Interband transitions and electronic Raman continuum in systems with strong inelastic scattering: applications to YBa$_2$Cu$_3$O$_{7-\delta}$

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Abstract. We consider a model for the electronic Raman continuum which takes into account strong inelastic scattering and interband transitions. Calculations are based on four-vertex Raman scattering diagrams (Kawabata formalism) within the RPA for Coulomb interaction and the ladder diagram Bethe-Salpeter equation for the vertex. We apply this method to an analysis of the nature of the electronic Raman continuum in the normal state of the high-$T_c$ superconductor YBa$_2$Cu$_3$O$_{7-\delta}$. In numerical calculations we take into account all the self-energy effects and make simulations for vertex corrections assuming that inelastic scattering is due to electron-phonon interaction. The $ab$-plane polarized continuum contains a large contribution from interband processes and does not depend strongly on temperature and inelastic scattering strength. The in-plane anisotropy is determined by interband transitions rather than by anisotropy of the Fermi surface. The ZZ continuum contains only weak contribution from interband transitions. It can be crudely described within a single band model with inelastic scattering and is strongly dependent on the relaxation rates of inelastic scattering. The nature of the oxygen-deficiency dependence of the Raman spectra is also commented upon.

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I. Introduction

The anomalous Raman scattering continuum is one of the most unusual properties of high-$T_c$ materials. The discovery of this feature of the Raman spectra in YBa$_2$Cu$_3$O$_{7-\delta}$ [1–3] generated a great challenge for theory because of the possibility that it may have some relevance for the high temperature of the superconducting transition in the cuprates. Later these flat continua have been found in practically all of the high-$T_c$ cuprates as well as in the copperless superconductor Ba$_{1-x}$K$_x$BiO$_3$ [4], which does not show spin fluctuations like the copper oxides. The insulating antiferromagnetic phases of the cuprates such as YBa$_2$Cu$_3$O$_6$ and orthorhombic La$_2$CuO$_4$ and Sm$_2$CuO$_4$ are also characterized by similar features of the Raman spectra, but in addition there is a broad peak usually attributed to two-magnon scattering [4–6]. The polarization, doping, temperature and laser frequency dependence of this continuum also shows a rich collection of unusual properties [4, 6–8], and provides extremely important information about these materials in both doped and insulating cases.

It is well known that Raman scattering by single particle excitations in metals must be very weak and will appear in a very low energy region. This is because the cross section is proportional to the structure factor $S(q, \omega)$ of the Fermi gas [9] and vanishes as $q^2$ when $q \to 0$. $S(q, \omega)$ is therefore very small at the momentum transfers of the light scattering. For the explanation of the strong Raman continuum in high-$T_c$ compounds several different theories have been proposed [10–16]. In spite of the formal differences, the electronic system of the material in all of these approaches, such as the phenomenological marginal Fermi liquid concept [10], nested Fermi liquid theory [11], fluctuations in Mott-Hubbard systems [12], Luttinger liquid theory [13], etc., is very different from the predictions of the normal Fermi liquid (FL) theory. For example, the concept of marginal Fermi liquid (MFL), inspired by a large amount of experimental results for high-$T_c$ superconductors, presents a special form for the one-particle self-energy; the nested Fermi liquid theory (NFL) considers the energy dependent damping from the electron-electron scattering between nearly parallel sections of the Fermi surface; etc.

It has also been demonstrated that in systems with strong electron-phonon interaction the behavior of the electron system is very far from the normal FL. [15–17]. Using some simple model for the Eliashberg function $\alpha^2 f(\omega)$ [15, 16], one can obtain very flat frequency dependence of the imaginary part of the electronic suscepti-
ibility in the $q \to 0$ limit extending up to high energies. More realistic Eliashberg functions $a^2 f(\omega)$ constructed from tunneling and neutron data for the high-$T_c$ cuprates produce one-particle spectral functions $A(k, \omega)$ with a width comparable to the energy distance from the Fermi level, a behaviour quite similar to the MFL model \[17\]. The resulting optical conductivity is in quite good agreement with experiment and gives rise to a linear $\omega$-dependence of the transport relaxation rate if interpreted within an extended Drude model.

In a previous paper \[18\] we developed this approach in order to investigate the role of conduction electron scattering for the Raman continuum and its polarization, temperature and laser frequency dependence in a normal state of the high-$T_c$ material $\text{YBa}_2\text{Cu}_3\text{O}_7$. We took into account both strong inelastic scattering and interband transitions. It was found that there is a large difference between the plane polarized and $c$-axis polarized components of the Raman tensor describing the electronic Raman continua. The present paper gives a full account both strong inelastic scattering and interband transitions. We also discuss the oxygen deficiency dependence of the continua.

Section II is devoted to a derivation of the main formulas which describe the contribution of conduction electrons to the Raman scattering cross section in a system with strong inelastic scattering. We use the Kawai- bata formalism and taken into account the ladder diagram Bethe-Salpeter equation for the vertex as well as the Coulomb interaction within RPA. It is shown that such an approach gives results which are close to those of the commonly used polarization operator formalism. The only formal difference is the dependence of effective masses on the energy of the electron. Such a dependence becomes important in systems with strong inelastic scattering and low energy interband electronic transitions.

In Sect. III we discuss the experimental and theoretical results concerning the nature of the electronic states near the Fermi level in $\text{YBa}_2\text{Cu}_3\text{O}_7$. We show that strong inelastic scattering due to electron-phonon interaction can significantly change the low-energy behavior of different polarization operators in this material. It seems doubtful that one can observe low-energy interband electronic transitions either in optical conductivity or in electronic Raman continua because of the strong smearing of the spectral functions for electrons near the Fermi level.

Section IV describes the results of numerical calculations of the electronic Raman continuum in the normal state of $\text{YBa}_2\text{Cu}_3\text{O}_7$. Calculations have been performed within the framework of Eliashberg strong-coupling theory for the electron-phonon interaction. We take into account all of the self-energy effects and make approximations for vertex corrections. We find that the difference between the $a$- and $c$-polarized continua is mostly due to the interband transitions. The nature of the oxygen-deficiency dependence of the Raman spectra is also commented upon.

II. Raman cross section

We consider the Raman scattering process using Kawabata formalism \[19-21\], which implies analysis of the four-vertex function $\mathcal{F}(q, \omega_n, i\omega_n, i\omega_n)$. The expression for the scattering cross section can be obtained by analytical continuation,

$$I_R(q, \omega) = \frac{1}{n(\omega)} \int \frac{d^4q}{(2\pi)^4} \int \frac{d^4\omega}{(2\pi)^4} \mathcal{F}(q, \omega, \omega, \omega, \omega, \omega)$$

where $r_0$ is the Thomson radius, $q$ and $\omega$ represent the momentum and energy transfer of the scattered photon, $\omega_1$ and $\omega_2(\omega_3 = \omega_4 = \omega)$ are incident and scattered light frequencies, and $n(\omega)$ is the Bose distribution function.

Let us at first consider the Raman cross section for the non-interacting system, i.e. we neglect the Coulomb interaction as well as contributions from impurity and inelastic scattering processes to vertices. The calculation in the $q \to 0$ limit of the four noninteracting four-vertex Raman scattering diagrams (Fig. 1; see also \[19-21\]) is based on the “dressed” Matsubara Green’s functions,

$$G_{kk}(\omega) = \frac{1}{i\omega - \epsilon_{kk} - \Sigma(i\omega_n, k)}$$

where $\epsilon_{kk}$ is the “bare” (unrenormalized) one-electron energy in a band $a$ at a given point $k$ in the Brillouin zone. The self-energy $\Sigma(i\omega_n, k)$ contains information about inelastic scattering processes and is taken to be independent of the band index $a$.

By taking into account the branch cuts of $\Sigma(\omega_n, k)$ on the real frequency $\omega$ axis in the complex plane, the summation of the product of four Green’s functions over Matsubara frequencies $i\omega_n$ can easily be performed, and one obtains:

$$G_{kk}(\omega) = \frac{1}{i\omega - \epsilon_{kk} - \Sigma(i\omega_n, k)}$$

Fig. 1. Four-vertex diagrams based on independent-particle Green's functions from (2) (see also \[20\]). Vertices 1 and 4 are associated with the operator $(p, e_1)$, and vertices 2 and 3 with $(p, e_3)$. 