Renormalization Group Study of the Electron-phonon Interaction in High $T_c$ Cuprates

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We generalize the numerical renormalization group scheme of Ref. [1–3] to study the phonon-mediated retarded interactions in the high $T_c$ cuprates. We find that three sets of phonon-mediated retarded quasiparticle scatterings grow under RG flow. These scatterings share the following common features: 1) the initial and final quasiparticle momenta are in the antinodal regions, and 2) the scattering amplitudes have a $x^2−y^2$ symmetry. All three sets of retarded interaction are driven to strong coupling by the magnetic fluctuations around $(\pi, \pi)$. After growing strong, these retarded interaction will trigger density wave orders with d-wave symmetry. However, due to the d-wave form factor they will leave the nodal quasiparticle unaffected. We conclude that the main effect of electron-phonon coupling in the cuprates is to promote these density wave orders.

One of the most prominent puzzles to emerge from experimental studies of the high-temperature superconducting cuprate materials is the strong momentum-space dependence of the properties of the electronic excitations. This can be seen most clearly in angle-resolved photoemission spectroscopy (ARPES) of LSCO: at optimum doping, sharp quasiparticle peaks can be distinguished near the Fermi surface in both nodal and antinodal directions. However, when the system is underdoped, the antinodal quasiparticle peaks disappear, while the nodal quasiparticle peaks remain[4]. Another beautiful demonstration of the robustness of the nodal quasiparticles is obtained in the NaCCOC materials. Recent STM studies have shown the presence of a commensurate, 4 lattice constant, checkerboard order which is independent of doping[5] (indicating the importance of lattice pinning). Despite this, ARPES studies of the same system reveal nodal quasiparticle peaks[6]. Finally, ARPES experiments probing the isotope effect in optimally doped Bi2212 reveal a substantial isotope shift in the ARPES spectra near the antinode, but little shift in the nodal spectrum[7].

The broad picture emerging from these experiments is of nodal quasiparticles which are insensitive to doping, disorder, charge and spin order, and lattice vibration, while antinodal excitations are sensitive to all these perturbations. One of us (DHL) has dubbed this the “nodal-antinodal dichotomy”[4].

In the cuprates it is widely accepted that in the overdoped regime, quasiparticles are well-defined excitations all along the normal state Fermi surface. We view the effect of decreasing doping as changing the Fermi surface geometry and increasing the strength of the residual quasiparticle interaction. We model this residual interaction with a momentum independent quasiparticle scattering. It is important not to confuse this effective residual quasiparticle scattering with the bare local electron correlation. Previously Honerkamp et al have performed a one-loop renormalization group (RG) study of this residual interaction[1]. Here we generalize their method to study the phonon-mediated retarded interaction. The RG treatment of the retarded interaction is similar to that used for one dimensional systems in Ref.[8–10]. Our motivation for studying the electron-phonon interaction in the cuprates are twofold: 1) we hope to better understand the electron-phonon interaction in doped Mott insulators, and 2) we hope to gain some insight about the origin of the nodal-antinodal dichotomy.

In a recent paper Devereaux et al pointed out the importance of the momentum dependence in the electron-phonon coupling constant when interpreting ARPES data[11]. In particular they showed that as the initial electron momentum is varied along the Fermi surface, the matrix element that couples the electron to the Bi$_2$Y phonon exhibits a $x^2−y^2$ symmetry. Meanwhile studies including weak to intermediate Hubbard interaction ($U < 6t$) have come to the conclusion that the $s$-symmetry electron-phonon coupling is suppressed by electron-electron repulsion[12–15], especially for large momentum transfer processes[13–15].

In this study we follow the RG flow of both the instantaneous and retarded electron-electron scattering amplitude in the full first Brillouin zone. We compare the flow of retarded interaction with different symmetry. We start with a tight binding dispersion given by

$$\epsilon(k) = -2t(x_2 + y_2) + 4t'\cos(k_x)\cos(k_y) + 4t''\cos^2(k_x) + \cos^2(k_y) - 1,$$

with $t' = 0.3t$, $t'' = -0.1t$, and $\mu = -0.7t$. This set of parameter choice produces a rather realistic Fermi surface. Following Ref.[1] we choose the bare residual quasiparticle scattering amplitude $U = 3t$. As in Ref.[1] we perform a one-loop Wilsonian RG for the one-particle-irreducible four-point vertex functions. At each energy scale the renormalized four-point function serves as an effective interaction for particles with excitation energies $|\epsilon(k)|$ below the cutoff scale $\Lambda$. The results we
report are obtained for a temperature $k_B T = 0.04 t$, and
the RG flow is integrated between initial cutoff $\Lambda = 4 t$
and final cutoff $0.2 t$. With spin-rotational invariance, the
cutoff-dependent effective interaction is given by

$$S_{\text{int}} = \sum_{\sigma, \sigma'} \int d^3k_i d^3\omega_i V_A(k_1, k_2, k_3) \psi_{\sigma'}(k_4, \omega_i) \psi_{\sigma}(k_1, \omega_i).$$

In the above $\psi_{\sigma}(\omega_i, k_i)$ annihilates an electron with quan-
tum numbers $\omega_i, k_i, \sigma$; furthermore $\omega_4 = \omega_1 + \omega_2 - \omega_3$
and $k_4 = k_1 + k_2 - k_3$. The contribution to the RG
flow $\partial \Lambda V_A$ is summarized by the Feynman diagrams in
Fig. (1), where the label “I” or “R” denotes instan-
taneous or retarded interaction respectively. For the mo-
moment we discuss the instantaneous interaction, hence all
interactions are the “I” type. In each diagram, there are
two internal lines. One represents the Greens function

$$G_A(k, \omega) = \frac{\chi_A(k)}{i\omega - \epsilon(k) - \chi_A(k) \Sigma(k, i\omega)},$$

while the other represents

$$S_A(k, \omega) = \frac{\chi_A'(k)[i\omega - \epsilon(k)]}{[i\omega - \epsilon(k) - \chi_A(k) \Sigma(k, i\omega)]^2}.$$  

Here $\chi_A(k) = 1 - 1/\{\exp[(\epsilon(k) - \Delta)/0.05\Delta] + 1\}$
cuts off contributions from $|\epsilon(k)| > \Lambda$, and $\chi_A'(k) = \delta_{k, \Lambda} \chi$
is nonzero only for $|\epsilon(k)|$ near the cutoff $\Lambda$. Each diagram
stands for two contributions since there are two ways to assign
$G_A$ and $S_A$ to the internal lines. As in previous
works[1, 2] our calculation ignores higher order vertices
and self-energy corrections (i.e. $\Sigma_A$ is set to zero). There-
fore the RG flow has to be stopped before the interactions
get too large and the lowest energy scales cannot be ac-
cessed in a controlled way.

We perform the RG numerically by dividing the Bril-
loin zone into 32 patches. Each patch is centered on a
“radial” line, as shown in Fig. (1). By standard Taylor
expansion and power counting arguments, the most rele-
vant vertex functions are the ones with incoming and
outgoing at the Fermi surface and the $\omega_i = 0$. In the
following we only keep track of these most relevant vertex
functions, which means we ignore the momentum depend-
ence in directions transverse to the Fermi surface. For
the instantaneous electron-electron scattering we thus
approximate the value of $V_A(k_1, k_2, k_3)$ by its value
$V_A(k_F(i), k_F(j), k_F(l))$, where $k_F(j)$ is the momentum
on the fermi surface at the center of the jth patch. This
leaves us with $32^3$ couplings $V(k_F(i), k_F(j), k_F(l))$ to
keep track of. We calculate the contributions to the flow of these couplings using the diagrams in Fig. (1).
The frequency sums are performed analytically, and the
loop momentum integration is performed by a sum over
patches and integration along the radial lines.

![Fig. 1: a) One loop Feynman diagrams contributing to $\partial \Lambda V_A$;
Spin is conserved along solid lines. The labels “I” and “R” represent
the instantaneous and retarded interaction (the gray bars) respectively. While all interactions can be the “I” type,
only those with both “I” and “R” labels can be retarded.]
scattering alone with band parameter $t'' = 0$ has been obtained by Honerkamp et al. We obtain similar results when including $t'' = -0.1t$. Depending upon the doping level, several groups have found that the renormalization flow enhances instantaneous couplings which favor either SDW formation or d-wave superconductivity as the most prominent ordering tendency[1–3]. These can be seen in Fig. (2) where $V_{\Lambda=0.2l}(k_F(i), k_F(j), k_F(l))$ is plotted as a function of $i$ and $j$ for a fixed $l = 2$. The couplings which favor SDW ordering have a positive amplitude and constant momentum transfer $k_F(j) - k_F(l)$[1]. They show up as the vertical bands in boxes (A) of Fig. (2). The values $k_F(j) - k_F(l)$ of these scattering processes are around $(\pi, \pi)$. In particular they include $(\pi \pm 2\pi/8a, \pi)$, indicating “incommensurate” SDW ordering. The couplings which favor d-wave superconductivity are the diagonal lines enclosed in boxes (B) of Fig. (2). These scatterings occur in the cooper channel where $k_F(i) + k_F(j) = 0$, and have an alternating sign structure indicative of d-wave symmetry. The fact that the couplings favoring superconducting pairing overlap with the couplings favoring SDW ordering signifies that physically, these ordering tendencies are linked. Since the phonon-mediated retarded couplings do not influence the flow of the instantaneous interactions, the d-wave superconducting pairing seen above can not be due to the electron-phonon interaction. In the present calculation, due to the choice of chemical potential and $U$, the spin-density waves are always the leading ordering tendency.

In addition to these two types of interactions, there also exist weaker scattering processes which favor other types of ordering. Couplings which lead to these ordering tendencies are also indicated in Fig. (2). The first is the Pomeranchuk instability, which leads to a $x^2 - y^2$-symmetry deformation of the Fermi surface[3]. The second leads to a charge-density wave order with ordering wavevector equal to the vectors connecting the parallel segments of the Fermi surface near the Brillouin zone face. These wavevectors correspond to a spatial period near four lattice constants. It is worth noting that the $t'$ and $t''$ terms in the band structure are responsible for the almost nested Fermi surface near the Brillouin zone face. They enhance the charge ordering tendency.
Now we investigate the flow of the retarded couplings. By experimenting with the symmetries of the initial scattering amplitude, we find three independent sets of retarded interactions that are most strongly enhanced by the RG (Fig. (3)). In all three sets the scattering amplitude shows \( x^2 - y^2 \) symmetry in momentum space. This type of sign structure can arise from phonon mediation if \( g(\mathbf{k}, \mathbf{k} + \mathbf{Q}) \) in Eq. (4) transforms as \( \cos(k_x) \rightarrow -\cos(k_y) \). For the interaction in Figs. (3a), (3b), and (3c), \( \mathbf{Q} \sim (\pm \pi, \pm \pi) \), \( \mathbf{Q} \sim (\pm 2\pi/4a, \pm 2\pi/4a) \), and \( \mathbf{Q} \sim (\pm 2\pi/4a, 0) \). For example, it can arise from coupling to the half breathing or the B\(_1g\) \[11\] phonons. Note that the electron-phonon interaction with the B\(_1g\) buckling mode has no amplitude for momentum transfer \((\pi, \pi)\) and so will not contribute appreciably to retarded interaction (3a). Consistent with previous results \[12–15\], the same analysis indicates that an s-symmetry electron-phonon coupling will be suppressed under RG. (Monte Carlo studies \[15\] find that s-symmetry electron-phonon couplings in the Hubbard model for large \( U > 6t \); it would be of interest to see the behavior of \( x^2 - y^2 \) couplings.) Another common feature among the three sets is that the involved initial and final momenta are all within the antinodal region.

We find that the most important contribution to the RG flow of the retarded interaction comes from the “bub-ble” diagram in the lower left of Fig. (1)(a), when one of vertices is an instantaneous interaction from the boxes (A) of Fig. (2) and the other is a retarded interaction. The \( x^2 - y^2 \) sign structure discussed above is essential for the growth of the scattering amplitude: the positive(negative) retarded coupling combines with the instantaneous interactions to drive the negative(positive) retarded interaction to strong coupling. Since the boxes (A) enclose interactions that favor SDW ordering near \((\pi, \pi)\), we conclude that commensurate and incommensurate magnetic fluctuations are responsible for driving the relevant retarded interactions to strong coupling.

The key features of each set of retarded interactions in Fig. (3) appear as horizontal bands. In a horizontal band the momentum transfer \( \mathbf{k}_F(i) - \mathbf{k}_F(l) \) is fixed, suggesting that these couplings promote some type of density wave order. However, the \( x^2 - y^2 \) sign structure makes the corresponding density wave order an unconventional one. The density wave order parameter driven by the retarded interactions in Fig. (3) has the form

\[
\mathcal{O} = \sum_{\mathbf{k}, \sigma} f(\mathbf{k}) < c^\dagger_{\mathbf{k}+\mathbf{Q}\sigma} c_{\mathbf{k}\sigma} > ,
\]

where \( f(\mathbf{k}) \) transforms like \( \cos(k_x) \rightarrow -\cos(k_y) \) under rotation. These are examples of generalized d-wave density orders, which in general can have bond averages \( < c^\dagger_i c_j > \) with any complex phase, leading to both bond current and charge density orders \[19\]. We have verified via mean field calculations (details in a later publication) that all three interactions can promote real space modulations in both charge density and current. In particular, the interaction of Fig. (3c) can lead to periodic charge density modulations with period \( \sim 4a \). Note that the chemical potential \( \mu \) can change the nesting wavevector and hence the period of modulations. Thus we find that in the cuprates the most important effect of the electron-phonon interaction is to promote density wave order. Interestingly, for any order described by Eq. (5), the nodal quasiparticles will be unaffected. In particular the density wave order in Fig. (3c) is consistent with the STM experiment of Hanaguri et al and the ARPES experiment by Shen et al. In addition, the fact that all the enhanced retarded interactions in Fig. (3) involve scattering processes with initial and final momentum states in the antinodal region is also consistent with the isotope-dependent ARPES study of Ref. \[7\].

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