of an important role of the phonons. The most remarkable ones are, for instance, the discovery of an isotope effect on $T_c$ larger than the BCS value ($\alpha T_c > 0.5$) in the underdoped regime\textsuperscript{12}, the report of a sizable isotope shift on the effective electronic mass $m^*\$ and on the onset of the pseudogap\textsuperscript{12} the observation of phonon renormalization\textsuperscript{12} and phonon anomalies at $T < T_c$.\textsuperscript{12}

More recently, ARPES measurements pointed out a kink in the electron dispersion the origin of which is probably phononic.\textsuperscript{12} Clearly, if phonons are relevant for superconductivity in these materials, this cannot be described in a BCS-like framework, but some non-conventional approach including strong electronic correlation is necessary. The study of the interplay between electron-phonon interaction and the electronic correlation is a challenging task which has attracted much scientific work along different lines.

An interesting issue concerns the momentum modulation of the electron-phonon coupling induced by the electronic correlation. In Ref.\textsuperscript{12} using a variety of theoretical and experimental findings, it is shown that in correlated systems small-$q$ scattering in the electron-phonon interaction is strongly favored. A strong enhancement of the forward scattering at $q \sim 0$ in correlated systems close to the metal-insulator transition, accompanied by a suppression of scattering at large $q$, was reported for example in Refs.\textsuperscript{13,14,15,16} by using $1/N$ expansion techniques.

A recent numerical work based on Quantum Monte Carlo technique confirms this picture.\textsuperscript{12}

Different but somehow complementary argumentations based on poor screening effects in correlated systems have been also discussed in literature. The basic idea is that, as a metal loses its coherence as function of the correlation degree approaching a metal-insulator transition, the screening properties of the bare long-range electron-phonon interaction become less effective resulting in a net predominance of small $q$ scattering.\textsuperscript{13,14,15,16} A similar physical argument applies, for example, to doped semiconductors which are commonly described in terms of the Fröhlich Hamiltonian, with electron-phonon matrix elements $|g_q|^2 \propto 1/|q|^2$.

The momentum structure of the electron-phonon scattering induced by the electronic correlation has been shown to play a crucial role in the context of nonadiabatic superconductivity.\textsuperscript{17,18,19} In narrow band systems, such as cuprates and fullerenes, the Fermi energy $E_F$ is so small to be comparable with the phonon frequencies $\omega_{ph}$, and the adiabatic assumption ($\omega_{ph} \ll E_F$) breaks down. In this context Migdal’s theorem\textsuperscript{12} does not apply and one needs to take into account nonadiabatic effects not included in the Migdal-Eliashberg (ME) theory of superconductivity. Detailed studies have shown that the nonadiabatic contributions, which are well represented by the vertex function, present a complex momentum-frequency structure, in which small $q$-scattering leads to an enhancement of the effective superconducting pairing, while large-$q$ scattering leads to a reduction of it.\textsuperscript{17,18,19} The strong $q$-modulation of the electron-phonon interaction due to the electronic correlation is thus expected to give rise to a net enhancement of the superconducting pairing.

The purpose of the present paper is twofold. On one hand we wish to quantify the microscopic dependence of the screening properties of a correlated system on relevant quantities as the electron density of the Hubbard repulsion; in addition we apply the derived screened
electron-phonon interaction to evaluate the role of the electronic correlation in the context of the nonadiabatic superconductivity and to derive a qualitative superconducting phase diagram. To this aim we introduce a model for the electronic Green’s function of the system, based on the decomposition of the total spectral function in a coherent, itinerant part, and an incoherent localized background corresponding to the Hubbard subbands. The relative balance between the two parts varies as a function of doping and electronic correlation. This will have important consequences on the electronic screening and hence on the $\mathbf{q}$-modulation of the effective electron-phonon scattering, as well as on the superconducting properties. We shall show that:

- the coherent excitations dominate the screening properties as well as the superconducting ones.
- the loss of coherent spectral weight approaching half-filling is thus responsible for the reduction of the screening properties and for the increase of the forward scattering in the electron-phonon interaction.
- in the strongly correlated regime the selection of forward scattering gives rise to an enhancement of the effective electron-phonon interaction within the context of the nonadiabatic superconductivity. These effects however compete with the reduction of the quasi-particle spectral weight which is detrimental for superconductivity.
- the resulting phase diagram shares many similarities with the one of the cuprates. In particular it shows an overdoped region, where superconductivity is suppressed by negative nonadiabatic effects, an underdoped region, in which superconductivity is destroyed by the loss of coherent spectral weight, and an intermediate region in which the predominance of small-$\mathbf{q}$ scattering leads to an enhancement of the nonadiabatic el-ph pairing which overcomes the reduction of the coherent spectral weight.

We hereby wish to point out that a complete description of the rich phenomenology of the cuprates is well beyond the aim of the present paper. In particular, we shall not discuss, for reason of simplicity, the symmetry of the gap, which of course is of fundamental importance if one wishes to give a quantitative description of these systems. We would like just to remark on this point that a $d$-wave symmetry of the superconducting order parameter was shown by many authors to naturally arise in the context of a phonon pairing with a significant predominance of forward scattering. The competition between $s-$ and $d-$wave symmetry in a nonadiabatic electron-phonon system was also studied in Ref. 25. Taking into account explicitly the $d$-wave symmetry of the gap would not change in a qualitative way the results of the present work.

This paper is organized as follows: in section II we introduce our model Green’s function; in section III we derive an effective form for the electron-phonon interaction. In the last section we write and solve the generalized Migdal-Eliashberg equations, in the adiabatic and nonadiabatic limit, and discuss in detail the competition of the different factors which determine the superconducting critical temperature of our system.

II. A MODEL FOR CORRELATED ELECTRON SYSTEMS

As briefly discussed in the introduction, one of the main aims of the present paper is to investigate how the screening properties are affected by the presence of strong electronic correlation, and to parametrize these effects in terms of microscopical quantities. In particular we have in mind a Hubbard-like system where itinerant electrons, with band dispersion $\epsilon_k$ and bandwidth $E$, interact each other through an onsite Coulomb repulsion $U$. As we are going to see, a crucial role is played in this context by the transfer of spectral weight as a function of the correlation degree from low energy coherent states to the high energy (Hubbard-like) incoherent ones.

In this section we present a simple, minimal model for the electron spectral function which takes into account these main effects and which can thus represent a proper starting point to evaluate screening effects in correlated systems.

All the possible information about the single-particle properties of the system is contained in the one-electron Green’s function $G(\mathbf{k}, \omega)$. Without loss of generality we assume that the Green’s function $G$ can be split in a coherent and an incoherent contribution:

$$G(\mathbf{k}, \omega) = G_{\text{coh}}(\mathbf{k}, \omega) + G_{\text{inc}}(\mathbf{k}, \omega),$$

(1)

where the coherent part $G_{\text{coh}}$ describes the itinerant, quasi-particle like properties of the electron wavefunction, while the incoherent part $G_{\text{inc}}$ accounts for the incoherent high energy excitations. Due to its localized nature $G_{\text{inc}}(\mathbf{k}, \omega)$ is only weakly dependent on the momentum quantum number, so that the dependence on $\mathbf{k}$ can be reasonably neglected.

An important quantity which parametrizes the relative balance between coherent and incoherent contributions is the quasi-particle spectral weight $Z$, which is simply given by:

$$\int d\omega \frac{1}{\pi} \text{Im} [G_{\text{coh}}(\mathbf{k}, \omega + i\delta)] = Z,$$

(2)

whereas the incoherent part obeys the sum rule:

$$\int d\omega \frac{1}{\pi} \text{Im} [G_{\text{inc}}(\mathbf{k}, \omega + i\delta)] = 1 - Z.$$

(3)

The quasi-particle spectral weight $Z$ can vary between 0 and 1, the two limits corresponding to the insulating
and metallic limit respectively. It depends on the internal parameters $U$ and $\delta$, where $\delta$ is the hole doping ($\delta = 1-n$) and $n$ the total number of electrons ($n = 1$ half-filled case).

Several techniques have been developed to investigate the Hubbard model. Different starting points are employed according to whether main emphasis has to be paid on the coherent (itinerant) or on the incoherent (localized) features. For instance the so-called Hubbard I approximation, which is exact in the atomic limit, is mainly aimed at a schematic representation of the localized states, described by an upper and a lower Hubbard band spaced by an energy gap of width $U$. On the other hand the Gutzwiller technique and the mean field slave bosons solution offer an useful tool to deal with the coherent spectral weight of the electron Green’s function: in this case the quasi-particle spectral properties in the presence of strong correlation are described in terms of an effective band of non-interacting fermions with spectral weight $Z$ and bandwidth $ZE$.

In this paper we introduce a new phenomenological model to take into account in the simplest way and at the same level the coherent and incoherent parts of the Green’s function. We approximate the exact (unknown) coherent and incoherent parts of $G(k,\omega)$ in Eq. (1) respectively with the Gutzwiller and Hubbard solutions, namely:

$$G_{\text{coh}}(k,\omega) = \frac{Z}{\omega - Z\epsilon_k + \mu \pm i0^+},$$

$$G_{\text{inc}}(\omega) = \frac{1-Z}{N_s} \sum_k \left[ \frac{(1-n/2)}{\omega - (1-n/2)\epsilon_k + \mu - U/2} + \frac{n/2}{\omega - (n/2)\epsilon_k + \mu + U/2} \right],$$

where $\mu$ is the chemical potential, $N_s$ is the total number of sites and $Z$ is the quasi-particle weight obtained in the Gutzwiller approximation in the paramagnetic state at finite $U$ and generic filling (Appendix A). Due to the localized nature of the incoherent part we have replaced the $G_{\text{inc}}(k,\omega)$ given by the Hubbard I approximation with its momentum average. Numerical calculations based on Dynamical Mean-Field Theory (DMFT) confirm our qualitative picture of a spectral weight transfer from a central coherent peak to an incoherent Hubbard-like background with increasing $U$.

The behaviour of $Z$ as function of the particles density $n$ and of the Hubbard energy $U$ is shown in Fig. 1. We show typical density of states $N(\omega)$ for the correlated system described by our model [Eqs. (4)-(5)].

We would like to stress that the phenomenological model described by Eqs. (4)-(5) is not meant at all to be exhaustive of the complex physics of a strongly correlated system. In fact, retardation effects are neglected, since we are assuming the separation into two species of electrons to be independent of frequency. More sophisticated methods of solution, including DMFT, permit to treat the self-energy of a strongly correlated system in a more careful way, retaining the correct frequency dependence of the self-energy.

Our model has the advantage of being extremely simple and easy to handle, and it allowed us to obtain explicit expressions for all the relevant quantities of the coupled electron-phonon system: in particular, we focus on the density of states $N(\omega)$ given by the Hubbard I approximation with its momentum average. Numerical calculations based on Dynamical Mean-Field Theory (DMFT) confirm our qualitative picture of a spectral weight transfer from a central coherent peak to an incoherent Hubbard-like background with increasing $U$.

FIG. 1: Quasi-particle spectral weight as determined by the Gutzwiller solution at finite $U$ and $n$. Left panel: $Z$ as function of $n$ for (from top to the bottom) $U/U_c = 0.4, 0.8, 1.2, 1.6, 2.0$. Right panel: $Z$ as function of $U/U_c$ for (from top to the bottom) $n = 0.6, 0.8, 0.9, 1.0$.

FIG. 2: Density of states $N(\omega) = (1/\pi) \sum \text{Im} G(k,\omega + i0^+)$ resulting from our model, for $U = 2U_c$ and different values of doping. At half-filling the system is an insulator, and its density of states is represented by two Hubbard-like features at distance $U$ from each other; moving away from half-filling a coherent peak starts forming, with increasing weight $Z$. Dashed regions represent filled states up to the chemical potential $\mu$ (dotted line).
on the spectral weight transfer from the coherent to the incoherent part of the Green’s function when increasing the degree of electronic correlation. As we are going to see, this feature will have important consequences on the electronic screening and on the momentum dependence of the electron-phonon coupling.

III. SCREENING AND ELECTRON-PHONON INTERACTION

A. Correlation effects on Thomas-Fermi screening

The momentum dependence of the electron-phonon interaction usually plays a marginal role in determining the electron-phonon properties of common metals. The basic reason for this is that the bare long-range electron-phonon interaction is effectively screened by the long-range Coulomb repulsion leading to a weak momentum dependence.

The conventional Migdal-Eliashberg theory, which describes electron-phonon effects both of the normal and superconducting states, is formally derived starting from an effective electron-phonon Hamiltonian, in which the Coulomb electron-electron repulsion does not appear, apart from a weak residual electron-electron contribution in the Cooper channel, $U_{\vec{k},\vec{q}}$, which gives rise to the Morel-Anderson “pseudopotential” term $\mu = N(0)U_{\vec{k}\vec{q}}$. The physical quantities appearing in this effective Hamiltonian are thus considered to have been already renormalized by the long-range Coulomb interaction. In particular the electron-phonon matrix elements $g_{\vec{k},\vec{k}+\vec{q}}$ and the residual electron-electron repulsion are usually considered to have a negligible momentum dependence, so that the Eliashberg equations depend only on the frequency variables.

This drastic assumption works quite well in many conventional low temperature superconductors with large carrier density since, in this case, the long-range $\vec{q}$-dependence of the bare electron-phonon and electron-electron interaction $[V(\vec{q},\omega) \propto 1/|\vec{q}|^2]$ is removed by the large metallic screening. This well-known effect is usually expressed in terms of the (static) dielectric function $\epsilon(\vec{q})$, which in the RPA approximation reads:

$$\epsilon(\vec{q}) = 1 + \frac{k_{TF}^2}{|\vec{q}|^2},$$

where $k_{TF}$ is the Thomas-Fermi screening momentum defined as

$$k_{TF}^2 = -\lim_{q \to 0} 4\pi e^2\Pi(\vec{q},\omega = 0),$$

and $\Pi(\vec{q},\omega)$:

$$\Pi(\vec{q},\omega) = \frac{2}{N_s} \sum_k \int d\omega' G(\vec{k} + \vec{q},\omega + \omega')G(\vec{k},\omega').$$

The effective long-range interaction results thus screened by conduction charge to give the Thomas-Fermi expression:

$$V_{\text{eff}}(\vec{q},\omega) = \frac{V(\vec{q},\omega)}{\epsilon(\vec{q})} \propto \frac{1}{|\vec{q}|^2 + k_{TF}^2}. \quad (9)$$

In free electron systems the Thomas-Fermi vector is directly related to the bare density of states via the simple relation $\lim_{q \to 0} \Pi(\vec{q},\omega = 0) = -2N(0)$, where $N(0)$ is the density of states per spin at the Fermi level, so that $k_{TF}^2 = 8\pi e^2 N(0)$. In common metals, since $k_{TF}$ is typically larger than the Brillouin zone size ($k_{BZ}$), the effective (electron-electron, electron-phonon) interaction $V_{\text{eff}}(\vec{q},\omega)$ can be considered in first approximation almost independent of the exchanged momentum $\vec{q}$.

Things are expected to be very different in correlated, narrow band systems. As we have mentioned before, strongly correlated electrons, due to their reduced mobility, are much less effective in screening external perturbations, especially at small wavelengths. For instance, the reduction of the screening properties approaching a metal-insulator transition in disorder alloys as well as in cuprates has been experimentally signaled in Refs. 40,41.

In this section we employ the simple model above introduced for the description of the Green’s function to quantify the reduced screening properties of correlated systems and their dependence on microscopic parameters, such as the hole doping $\delta$ or the Hubbard repulsion $U$. In order to do this, we compute the Thomas-Fermi vector $k_{TF}$, defined in Eq. (7), using the model described by Eqs. (1-3) to evaluate the RPA response function $\Pi(\vec{q},\omega)$ according to Eq. (3). While higher order (vertex) diagrams are not taken into account in this framework, we shall show that this simple model is already sufficient to describe the reduction of screening properties due to transfer of spectral weight from the coherent to incoherent states.

Using Eqs. (1-6) the response function $\Pi$ can be written as a sum of three different contributions:

$$\Pi = \Pi_{-\epsilon - \epsilon} + \Pi_{-\epsilon - \epsilon} + \Pi_{-\epsilon - \epsilon},$$

where the first one describes scattering processes which involve only coherent states; the second term describes scattering between the coherent peak and the Hubbard lower/upper (incoherent) bands; the last one describes processes which involve only localized incoherent states in both the Green’s functions of Eq. (3). In general we expect that the total screening will be dominated by the first contribution $\Pi_{-\epsilon - \epsilon}$ since the itinerant coherent states are much more effective, because of their mobility, in screening external perturbations than the localized ones.

In Fig. 3 we plot the RPA response function in units of the bare DOS: $-\lim_{\omega \to 0} \Pi(\vec{q},\omega = 0)/2N_0$, as function of the electron filling. Since for $n \to 0$ the screening properties are determined only by the coherent part regardless
Coulomb interaction renormalizes both the bare electron-phonon matrix element $g_{k}^{0}$ and the phonon frequencies $\Omega_{n}$. The el-ph matrix element can be usefully written as $g_{k}^{0} = c(\Omega_{n})/|q|$, where $c(\Omega_{n})$ is a well behaved function of $q$ in the limit $lim_{q \to 0}$ and it mainly depends on the phonon frequency $\Omega_{n}$. If both the screening effects on $g_{k}^{0}$ and $\Omega_{n}$ are properly taken into account one can get an expression for the effective total electron-phonon interaction:

$$V_{\text{eff}}^{\text{el-ph}}(q, \omega) = \frac{c^{2}(\omega_{q})}{|q|^{2}c(q)} D_{q}(\omega), \quad (11)$$

where both the phonon propagator $D_{q}(\omega)$ and the coupling function $c(\omega_{q})$ are written in terms of the screened phonon frequency $\omega_{q}$. Eq. (11) shows that the long-range behaviour of the total el-ph interaction $\propto 1/|q|^{2}$, when written as function of the screened phonon frequency, is correct by the dielectric function $c(q)$.

For an optical mode, $\omega_{q}$ is only weakly dependent on $q$ and the leading dependence on $q$ of Eq. (11) comes from the term $\propto 1/[c(q)|q|^{2}]$. These screening effects can be conveniently dealt with by introducing the screened el-ph matrix element $g_{q}$:

$$g_{q}^{2} = \frac{|g_{q}|^{2}}{c(q)} \propto \frac{1}{|q|^{2} + k_{TF}^{2}}. \quad (12)$$

The el-ph scattering is thus roughly described (we remind these expression were derived in the limit $q \to 0$) by a lorentzian function in the space $|q|$. It is also useful to introduce the dimensionless variables $Q = |q|/2k_{F}$ and $Q_{c} = k_{TF}/2k_{F}$, so that:

$$|g(Q)|^{2} \approx g^{2} \frac{1}{Q^{2} + Q_{c}^{2}}. \quad (13)$$

The parameter $Q_{c}$ represents a cut-off for the exchanged phonon momenta: the electron-phonon scattering will be operative for $Q \lesssim Q_{c}$, and negligible for $Q \gtrsim Q_{c}$.

The momentum structure resulting in Eq. (13) plays a crucial role in the Cooper pairing in the coherent-coherent channel where the momentum is a good quantum number. For these contributions the total strength of the electron-phonon coupling is linked with the momentum average of Eq. (11) over the Fermi surface. For an isotropic system, using polar coordinates $d\Omega = 2\pi d\phi \int_{0}^{1} d\cos \theta$ and reminding that $Q = \sin(\theta)/2$, we obtain:

$$\langle |g(Q)|^{2} \rangle_{FS} = \frac{\int d\phi \int_{0}^{Q} QdQ \frac{g^{2}}{Q^{2} + Q_{c}^{2}}}{\int d\phi \int_{0}^{Q} QdQ} = g^{2} \ln \left( \frac{1 + Q_{c}^{2}}{Q_{c}^{2}} \right). \quad (14)$$

In common metals $Q_{c} \sim 0.5 - 1$ so that $\ln \left( (1 + Q_{c}^{2})/Q_{c}^{2} \right)$ is of the order of 1. On the other hand, in poorly screened
systems \( Q_c \ll 1 \) and the resulting el-ph coupling is sensitively enhanced. In the following we shall consider \( Q_c \simeq 0.7 \) as representative case of uncorrelated usual metals.

For practical purposes, following Refs. [18-19] we approximate the lorentzian behaviour of Eq. (14) with a Heaviside \( \theta \) function:

\[
|g(Q)|^2 \rightarrow g^2 \alpha \theta(Q_c - Q). \tag{15}
\]

In order to preserve in this mapping the total strength of the el-ph coupling, the prefactor \( \alpha \) has to be determined by requiring the resulting el-ph coupling strength, namely the average of \( g^2 \) over the Fermi surface, to be equal for Eqs. (13) and (15). With this condition we find:

\[
|g(Q)|^2 = g^2 \frac{1}{Q_c^2} \ln \left( \frac{1 + Q_c^2}{Q_c^2} \right) \theta(Q_c - Q). \tag{16}
\]

As a final remark of this section we note that the momentum dependence of \( |g(Q)|^2 \) is not expected on the other hand to be effective in the incoherent-coherent and incoherent-incoherent contributions to the electron-phonon interaction, where the exchanged momentum \( q \) is no more a good quantum number. In this case the effective incoherent electron-phonon coupling is roughly given by its momentum average on the Brillouin zone, which we shall set in the following to be equal to \( g^2 \).

IV. GENERALIZED MIGDAL-ELIASBERG EQUATIONS

In the previous sections we have introduced a simple model for an electron-phonon system in the presence of electronic correlation. In particular we have reduced, in an approximate way, the complex problem of the interplay between electron-phonon and electron-electron interactions to a purely electron-phonon system described by an effective one-particle Green’s function [Eqs. (1), (4), (5)] and an effective electron-phonon matrix element \( g(Q) \) [Eq. (13)]. After this mapping, the Baym-Kadanoff theorem assures that the functional form of the superconducting equations will be the same of a purely electron-phonon system:

\[
\Phi = \Phi_{el-ph}[g, G, \Phi], \tag{17}
\]

\[
Z = Z_{el-ph}[g, G, \Phi], \tag{18}
\]

where \( \Phi \) is the superconducting order parameter; the Green’s function \( G \) and the matrix element \( g \) are defined by Eqs. (13), (4), (5), as mentioned above. In order to obtain an explicit expression for Eqs. (17)-(18) we should specify in which framework we are going to treat the electron phonon interaction. In particular, we observe that the conventional ME theory, in particular, is based on the assumption that the phonon frequencies are much smaller than the electronic Fermi energy, \( \omega_{ph} \ll E_F \) (adiabatic limit). This theory works quite well in the conventional low temperature superconductors, where no electronic correlation is present and \( E_F \) is of the order of 5 – 10 eV. On the other hand, the strong band renormalization in correlated systems described in Sec. III questions the adiabatic assumption, especially as, approaching half-filling, the renormalized bandwidth \( \sim ZE \) can be comparable with \( \omega_{ph} \). In these systems a more suitable description can be obtained in the framework of the non adiabatic theory of superconductivity [17]. Eqs. (17)-(18) can be rewritten as:

\[
Z_n = 1 + \frac{T_c}{\omega_n} \sum_m \Gamma_Z([G]; \omega_n, \omega_m) \eta_m [G], \tag{19}
\]

\[
\Phi_n = T_c \sum_m \Gamma_\Phi([G]; \omega_n, \omega_m) \frac{\Phi_m}{\omega_m \omega_m} \eta_m^A [G], \tag{20}
\]

where the electron-phonon kernels \( \Gamma_Z([G]; \omega_n, \omega_m) \) and \( \Gamma_\Phi([G]; \omega_n, \omega_m) \) contain the nonadiabatic vertex \( (P) \) and cross \( (C) \) contributions to the self-energy and to the Cooper pairing channels:

\[
\Gamma_Z([G]; \omega_n, \omega_m) = \lambda_{n-m} \left[ 1 + \lambda P([G]; \omega_n, \omega_m, Q_c) \right],
\]

\[
\Gamma_\Phi([G]; \omega_n, \omega_m) = \lambda_{n-m} \left[ 1 + 2 \lambda P([G]; \omega_n, \omega_m, Q_c) \right] + \lambda C([G]; \omega_n, \omega_m, Q_c) - \mu.
\]

Here \( \lambda_{n-m} \) is linked with the electron-phonon spectral function \( \alpha^2 F(\omega) \) through the relation \( \lambda_{n-m} = 2 \int d\omega \alpha^2 F(\omega) \omega/[\omega^2 + (\omega_n - \omega_m)^2] \), \( \lambda = \lambda_{n-m=0} \) and \( \mu \) is the short-range residual electron-electron repulsion. The breakdown of the adiabatic hypothesis determines the need for the explicit inclusion of the vertex \( (P) \) and cross \( (C) \) functions in Eqs. (19)-20 and it affects the expression of \( \eta_m [G] = \sum_k G(k, \omega) \) and \( \eta_m^A [G] = \sum_k G(k, \omega) G(-k, -\omega) \) through finite bandwidth effects. The momentum dependence of the superconducting equations has been averaged on the Fermi surface and it gives rise to the strong dependence on \( Q_c \) in the vertex and cross terms. In Eq. (19)-20 we have moreover implicitly expressed the functional dependence of the electron-phonon kernels \( \Gamma_Z, \Gamma_A \) as well as of the quantities \( P, C \) and \( \eta \) on the Green’s function \( G \) which we remind is modeled as in Eqs. (13), (4), (5).

Before solving Eqs. (19)-20 in the whole range of doping, we would like to discuss the different role of the coherent (itinerant) states and the incoherent (localized) states, described respectively by Eqs. (13), (5) on the superconducting properties. As we have seen in Sec. III the electronic screening is mainly dominated by the coherent term of the electronic Green’s function, which describes mobile electrons for which \( k \) is a good quantum number.

Similar considerations can be made also for superconductivity: we expect, in fact, that the coherent electrons, which have a high mobility, will give a more relevant contribution to the superconducting critical temperature. To check the validity of this hypothesis, we have solved Eqs. (19)-20 in the ME limit \( (i.e., \text{neglecting vertex corrections}) \), once using an integral kernel containing the
Incoherent couplings is negligible. The increase of sets of data are hardly distinguishable, pointing out that with the full kernel, and with solid line the critical temperature of Eq. (4), as a function of the Hubbard repulsion $U$. In Fig. (4), we show as empty circles the results obtained with only the coherent part (solid line).

After this observation, in the following the functional dependence on the total Green’s function $G$ in Eqs. (19)-(20) can be in good approximation replaced by the only coherent part, explicitly: $\Gamma = \Gamma(G_{\text{coh}})$, $\Phi = \Phi(G_{\text{coh}})$, $P = P(G_{\text{coh}})$, $C = C(G_{\text{coh}})$, $\eta_m = \eta_m(G_{\text{coh}})$. As we show in Appendix B when the reduced spectral weight and bandwidth are taken into account, this corresponds to a proper rescaling of the analytical expressions for these quantities evaluated in the absence of correlation in Refs. 30, 37.

It is interesting to compare our model with the two-band superconductivity, which has recently driven a considerable attention due to MgB$_2$. In that case, the opening of inter-band scattering channels leads to an enhancement of the critical temperature. For some respects, our model could also be seen as an effective two-band system, made up of a very narrow band of mobile electrons and another band of localized electrons, coupled to each other. However, we note that, since the spectral weight of each single band is not conserved, the onset of the high-energy bands of localized electrons is accompanied by a decrease of the quasi-particle spectral weight, resulting in an effective reduction of the Cooper pairing.

### A. Doping effects and phase diagram of the nonadiabatic superconductivity

Eqs. (19)-(20) represent our tool to investigate the loss of the superconducting properties due to the electronic correlation approaching half-filling. We can in fact evaluate all the relevant quantities, such as the electron-phonon interaction kernels $\Gamma_Z$, $\Gamma_\Delta$, the electron Green’s function $G$, the vertex and cross functions $P$, $C$, and the momentum cut-off $Q_c$ as a function of the microscopic parameters such as the hole doping $\delta$ and the Hubbard repulsion $U$. We shall show that the phase diagram as a function of the doping is governed by two competing effects: one driven by the reduction of the coherent spectral weight approaching half-filling, which is detrimental for superconductivity, and the other by the complex behaviour of the non-adiabatic terms, which increase the effective pairing as $\delta \rightarrow 0$ and decrease it as $\delta \rightarrow 1$.

Since we are mainly interested in the region $\delta \rightarrow 0$ of the phase diagram, we disregard for simplicity the analytical dependence of the non-adiabatic terms on the chemical potential. The behaviour of the “bare” $P$ and $C$ as a function of doping is in fact determined by the density of electrons ($n = 1 - \delta$); this dependence is much weaker than the dependence of $Z$ and $Q_c$ close to half-filling (see Figs. 3, 4).

Before solving Eqs. (19)-(20) numerically to obtain the critical temperature $T_c$ as a function of doping, we wish to discuss the phase diagram of our model in terms of simple intuitive physical arguments, based on an effective electron-phonon coupling. Let us consider for the moment the electron-phonon interaction alone, without any residual Coulomb repulsion, namely $\mu = 0$. Eq. (20) can be rewritten in a simplified way as:

$$\Phi_n \simeq T_c \sum_m Z\lambda [1 + 2Z\lambda P + Z\lambda C] K_{n-m} \Phi_m, \quad (21)$$

where we have simplified, according Appendix B, the main dependences on $Z = Z(U, \delta)$ of each quantity. In this way, we can roughly see the total electron-phonon coupling as the product of two terms: an effective electron-phonon coupling of ME theory renormalized by the electronic correlation, $\lambda_{\text{ME}}$, and the enhancement due to nonadiabatic vertex and cross (VC) diagrams $\gamma_{\text{VC}}$:

$$\lambda_{\text{eff}} = \lambda_{\text{ME}} \gamma_{\text{VC}},$$
$$\lambda_{\text{ME}} = Z\lambda,$$
$$\gamma_{\text{VC}} = 1 + 2Z\lambda P(Q_c) + Z\lambda C(Q_c).$$

The schematic behaviour of these quantities as a function of the hole doping $\delta$ is shown in the upper panel of Fig. 5. The physics behind the $\delta$-dependence of $\lambda_{\text{ME}}$ can be easily related to the loss of spectral weight approaching the metal-insulator transition for $\delta \rightarrow 0$. This effect, which is present also in $\gamma_{\text{VC}}$, is however in that case competing with the enhancement of the effective coupling due to $P(Q_c)$ and $C(Q_c)$ which will be maximum and positive close to half-filling (where $Q_c \rightarrow 0$) and negative at
high dopings. The interplay between these two effects will give rise to a maximum of $\gamma_{VC}$, and hence of $\lambda_{\text{eff}}$, somewhere in the small doping region where the competition between the spectral weight loss and the positive nonadiabatic effects is stronger (see upper and middle panels in Fig. 5).

We can now also consider the effect of the residual Morel-Anderson-like repulsion $\mu$: first of all, we observe that the reduction of spectral weight will lead to an effective repulsion $\mu_{\text{eff}} \approx Z\mu$. Superconductivity will be possible only when the net electron-phonon attraction overcomes the repulsion term: $\lambda_{\text{eff}} - \mu_{\text{eff}} > 0$ (see lower panel of Fig. 5). The resulting total coupling is expected to exhibit a “bell” shape which is mostly due to the $\delta$-dependence of the nonadiabatic factor $\gamma_{VC}$. It is interesting to note two things. First, in the extreme case $\lambda_{\text{ME}} < \mu_{\text{eff}}$, where no superconductivity would be predicted in the whole $\delta$ range by the conventional ME theory, we could expect finite $T_c$ in a small $\delta$ region, due to purely nonadiabatic effects $\lambda_{\text{eff}} = \lambda_{\text{ME}}\gamma_{VC} > \mu_{\text{eff}}$. Secondly, it is clear that within the ME framework a net attractive interaction in the Cooper channel at a certain doping $\delta$, which corresponds to $\lambda_{\text{ME}} > \mu_{\text{eff}}$, would imply a superconducting order also at larger $\delta$ since the two quantities $\lambda_{\text{ME}}, \mu_{\text{eff}}$ scale in the same way $\propto Z$; on the other hand, in the nonadiabatic theory superconductivity, $T_c$ is expected to be limited to some maximum value of doping, due to the negative contribution of the nonadiabatic diagrams $P$ and $C$ at large $\delta$ (large $Q_c$’s).

We can now quantify the simple arguments discussed so far. A quantitative estimate of the strength of the superconducting pairing is given by the highest eigenvalue $v_{\text{max}}$ of the superconducting integral kernel in Eq. (20), computed at low $T$; at a given temperature $T$ and doping $\delta$ superconductivity occurs if $v_{\text{max}} \geq 1$ and the superconducting pairing (and $T_c$) is stronger as $v_{\text{max}}$ is larger.

In Fig. 6, we compare the behaviour of $v_{\text{max}}$ as a function of $\delta$, obtained at $T = 0.01\omega_0$ using an Einstein spectrum for different values of $\mu$ in ME (open symbols, dashed lines) and in the nonadiabatic theory (full symbols, solid lines). The Hubbard repulsion was set at $U = 8U_c$ and the phonon frequency at $\omega_0 = 0.8E/2$, where $E/2$ is the bare half-bandwidth (unrenormalized by correlation effects). The corresponding phase diagram $T_c$ vs. $\delta$ is reported in Fig. 7. In agreement with our previous discussion in the ME framework $v_{\text{max}}$ and $T_c$ de-
crease monotonously as the hole doping is reduced. On the other hand, the corresponding results in the nonadiabatic theory display a more complex behaviour, showing that the effective nonadiabatic pairing is larger than the ME one at low doping and smaller at high doping.

As we have already discussed, the bell-shape of the highest eigenvalue \( v^{\text{max}} \) and of the critical temperature \( T_c \) can be attributed to the dependence of the magnitude and sign of the nonadiabatic terms on \( Q_c \), which, in turn, strongly depends on doping. For high doping the nonadiabatic contributions are negative and decrease \( v^{\text{max}} \) and \( T_c \) with respect to their ME values. Decreasing \( \delta \) the nonadiabatic terms turn from negative into positive and \( v^{\text{max}} \) and \( T_c \) increase up to a maximum value. As the hole doping is further decreased (\( \delta \to 0 \)), the loss of spectral weight becomes the dominant effect and it finally leads to the complete suppression of superconductivity. The inclusion of the residual Coulomb repulsion in the Cooper channel, \( \mu \), leads to an overall reduction of the superconducting pairing. The effect is more pronounced in the nonadiabatic theory than in ME, since in this case a very small value of \( \mu \) is enough to suppress superconductivity in a large region of phase space at high dopings.

**V. DISCUSSION AND CONCLUSIONS**

The main aim of the present paper is the description, on microscopical grounds, of the hole doping dependence of the electron-phonon and superconducting properties of a strongly correlated system within the context of a nonadiabatic electron-phonon theory. The need for a nonadiabatic treatment of the electron-phonon interaction in correlated systems comes from the fact that, as a metal-insulator transition is approached, the electronic bandwidth is strongly reduced, and the adiabatic assumption \( \omega_{\text{ph}}/E_F \) on which Migdal’s theorem is based breaks down.

Past studies have shown that the inclusion of nonadiabatic effects can lead to a strong enhancement or depression of \( T_c \) depending on the value of the exchanged momenta and frequencies: if a microscopic mechanism leads to a predominance of the forward scattering in the electron-phonon interaction, \( T_c \) is strongly enhanced. This effect was schematized in the past with the introduction of an effective cut-off in the electron-phonon interaction \( (Q_c) \), which was argued to be due to strong correlations effects.

In this work we have related the existence of \( Q_c \) with the reduction of the screening properties due to correlation of a metal approaching a metal-insulator transition. The same effects which are responsible for the reduction of the screening (namely the loss of k-space coherence) are however also strongly detrimental to superconductivity. In this work we have analyzed how the interplay between these effects is reflected on a \( T_c \) vs doping phase diagram.

We have introduced a simple analytical model to simulate the effects of the strong correlation on the one electron Green’s function. This model has also been employed to estimate the role of the electronic screening on the electron-phonon scattering in correlated systems. We have shown that the reduction of the metallic character due to the electronic correlation implies a reduction of the “effective” Thomas-Fermi screening approaching \( \delta = 0 \), where correlation is stronger. This results in a predominance of forward (small-q) scattering, which has been parametrized in terms of a phonon momentum cut-off \( Q_c = k_{\text{TF}}/2k_F \), where \( k_{\text{TF}} \) and \( k_F \) are respectively the Thomas-Fermi and the Fermi vectors.

We have also shown how the different parts of the electronic Green’s function contribute to the superconducting pairing; in particular, we have shown that the superconducting critical temperature is mainly determined by the coherent excitations. The similarities and differences between our model and the two-band superconductivity\(^{38,39}\) have also been discussed.

Solving the nonadiabatic generalized ME equations, we obtained a \( T_c \) vs. \( \delta \) diagram, which can be ideally divided into three regions:

(a) a high doping region, where superconductivity is suppressed by the negative contribution of the nonadiabatic channels to the electron-phonon pairing;

(b) an extremely low doping region, where the poor metallic character is reflected in a vanishing coherent spectral weight. In this region, superconductivity is extremely unstable and it can be overwhelmed by other electronic or structural instabilities induced by spin and charge degrees of freedom (antiferromagnetic fluctuations, stripes, charge-density-waves, pseudogaps, \ldots).
(c) an intermediate doping region, in which the loss of coherent spectral weight is not large enough to prevent superconductivity, which is in turn enhanced by the positive contribution of the nonadiabatic channels of interactions.

The resulting phase diagram bares strong resemblance with that of cuprates. We have in fact an overdoped region, where superconductivity is triggered on by the positive contribution of the nonadiabatic channels as doping is decreased; an optimal doping, where the enhancement due to the nonadiabatic interaction is counterbalanced by the reduction of the metallic character, and an underdoped region, where superconductivity disappears due to the incipient metal-insulator transition. In the qualitative scenario outlined here the origin of superconductivity in cuprates can be understood by focusing on the overdoped region, where the materials retain defined metallic properties; on the other hand, the exotic phenomenology of the underdoped region is only marginal. The occurrence of different kinds of electronic/structural instabilities, not discussed in the present paper, is thus thought to be a by-product of the loss of metallic character which also drives the suppression of $T_c$ as $\delta \to 0$ more than to be the secret of the superconducting pairing.

Once more, we wish to stress that what we present in this paper is a general scenario, based on the microscopic description of the interplay between nonadiabatic effects and strong electronic correlation. A quantitative understanding of the specific phase diagram of cuprates should of course take into account specific features of these materials, such as Van Hove singularities and the $d$-wave symmetry of the gap. The possibility of a $d$-wave pairing within the context of electron-phonon superconductivity has been discussed elsewhere, we remind here that $d$-wave symmetry was shown to be favoured by forward scattering, which in our model is enhanced as $\delta \to 0$.

The qualitative behaviour of our results would be however left unchanged by the inclusion of these effects.

On the experimental ground we observe that the present scenario is supported by a detailed analysis of $T_c$ vs. normal state properties in different families of cuprates. In Ref. [41] for example, the complex behaviour of $T_c$ approaching the metal-insulator transition either by reducing the doping or by increasing the disorder was nicely pointed out by Ososky et al. The relation between $T_c$ and reduced screening properties was also discussed there. Although we do not attempt to discuss the scaling relations close to the metal-insulator transition in region (b), where a more specific treatment of the electronic correlation is needed, we think our analysis is somehow complementary to that of Ref. [41]. This scenario can also open new perspectives on the remarkable increase of $T_c$ in granular metals and alloys.

Furthermore, a strong doping dependence of the electron-phonon properties in cuprates has also been reported by inelastic X-ray measurements of the phonon dispersion. Experimental data in NCCO compounds were shown to be compatible with the theoretical calculations, based on the shell model, assuming a negligible Thomas-Fermi vector ($Q_c = 0$) for the strongest correlated undoped compound ($\delta = 0$), whereas a Thomas-Fermi momentum $k_{TF} \approx 0.39 \AA^{-1}$, comparable to that for LSCO, was estimated for $\delta \simeq 0.14$. The corresponding dimensionless cut-off $Q_c$ would be hence estimated $Q_c \approx 0.26$ by using an in-plane Fermi vector $k_F^0 \approx 0.74 \AA^{-1}$.

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APPENDIX A: GUTZWILLER SOLUTION FOR GENERIC $U$ AND $n$

In this appendix we provide a brief overview about the analytical solution of the Gutzwiller approximation for generic filling and Hubbard repulsion.

Let us write the Hubbard Hamiltonian within the Gutzwiller approximation (in the paramagnetic state) as:

$$H = -\gamma(U, n, d)|\bar{\epsilon}| + Ud, \quad (A1)$$

where $n$ is the total electron filling, $d$ the density of double occupancy sites, $\bar{\epsilon}$ the kinetic energy for site, and

$$\gamma(U, n, d) = \frac{2(n - 2d)}{n(2 - n)} \left(\sqrt{1 - n + d} + \sqrt{d}\right)^2. \quad (A2)$$

Minimizing Eq. (A1) with respect to $d$ yields:

$$0 = \left[\sqrt{1 - n + d} + \sqrt{d}\right]^2 - \left(\frac{n}{2} - d\right) \frac{\left(\sqrt{1 - n + d} + \sqrt{d}\right)^2}{\sqrt{d(1 - n + d)}} + 2\left(\frac{U}{U_c}\right) n(2 - n), \quad (A3)$$

where we have introduced as usual $U_c = 8|\bar{\epsilon}|$.

After expanding the squares $\left[\sqrt{\ldots} + \sqrt{\ldots}\right]^2$ one can now isolate on the right side the remaining square roots:

$$2n(2 - n) \left(\frac{U}{U_c}\right) + (1 - 2n + 4d) = \left(\frac{n}{2} - d\right) \frac{\left(1 - n + 2d\right)}{\sqrt{d(1 - n + d)}} - 2\sqrt{d(1 - n + d)} \quad (A4)$$

and, by squaring both the sides of Eq. (A4), all the remaining square roots are removed and we are left with a third order polynomial expression for $d$. We obtain namely:

$$A_3 d^3 + A_2 d^2 + A_1 d + A_0 = 0, \quad (A5)$$
where
\[ A_3 = 16n(2 - n)\left(\frac{U}{U_c}\right), \]  
\[ A_2 = 4n(2 - n)\left(\frac{U}{U_c}\right)\left[n(2 - n)\left(\frac{U}{U_c}\right) - 6n + 5\right], \]  
\[ A_1 = (1 - n)\left[4n^2(2 - n)^2\left(\frac{U}{U_c}\right)^2 + 4n(2 - n)(1 - 2n)\left(\frac{U}{U_c}\right) - n\right], \]  
\[ A_0 = -\frac{n^2(1 - n)^2}{4}. \]

Eq. (A6) can be easily solved to obtain \( d_{\text{min}} \), and, in the standard notations, the Gutzwiller factor \( Z(U, n) = \gamma(U, n, d_{\text{min}}) \).

**APPENDIX B: ANALYTICAL EXPRESSION OF DIFFERENT PHYSICAL QUANTITIES**

1. **Thomas-Fermi Screening**

In this section we provide some useful analytical expressions for the different contributions (\( \Pi_{-c}, \Pi_{-1}, \Pi_{i-1} \)) to the response function \( \Pi \) involved in the evaluation of the Thomas-Fermi screening as limit \( k_F^2 \propto \lim_{q \to 0} \Pi(q, \omega = 0) \).

In the RPA approximation \( \Pi(q, \omega) \) is given by:

\[ \Pi(q, \omega) = \sum_{k} \int d\omega' G(k + q, \omega + \omega') G(k, \omega'). \]  

We employ the simple model of Eqs. (1), (3), (5) for the electron Green’s function in the presence of correlation. From simple scaling relation it is straightforward to recognize that

\[ \Pi_{-c} = Z\Pi(Z = 0) = -ZN_0. \]  

The analytical expressions for \( \Pi_{-1}, \Pi_{i-1} \) are straightforward but more cumbersome since they involved the explicit integration over the upper/lower Hubbard bands. One obtains:

\[ \Pi_{-c} = -2N(0)^2(1 - Z)\left[(ZE/2 + U/2 + (1 - n)E/2) \times \right. \]
\[ \left. \times \ln \left(ZE/2 + U/2 + (1 - n)E/2\right) + \left(ZE/2 + U/2 - (1 - n)E/2\right) \times \right. \]
\[ \left. \times \ln \left(ZE/2 + U/2 - (1 - n)E/2\right) + \left(U/2 + \mu - (1 - n)E/2\right) \times \right. \]
\[ \left. \times \ln \left(U/2 + \mu + (1 - n)E/2\right) \right], \]  
\[ \Pi_{-1} = \frac{-n^2(1 - n)^2}{4}. \]  
\[ (A9) \]

The incoherent-incoherent contribution gives:

\[ \Pi_{i-1} = -2N\left(1 - Z\right)^2 \left[(U + E/2) \ln(U + E/2) + (U - E/2) \ln(U - E/2) + (U + (n - 1)E/2) \ln(U + (n - 1)E/2) + (U + (1 - n)E/2) \ln(U + (1 - n)E/2) \right] \]

2. **Superconducting properties**

Here we report the explicit expressions for the coherent contribution to different quantities in Eqs. (13, 14).

Let us consider for instance \( \eta_m[G_{\text{coh}}] \). In this case

\[ \eta_m[G_{\text{coh}}] = \eta_m^A[G_{\text{coh}}] \]  

and:

\[ \eta_m[G_{\text{coh}}] = \int \frac{d\varepsilon}{2\omega_m} \left[ \frac{Z}{\omega_m \left[\arctan \left(\frac{ZE - \mu}{2\omega_m}\right) + \arctan \left(\frac{ZE + \mu}{2\omega_m}\right)\right]} \right]. \]  

The expression (12) corresponds just to the \( \eta_m(E) \) for an uncorrelated system with reduced spectral weight \( Z \) and rescaled bandwidth \( ZE \): \( \eta_m[G_{\text{coh}}](E) = Z \eta_m(ZE) \).

Similar considerations apply for the vertex and cross function:

\[ P^{G_{\text{coh}}}(E, Q_c; n, m) = ZP(ZE, Q_c; n, m), \]
\[ C^{G_{\text{coh}}}(E, Q_c; n, m) = ZC(ZE, Q_c; n, m), \]

where \( P(E, Q_c; n, m) \) and \( P(E, Q_c; n, m) \) in the absence of electronic correlation were computed in Refs. [17, 18, 30].

\[ P(E, Q_c; n, m) = T \sum_{l} D(\omega_n - \omega_l) \left\{ B(n, m, l) + \frac{A(n, m, l) - B(n, m, l)\omega_l - \omega_{l-n+m})^2}{EQ^2} \times \right. \]
\[ \left. \times \left[ \frac{1}{2} \ln \left(\frac{2EQ^2}{\omega_l - \omega_{l-n+m}}\right)^2 \right] \right\}, \]
\[ (B5) \]
\[ C(E, Q_c; n, m) = D(\omega_n - \omega_l)D(\omega_l - \omega_m) \times \]
\[
\times \left\{ 2B(n, -m, l) + \arctan \left( \frac{2E Q_c^2}{|\omega_l - \omega_{l-n+m}|} \right) \times \frac{A(n, -m, l) - B(n, -m, l)(\omega_l - \omega_{l-n+m})}{E Q_c^2 |\omega_l - \omega_{l-n+m}|} \right\} \right\} \tag{B6}
\]

where

\[
A(n, m, l) = (\omega_l - \omega_{l-n+m}) \left[ \arctan \left( \frac{E}{2\omega_l} \right) + \arctan \left( \frac{E}{2\omega_{l-n+m}} \right) \right]. \tag{B7}
\]

\[
B(n, m, l) = (\omega_l - \omega_{l-n+m}) \frac{E \omega_{l-n+m}}{2 \left[ (E/2)^2 + \omega_{l-n+m}^2 \right]^2} + \frac{E}{2 \left[ (E/2)^2 + \omega_{l-n+m}^2 \right]^2}. \tag{B8}
\]