Theory of the time-resolved spectral function of high-temperature superconductors

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Abstract. We have recently developed a three-temperature model to simulate the time evolution of the electron and phonon temperatures in high-temperature superconductors. This is the first model that is valid in the superconducting state. Based on this model, we calculated the time-resolved spectral function via the double-time Green’s functions. Our calculations show that the theory not only reveals the familiar dip-hump structure in the normal state, but also a new signature of the electron-phonon coupling in the superconducting state. We further show that this signature can only be observed when the phonons are pumped directly. In this proceeding, we provide detailed derivation of our theory.

1. Introduction
The physics underlying pairing in high-temperature superconconductors (HTSC) remains a topic of strong interest. The small isotope effect of optimally doped samples and the very nature of the $d$-wave pairing suggested the importance of a spin-based pairing interaction. Indeed the dip-hump structure of the density of states observed in electron tunneling spectroscopy [1] could be explained with the electronic coupling to spin fluctuations [2]. Due to the improvement of sample quality and momentum resolution, similar structures have been observed in angle-resolved photoemission spectroscopy (ARPES) [3]. These features have been equally well explained [4] with the electron-phonon (el-ph) coupling. This suggests that some phonon modes that are strongly coupled to electrons may be of relevance. To better understand the physics behind the superconductivity, a good knowledge of the el-ph coupling is essential.

However, the usual ARPES only provides the information of the el-ph coupling in thermally populated excitation. Accessing the thermally inaccessible states provides the ability to uncover novel signatures of the el-ph coupling, which may not be captured by the standard ARPES. For this reason, time-resolved (TR) ARPES has been developed to offer the capability to capture the single-particle (frequency domain) and collective (time domain) information, thus making it possible to directly probe the link between the collective modes and single-particle states. In this setting, either electrons or phonons (i.e., lattice vibrational modes) can be selectively excited with an ultrafast laser pulse. This new technique has been applied to the studies of transient electronic structure in Mott insulators [5, 6] and HTSC [7] with optical pump. The TR-ARPES with the capability of directly pumping vibrational or phonon mode has been developed to study the el-phonon coupling in manganites [8], though not yet in the cuprates.

To study the dynamics of the el-ph coupling in HTSC, We have recently proposed [9] a theory of the time-resolved spectral function, which is valid in the superconducting state where
the quasiparticle excitation is well defined [2]. The theory consists of two parts: (i) a three-
temperature model is proposed to simulate the time dependence of the electron and phonon
temperatures, and (ii) time-resolved spectral function up to second order in the coupling constant
is calculated with the double-time Green’s function approach. To illustrate the theory, we applied
it to the optimally doped cuprates to study the time evolution of the el-ph interaction between
electrons and phonons of the out-of-plane and out-of-phase buckling mode [10]. Numerical
calculations show that, when phonons are pumped directly, a new signature of the el-ph coupling
can be observed in the superconducting state and then immediately disappears when the system
evolves into the normal state with the increase of the electronic temperature. This enhancement
of the el-ph coupling in the superconducting state suggests that the role of the el-ph coupling
cannot be ignored when we explore the physics behind high-temperature superconductivity.

2. Three-temperature model

Our three-temperature model [9] is based on the two assumptions: (i) The system can be
divided into three subsystems, namely, electrons, hot phonons, and cold lattice, and (ii) the
energy transfer within each subsystem is much faster than that between different subsystems.
The first assumption requires three temperatures to characterize the system, while the second
guarantees that a local equilibrium within each subsystem can be reached quickly after pumping.
According to the energy conservation law, the rate equations for the electron, hot phonon, and
cold lattice temperatures [7] can be written as

\[ C_e \frac{\partial T_e}{\partial \tau} = \frac{\partial E_e}{\partial \tau} + P_e, \]  

\[ C_{ph} \frac{\partial T_{ph}}{\partial \tau} = -\frac{\partial E_e}{\partial \tau} + P_{ph} - \frac{C_{ph}(T_{ph} - T_0)}{\tau_\beta}, \]  

\[ C_l \frac{\partial T_l}{\partial \tau} = \frac{C_{ph}(T_{ph} - T_0)}{\tau_\beta}, \]

where \( P_e \) is the power for pumping electrons, \( P_{ph} \) is the power for pumping hot phonons, and
\( \tau_\beta \) is the time of the anharmonic decay of hot phonons. The specific heat of electrons can be
calculated from the Boltzmann entropy \( S_e = -2k_B \sum_k \{1 - f(E_k)\} \log[1 - f(E_k)] + f(E_k) \log f(E_k) \} \)
by \( C_e = T_e \partial S_e / \partial T_e \), while the specific heat of hot phonons for one-vibrational mode can be
calculated directly from the internal energy of phonons [which is given by the third term
of Eq. (6)] by \( C_{ph} = \hbar \Omega \partial N(\Omega) / \partial T_{ph} |_{\Omega=\Omega_0} \). In these expressions, \( E_k = \sqrt{\xi_k^2 + \Delta_k^2} \) is the
superconducting-state quasiparticle energy, \( f(E_k) = 1/(e^{\beta_k E_k} + 1) \) is the Fermi distribution
function of electrons, and \( N(\Omega_0) = 1/(e^{\beta_{ph} \Omega_0} - 1) \) is the Bose-Einstein distribution function of phonons,
with \( \beta_e = 1/k_B T_e \) and \( \beta_{ph} = 1/k_B T_{ph} \) being the temperature parameters of electrons and phonons. Simple algebra leads to the results

\[ C_e = \beta_k B \sum_k \left[ -\frac{\partial f(E_k)}{\partial E_k} \right] \left( 2E_k^2 + \beta_e \Delta_k \frac{\partial \Delta_k}{\partial \beta_e} \right), \]  

\[ C_{ph} = \frac{k_B}{4(\hbar \Omega_0 \beta_{ph})^2} \left[ \coth^2 \left( \frac{\hbar \Omega_0 \beta_{ph}}{2} \right) - 1 \right]. \]

Now we calculate the energy exchange rate \( \partial E_e / \partial \tau \) due to el-ph scattering. For this purpose,
we consider a two-dimensional superconductor exposed to a time-dependent laser field. The
model Hamiltonian for a vibrational mode $\nu$ can be written as

$$H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k} (\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow} + \text{h.c.}) + \sum_{q} \hbar \omega_q \left( b_{q\nu}^\dagger b_{q\nu} + \frac{1}{2} \right) + \frac{1}{\sqrt{N_L}} \sum_{kq\sigma} g_{\nu}(k, q) c_{k+q,\sigma} c_{k\sigma} A_{\nu q} + H_{\text{field}}(\tau), \quad (6)$$

where $c_{k\sigma}^\dagger$ ($b_{q\nu}$) and $c_{k\sigma}$ ($b_{q\nu}$) are the creation and annihilation operators for an electron with momentum $k$ and spin $\sigma$ (phonon with momentum $q$ and vibrational mode $\nu$), $A_{\nu q} = b_{\nu,-q}^\dagger + b_{q\nu}$, $\varepsilon_k$ is the normal-state energy dispersion [11], $\mu$ the chemical potential, $\Delta_k$ the gap function [12], and $g_\nu$ the coupling matrix. To simplify the calculation, we perform the Bogoliubov-de Gennes transformation [13] $c_{k\uparrow}^\dagger = u_k \alpha_k - v_k \beta_k^\dagger$ and $c_{-k\downarrow} = u_k \beta_k + v_k \alpha_k^\dagger$, where $u_k^2 = (1 + \varepsilon_k/E_k)/2$ and $v_k^2 = (1 - \varepsilon_k/E_k)/2$, and obtain the diagonalized expression for the electronic quasiparticle energy, $E_e = \sum_k E_k((\alpha_{k\uparrow}^\dagger \alpha_k) - \langle \beta_{k\beta_k}^\dagger \beta_k \rangle)$. The time evolution of $\langle \alpha_k \uparrow \alpha_k \rangle$ and $\langle \beta_k \beta_k \rangle$ can be calculated using the equations-of-motion approach. The results, correct to second order in $g_\nu$, are given by

$$\frac{\partial \langle \alpha_k \uparrow \alpha_k \rangle}{\partial \tau} = \frac{2\pi}{N_L} \sum_q g_q^2 (u_k u_{k-q} - v_k v_{k-q})^2 (\delta_{2e}^{\beta_k \Omega_k} - \delta_1) \left[ e^{(\beta_{k\beta_k} - \beta_k)\Omega_k} - 1 \right] (1 - f_k) f_{k-q} N_{\Omega_k} T \quad (\text{7})$$

and $\partial \langle \beta_k \beta_k \rangle / \partial \tau = -\partial \langle \alpha_k \uparrow \alpha_k \rangle / \partial \tau$, where $f_k = f(E_k)$, $N_{\Omega_k} = N(\Omega_k)$, $\delta_1 = \delta(E_{k-q} - E_k + \Omega_k)$, and $\delta_2 = \delta(E_{k-q} - E_k - \Omega_k)$. Here we have specifically set $\Omega_\nu = \Omega_0$. Differentiation of both sides of the expression for $E_e$ with respect to $\tau$ leads to

$$\frac{\partial E_e}{\partial \tau} = \frac{4\pi}{N_L} \sum_{kq} g_q^2 (u_k u_{k-q} - v_k v_{k-q})^2 \delta(E_{k-q} - E_k - \Omega_0) \Omega_0 \left[ e^{(\beta_{k\beta_k} - \beta_k)\Omega_k} - 1 \right] f_k (1 - f_{k-q}) N_{\Omega_k} T \quad (\text{8})$$

Equations (1)-(5) and (8) constitute our three-temperature model. The original version of this model was phenomenologically proposed [7] as an extension of the two-temperature model [14] for the normal state. Compared to the original version, the present model has the additional ingredients: (i) it incorporates the detailed band structure, (ii) it is valid for the superconducting state and will essentially reduce to the original version [7] in the normal state, (iii) it includes the anistropic effect on the el-ph coupling, and (iv) it offers the capability of selectively pumping electron and phonon degrees of freedom.

Finally we point out that in the calculation of the equations of motion for $\langle \alpha_k \uparrow \alpha_k \rangle$ and $\langle \beta_k \beta_k \rangle$, two cross terms $\langle \alpha_{k\beta_k} \beta_k \rangle$ and $\langle \beta_k \alpha_k \rangle$, which are coupled to the former two direct terms, have been neglected. These two terms describe the formation and breaking of the Cooper pairs arising from the time-dependent perturbation. At the initial state, they vanish. This negligence should not change the main physics discussed here, because they do not contribute to the energy directly.

3. Time-resolved spectral function

The time-resolved spectral function is defined as $A(k, \omega) \equiv -\frac{2}{\pi} \text{Im} G_{11}(k, \omega)$. Here $G_{11}$ is the one-one component of the retarded Green’s function $\hat{G}(k, \omega)$, which is related to the self-energy by $\hat{G}^{-1}(k, \omega) = \hat{G}_0^{-1}(k, \omega) - \hat{\Sigma}(k, \omega)$, with $\hat{G}_0^{-1}(k, \omega) = \omega \bar{\sigma}_0 - \Delta_k \bar{\sigma}_1 + \varepsilon_k \bar{\sigma}_3$. $\bar{\sigma}_{0,1,2,3}$ are the unit and Pauli matrices. As is known [4], in the equilibrium state with $T_e = T_{ph}$, the self-energy can be evaluated more conveniently within the imaginary-time Green’s function approach, in which a key step is to convert the Bose-Einstein distribution to the Fermi distribution, $n_B(\pm \omega_n, \pm E_{k-q}) = -n_F(\pm E_{k-q})$ (with $\omega_n = (2n+1)\pi T$, $T = T_e = T_{ph}$). For the current
situation, the temperatures of electrons and hot phonons are no longer tied to each other and the above conversions are not valid any more. To avoid this restriction, here we apply the double-time Green’s function approach to calculate $\tilde{\Sigma}(\mathbf{k}, \omega)$. The result is

$$\tilde{\Sigma}(\mathbf{k}, \omega) = \frac{1}{N_L} \sum_{\mathbf{q}} |g_{\nu}(\mathbf{k}, -\mathbf{q})|^2 \left\{ (\omega - \Omega_0) \Phi_1 - (\omega + \Omega_0) \Phi_2 + \Omega_0 (\Phi_3 + \Phi_4) \right\} \bar{\sigma}_0 + \left\{ 2E_{\mathbf{k} - \mathbf{q}} (\Phi_1 - \Phi_3) + 2\Omega_0 (\Phi_3 - \Phi_4) \right\} \bar{\sigma}_1 + \left\{ \xi_\mathbf{k} (\Phi_1 - \Phi_2) + (\Omega_0 \xi_\mathbf{k} / E_{\mathbf{k}}) (\Phi_3 - \Phi_4) \right\} \bar{\sigma}_3 \right\} (\mathbf{q})$$

where $\Phi_1 = N(\Omega_0) / [(\omega + \Omega_0 + E_{\mathbf{k} - \mathbf{q}}) (\omega - \Omega_0 - E_{\mathbf{k} - \mathbf{q}})]$, $\Phi_2 = N(-\Omega_0) / [(\omega + \Omega_0 + E_{\mathbf{k} - \mathbf{q}}) (\omega - \Omega_0 - E_{\mathbf{k} - \mathbf{q}})]$, $\Phi_3 = f(-E_{\mathbf{k} - \mathbf{q}}) / [(\omega + \Omega_0 - E_{\mathbf{k} - \mathbf{q}}) (\omega - \Omega_0 - E_{\mathbf{k} - \mathbf{q}})]$, and $\Phi_4 = f(E_{\mathbf{k} - \mathbf{q}}) / [(\omega + \Omega_0 + E_{\mathbf{k} - \mathbf{q}}) (\omega - \Omega_0 + E_{\mathbf{k} - \mathbf{q}})]$. In our calculation, a bare $\hat{G}_0$ is used. Since the coupling constant for the cuprates is small, self-consistency effect on the self-energy is small and is thus neglected in this work. Notice that the dynamics due to the perturbative Hamiltonian (6) enters the spectral function through the three-temperature model. From Eq. (9), we see that the dip-hum structure of the density of states, $\rho(\omega) = \frac{1}{N_L} \sum_{\mathbf{k}} A(\mathbf{k}, \omega)$, arise from the pole structure [15] of the self-energy $\tilde{\Sigma}(\mathbf{k}, \omega)$. Because of the inverse relationship between the Green’s function and the self-energy, the larger the self-energy is, the smaller the Green’s function and so is the spectral function, and vice versa.

In conclusion, we have explained in detail a theory of the time-resolved spectral function we recently proposed to study the time-evolution of the signature of the el-ph coupling in HTSC materials. The theory is valid in the superconducting state. Our study shows that in the superconducting state, the el-ph coupling signature gets enhanced, suggesting the relevance of the el-ph coupling to the superconductivity. In the viewpoint that the electronic spin fluctuations arise from the strong correlation within the electronic DoF itself, and if one can assume that the spin fluctuations will ride on the electrons and thus its effective temperature will be tied to the electronic temperature, direct pumping of hot phonons will provide a unique way to differentiating the bosonic modes being of electronic or phononic origin, to which electronic quasiparticles are strongly coupled.

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