

Effects of energy dependence in the quasiparticle density of states on far-infrared absorption in the pseudogap state

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We derive a relationship between the optical conductivity scattering rate $1/\tau(\omega)$ and the electron-boson spectral function $\alpha^2F(\Omega)$ valid for the case when the electronic density of states, $N(\epsilon)$, cannot be taken as constant in the vicinity of the Fermi level. This relationship turns out to be useful for analyzing the experimental data in the pseudogap state of cuprate superconductors.

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I. INTRODUCTION

Optical conductivity data on $\sigma(\omega)$ vs ω contains important information on electron dynamics. In general however the relationship between $\sigma(\omega)$ and the electron self-energy is rather complicated. Under such circumstances the reduction, if possible, of the complete expression for conductivity, to somewhat more approximate but simpler analytic form can be valuable. It can help our understanding of the basic physics as well as provide experimentalists with a simpler basis for the analysis of data.

In the specific case of an electron-phonon system, the analytic formula provided by Allen¹ has proved to be valuable. It relates the measured optical scattering rate through a simple integral to the underlying electron-phonon spectral function $\alpha^2F(\omega)$ which is, in the end, the fundamental quantity of interest. A generalization of Allen's formula to finite temperature was provided by Shulga *et al.*² In this paper we want to extend this previous work to the case when the underlying electronic density of states is energy dependent rather than constant. A motivation for this extension is to provide guidance in the interpretation and analysis of optical data in the pseudogap regime of the cuprates. In fact the formula derived herein has already been used in the experimental work of Hwang *et al.*³ on ortho-II YBCO.

II. PRELIMINARIES

The Drude formula for optical conductivity $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$,

$$\sigma(\omega, T) = \frac{\omega_p^2}{4\pi} \frac{1}{1/\tau - i\omega} \quad (1)$$

can be extended (see Refs. 4 and 5 and references therein) to include a frequency-dependent scattering rate

$$\sigma(\omega, T) = \frac{\omega_p^2}{4\pi} \frac{1}{1/\tau(\omega, T) - i\omega[1 + \lambda(\omega, T)]}, \quad (2)$$

where $1/\tau(\omega, T)$ is the frequency-dependent optical scattering rate and $\lambda(\omega, T)$ is the optical mass enhancement. For a spherical Fermi surface the plasma frequency $\omega_p^2 = 4\pi n e^2 / m$, where n is the free-carrier density and m is the carrier mass.

One can solve Eq. (2) for $1/\tau(\omega)$ and $1 + \lambda(\omega)$ in terms of the optical conductivity found from experiment,

$$\frac{1}{\tau(\omega)} = \frac{\omega_p^2}{4\pi} \operatorname{Re} \left(\frac{1}{\sigma(\omega)} \right) \quad (3)$$

and

$$1 + \lambda(\omega) = - \frac{\omega_p^2}{4\pi} \frac{1}{\omega} \operatorname{Im} \left(\frac{1}{\sigma(\omega)} \right). \quad (4)$$

The plasma frequency can be extracted from the experimental data using the sum rule $\int_0^\infty \sigma_1(\omega) d\omega = \omega_p^2 / 8$. Although the representations of experimental data using $\sigma_1(\omega)$, $\sigma_2(\omega)$ and $1/\tau(\omega)$ with $1 + \lambda(\omega)$ are formally equivalent, it has become rather popular to discuss the pseudogap behavior in high-temperature superconductors (HTSC) using the language of the optical scattering rate and mass enhancement. For example, a drop of $1/\tau(\omega)$ extracted from in-plane optical conductivity measurements in HTSC which is observed below a certain frequency for the temperatures $T < T_{ab}^*$ is associated with the above-mentioned pseudogap.⁴

Another advantage of $1/\tau(\omega)$ is that in an electron-phonon system it is related to the electron-phonon interaction spectral density, $\alpha^2F(\omega)$. For example, there is an approximate relationship⁶

$$\alpha^2F(\omega) = \frac{1}{2\pi} \frac{d^2}{d\omega^2} \left(\omega \frac{1}{\tau(\omega)} \right) \quad (5)$$

which is valid at $T=0$ in the normal state. Note that one can consider a general electron-boson interaction function, because instead of $\alpha^2F(\omega)$ one can, for instance, introduce electron-spin excitation spectral density, $I^2\chi(\omega)$.⁷ Thus below we imply this more general case, but preserve the historical notation $\alpha^2F(\omega)$.

Despite its “magic” simplicity, formula (5) works rather well (see, e.g., Refs. 8 and 9), but unfortunately its practical applications are limited because the experimental data must be (ambiguously) smoothed “by hand” before the second derivative can be taken. This problem was very recently circumvented in Ref. 10 by solving the corresponding integral equations for $\alpha^2F(\omega)$. For example, instead of differentiating $\omega/\tau(\omega)$, one can extract $\alpha^2F(\omega)$ using the well-known result of Allen¹

$$\frac{1}{\tau(\omega)} = \frac{2\pi}{\omega} \int_0^\omega d\Omega (\omega - \Omega) \alpha^2 F(\Omega). \quad (6)$$

The last expression was derived using the second order perturbation theory and in fact, Eqs. (6) and (5) are equivalent under the condition $1/\tau(\omega=0)=0$.

A finite temperature generalization of Eq. (6) was derived in Ref. 2 using the Kubo formula

$$\frac{1}{\tau(\omega)} = \frac{\pi}{\omega} \int_0^\infty d\Omega \alpha^2 F(\Omega) \left(2\omega \coth \frac{\Omega}{2T} - (\omega + \Omega) \coth \frac{\omega + \Omega}{2T} + (\omega - \Omega) \coth \frac{\omega - \Omega}{2T} \right). \quad (7)$$

In fact, there is no finite temperature equivalent of a ‘‘magic’’ equation (5) for Eq. (7), so that for finite T 's $\alpha^2 F$ can only be found by inversion of the last equation. The numerical method of inversion of Eq. (7), its limitations and the resulting doping and temperature dependences of the bosonic spectral function, $\alpha^2 F(\omega)$ in several families of HTSC were investigated in detail in Ref. 10.

There is, however, an important assumption used in deriving both the $T=0$ Eq. (6) and its finite temperature extension (7), viz. the electronic density of states (DOS), $N(\epsilon)$ is taken as a constant in the vicinity of the Fermi level. As shown in Ref. 10 when Eq. (7) is used for analyzing the experimental data in the pseudogap state of HTSC, the resulting $\alpha^2 F$ contains nonphysical negative values. This problem originates from the fact that the above-mentioned assumption $N(\epsilon)=\text{const}$ is definitely strongly violated in the pseudogap state. The essence of the pseudogap phenomenon is that $N(\epsilon)$ becomes a nontrivial function of energy and the form of $N(\epsilon)$ depends strongly on the temperature and doping.

Therefore it would be very useful to have a generalization of Eqs. (6) and (7) valid for $N(\epsilon) \neq \text{const}$. Interestingly, such a generalization of the zero temperature expression (6) was already done 20 years ago by Mitrović and Fiorucci¹¹ in relation to A15 compounds

$$\frac{1}{\tau(\omega)} = \frac{2\pi}{\omega} \int_0^\omega d\Omega \alpha^2 F(\Omega) \int_0^{\omega-\Omega} d\epsilon \frac{1}{2} \left(\frac{N(\epsilon)}{N(0)} + \frac{N(-\epsilon)}{N(0)} \right). \quad (8)$$

Equation (8) was derived using the method of Ref. 1 and it is easy to see that for $N(\epsilon)=\text{const}$ it reduces to Eq. (6).

The purpose of the present work is to obtain a generalization of the finite temperature expression (7) valid for $N(\epsilon) \neq \text{const}$. In contrast to Refs. 1 and 11 we base our derivation on the Kubo formula which turns out to be more useful for considering the $T \neq 0$ case.

We begin by presenting in Sec. III the expression for optical conductivity $\sigma(\omega)$ in terms of frequency-dependent self-energy $\Sigma(\omega)$ for the case $N(\epsilon) \neq \text{const}$. The corresponding expression for $\Sigma(\omega)$ is obtained in Sec. IV for the case of nonconstant quasiparticle DOS $\tilde{N}(\epsilon)$. The difference between the usual DOS $N(\epsilon)$ and the quasiparticle DOS $\tilde{N}(\epsilon)$ is

pointed out. In Sec. V we present the relationship between the optical scattering rate, $1/\tau(\omega)$, electron-boson interaction function $\alpha^2 F(\omega)$, and the quasiparticle DOS $\tilde{N}(\epsilon)$. The frequency-dependent impurity scattering rate $1/\tau_{\text{imp}}(\omega)$ is considered in Sec. VI. In the discussion, Sec. VII, we illustrate that the pseudogap opening results in the decrease of $1/\tau(\omega)$ and consider possible applications of our results.

III. OPTICAL CONDUCTIVITY FOR $N(\xi) \neq \text{const}$

We begin with the Kubo formula for electrical conductivity¹²

$$\sigma_{ij}(\omega) = \frac{i}{\omega + i0} [\tau_{ij} - \Pi_{ij}^R(\omega + i0)], \quad (9)$$

where τ_{ij} is the diamagnetic term and $\Pi_{ij}(\omega)$ is the retarded correlation function obtained by analytical continuation [$\Pi_{ij}^R(\omega) = \Pi_{ij}(i\Omega_m \rightarrow \omega + i0)$] of the imaginary time expression

$$\Pi_{ij}(i\Omega_m) = \frac{1}{V} \int_0^\beta d\tau e^{i\Omega_m \tau} \langle j_i(\mathbf{q}=0, \tau) j_j(\mathbf{0}, 0) \rangle, \quad \Omega_m = \frac{2\pi m}{\beta}. \quad (10)$$

Here $j_i(\mathbf{q}, \tau)$ is the Fourier transform of the paramagnetic electric current density operator, V is the volume of the system, $T=1/\beta$ and for the case of parabolic band $\tau_{ij} = \omega_p^2/4\pi \delta_{ij} = e^2 n \delta_{ij}/m$. The electrical conductivity (9) consists of a regular part

$$\sigma_{ij}^{\text{reg}}(\omega) = -\frac{i}{\omega} [\Pi_{ij}^R(\omega) - \Pi_{ij}^R(0)] \quad (11)$$

and singular part, related to the superconducting condensate,

$$\sigma_{ij}^{\text{SC}}(\omega) = \frac{i}{\omega + i0} [\tau_{ij} - \Pi_{ij}^R(0)]. \quad (12)$$

Since in what follows we restrict ourselves to considering the normal state of the isotropic two-dimensional system, we suppress the subscript reg and consider $\sigma(\omega) = \sigma_{xx}^{\text{reg}}(\omega) = \sigma_{yy}^{\text{reg}}(\omega)$ deriving, for example, $\Pi_{xx}(\omega)$.

Neglecting vertex corrections, the calculation of $\sigma(\omega)$ reduces to evaluation of the bubble diagram

$$\Pi_{ij}(i\Omega_m) = -2e^2 T \sum_{n=-\infty}^{\infty} \int \frac{d^2 k}{(2\pi)^2} v_{Fi}(\mathbf{k}) v_{Fj}(\mathbf{k}) G(i\omega_n) + i\Omega_m \mathbf{k} G(i\omega_n, \mathbf{k}), \quad (13)$$

where $v_{Fi}(\mathbf{k}) = \partial \xi(\mathbf{k}) / \partial k_i$ is the Fermi velocity and

$$G(i\omega_n, \mathbf{k}) = \frac{1}{i\omega_n - \xi(\mathbf{k}) - \Sigma(i\omega_n, \mathbf{k})} \quad (14)$$

is the fermionic Green's function with the self-energy $\Sigma(i\omega_n, \mathbf{k})$ and $\omega_n = \pi(2n+1)/\beta$. Using the spectral representation for the Green's function (14), one can easily sum over fermionic Matsubara frequencies in Eq. (13),

$$\begin{aligned} \Pi_{xx}(i\Omega_m) = & -2e^2 \int_{-\infty}^{\infty} d\xi \int \frac{d^2k}{(2\pi)^2} \delta[\xi - \xi(\mathbf{k})] \\ & \times v_{Fx}^2(\mathbf{k}) \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \frac{n_F(\omega_1) - n_F(\omega_2)}{\omega_1 - \omega_2 + i\Omega_m} \\ & \times A(\omega_1, \mathbf{k}) A(\omega_2, \mathbf{k}), \end{aligned} \quad (15)$$

where the spectral function

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \text{Im} G_R(\omega + i0, \mathbf{k}), \quad (16)$$

$n_F(\omega) = 1/(e^{\beta\omega} + 1)$ is the Fermi distribution, and we inserted the integral over ξ which is equal to 1. Since we are interested in the complex conductivity $\sigma(\omega)$ we cannot remove one of the integrations over ω in (15) by taking $\text{Im} \Pi(\omega + i0)$, but one of the integrations can be done by again using the spectral representation for retarded (advanced) Green's function

$$G_{R,A}(\omega, \mathbf{k}) = \int_{-\infty}^{\infty} d\omega_2 \frac{A(\omega_2, \mathbf{k})}{\omega \pm i0 - \omega_2}. \quad (17)$$

Then we obtain

$$\begin{aligned} \Pi_{xx}(\omega) = & -2e^2 \int_{-\infty}^{\infty} d\omega' n_F(\omega') \int_{-\infty}^{\infty} d\xi N(\xi) v_{Fx}^2(\xi) A(\omega', \xi) \\ & \times [G_R(\omega' + \omega, \xi) + G_A(\omega' - \omega, \xi)], \end{aligned} \quad (18)$$

where to isolate the effects of the energy dependence of the single-spin-band DOS,

$$N(\xi) = \int \frac{d^2k}{(2\pi)^2} \delta[\xi - \xi(\mathbf{k})], \quad (19)$$

the velocity $v_{Fx}^2(\xi)$ is defined as (see Refs. 11 and 13)

$$v_{Fx}^2(\xi) \equiv \frac{1}{N(\xi)} \int \frac{d^2k}{(2\pi)^2} v_{Fx}^2(\mathbf{k}) \delta[\xi - \xi(\mathbf{k})]. \quad (20)$$

Writing Eq. (18) we also assumed that $A(\omega, \mathbf{k})$ and, accordingly, $G_{R,A}(\omega, \mathbf{k})$ to be dependent only on $\xi(\mathbf{k})$.

Now we must make two important assumptions: The first one is quite common and states that the self-energy $\Sigma(i\omega, \xi)$ does not depend on ξ , so that the whole dependence of $G_{R,A}(\omega, \xi)$ is contained in the free-electron dispersion $\xi(\mathbf{k})$. The second assumption is that the energy dependence of the square of the plasma frequency

$$\frac{\omega_p^2(\xi)}{4\pi} = 2e^2 N(\xi) v_{Fx}^2(\xi) \quad (21)$$

can be ignored as compared to the dependence of $N(\xi)$ in the vicinity of $\xi=0$, so that in Eq. (18) we can replace $\omega_p^2(\xi)$ by $\omega_p^2(\xi=0)$. The validity of this approximation for A15 compounds was discussed in Ref. 11 and here we will assume that it is also valid for HTSC. In this respect, the first assumption can be considered as a statement that $\Sigma(\omega, \xi)$ is approximated by $\Sigma(\omega, \xi=0)$.¹⁶ After these two assumptions are made we can integrate over ξ and finally arrive at the

following representation for the optical conductivity (see, e.g., Refs. 2,14,15,16):

$$\begin{aligned} \sigma(\omega) = & \frac{\omega_p^2}{4\pi} \frac{i}{\omega} \int_{-\infty}^{\infty} d\epsilon [n_F(\epsilon) - n_F(\epsilon + \omega)] \\ & \times \frac{1}{\omega + i/\tau_{\text{imp}} + \Sigma^*(\epsilon) - \Sigma(\epsilon + \omega)}, \end{aligned} \quad (22)$$

where $\Sigma(\epsilon)$ is the retarded self-energy on the real axes and $\Sigma^*(\epsilon)$ its complex conjugate. In Eq. (22) we also included the electron-impurity scattering rate, $1/\tau_{\text{imp}}$, its frequency dependence will be considered in Sec. VI. One can check that for $T=0$ Eq. (22) reduces to the expression for $\sigma(\omega)$ written in Refs. 6, 8, and 9.

To investigate the effect of electron-boson interaction on $1/\tau(\omega)$ we must express $\text{Re}[1/\sigma(\omega)]$ in terms of the self-energy Σ in the simplest possible form. It can be anticipated if one substitutes Eq. (22) in Eq. (3) and rewrites it as follows:

$$\begin{aligned} \frac{1}{\tau(\omega)} = & \omega \text{Im} \left(\frac{1}{\omega + i/\tau_{\text{imp}}} \int_{-\infty}^{\infty} d\epsilon [n_F(\epsilon) - n_F(\epsilon + \omega)] \right. \\ & \left. \times \frac{1}{1 - [\Sigma(\epsilon + \omega) - \Sigma^*(\epsilon)]/(\omega + i/\tau_{\text{imp}})} \right)^{-1}. \end{aligned} \quad (23)$$

Now expanding the denominator of Eq. (23), doing the integration and then “de-expanding” the result (see Refs. 8 and 9) we obtain the following approximate representation:

$$\begin{aligned} \frac{1}{\tau(\omega)} = & \frac{1}{\tau_{\text{imp}}} - \frac{1}{\omega} \int_{-\infty}^{\infty} d\epsilon [n_F(\epsilon) - n_F(\epsilon + \omega)] \\ & \times \text{Im}[\Sigma(\epsilon + \omega) - \Sigma^*(\epsilon)]. \end{aligned} \quad (24)$$

In deriving Eq. (24) we used the assumption $|\Sigma(\epsilon + \omega) - \Sigma^*(\epsilon)| \ll |\omega + i/\tau_{\text{imp}}|$ to expand and then assumed that

$$\int_{-\infty}^{\infty} d\epsilon [n_F(\epsilon) - n_F(\epsilon + \omega)] |\Sigma(\epsilon + \omega) - \Sigma^*(\epsilon)| \ll \omega |\omega + i/\tau_{\text{imp}}|$$

to “de-expand.” Based on these inequalities one would expect that all results that follow from Eq. (24) are valid only for large ω . Nevertheless, the numerical comparison of the results obtained by the direct substitution of the self-energy (32) in Eq. (22) with $1/\tau(\omega)$ computed using Eq. (7) in Ref. 2 shows that the last equation is valid for a much wider range of the frequency ω . This is in spite of the fact that the derivation of Eq. (7) is based on the approximate Eq. (24). Finally we remind that since we did not include vertex corrections, $1/\tau(\omega)$ is expressed in terms of the usual self-energies instead of transport “self-energies” discussed in Ref. 15. Accordingly in Sec. V the optical scattering rate $1/\tau(\omega)$ will be expressed in terms of the tunneling $\alpha^2 F$ instead of the transport $\alpha_u^2 F$ considered by Allen in Ref. 1.

IV. SELF-ENERGY FOR $\bar{N}(\xi) \neq \text{const}$

Now we consider the influence of a nonconstant DOS on the usual relationship between the self-energy $\Sigma(\omega)$ and the

electron-boson interaction function $\alpha^2 F$. We begin with the well-known expression (see, e.g., Refs. 17 and 18)

$$\begin{aligned} \Sigma(i\omega_n) = T \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi \frac{N(\xi)}{N(0)} \int_0^{\infty} d\Omega \alpha^2 F(\Omega) \frac{2\Omega}{\Omega_m^2 + \Omega^2} \\ \times G(i\omega_n - i\Omega_m, \xi) \end{aligned} \quad (25)$$

written for the case when $\alpha^2 F(\Omega)$ does not depend on the electron energy. In Eq. (25),

$$G(i\omega_n, \xi) \equiv \frac{1}{N(\xi)} \int \frac{d^2 k}{(2\pi)^2} \delta[\xi - \xi(\mathbf{k})] G(i\omega_n, \mathbf{k}), \quad (26)$$

the DOS $N(\xi)$ is defined by Eq. (19) and its energy dependence usually is also neglected. Our goal is, however, to retain $N(\xi)$ and consider the influence of $N(\xi) \neq \text{const}$ on $\Sigma(\omega)$ and, accordingly, on $\sigma(\omega)$. Again using the spectral representation for the Green's function $G(i\omega_n, \mathbf{k})$, one can easily sum over Matsubara frequencies in Eq. (25) and obtain

$$\begin{aligned} \Sigma(i\omega_n) = \int_{-\infty}^{\infty} d\xi \frac{N(\xi)}{N(0)} \int_{-\infty}^{\infty} d\omega' \int_0^{\infty} d\Omega \alpha^2 F(\Omega) \\ \times \left(-\frac{1}{\pi} \text{Im} G_R(\omega + i0, \xi) \right) I(i\omega_n, \Omega, \omega'), \end{aligned} \quad (27)$$

where¹⁷

$$I(i\omega_n, \Omega, \omega') = \frac{n_B(\Omega) + 1 - n_F(\omega')}{i\omega_n - \Omega - \omega'} + \frac{n_B(\Omega) + n_F(\omega')}{i\omega_n + \Omega - \omega'} \quad (28)$$

with the Bose distribution $n_B(\Omega) = 1/(e^{\beta\Omega} - 1)$.

Let us now consider the quantity

$$\tilde{N}(\omega) \equiv -\frac{1}{\pi} \int_{-\infty}^{\infty} d\xi N(\xi) \text{Im} G_R(\omega + i0, \xi) \quad (29)$$

which enters Eq. (27). Using Eq. (26) and the definition of the spectral function (16) one can easily check that

$$\tilde{N}(\omega) = \int \frac{d^2 k}{(2\pi)^2} A(\omega, \mathbf{k}), \quad (30)$$

viz. this quantity represents the fully dressed quasiparticle DOS which could contain a pseudogap that has its origin in correlation effects. Finally making an analytical continuation $i\omega_n \rightarrow \omega + i0$ and taking the imaginary part of $\Sigma(\omega)$ we obtain

$$\begin{aligned} \text{Im} \Sigma(\omega) = -\pi \int_0^{\infty} d\Omega \alpha^2 F(\Omega) \left(\frac{\tilde{N}(\omega - \Omega)}{N(0)} [n_B(\Omega) + 1 \right. \\ \left. - n_F(\omega - \Omega)] + \frac{\tilde{N}(\omega + \Omega)}{N(0)} [n_B(\Omega) + n_F(\omega + \Omega)] \right). \end{aligned} \quad (31)$$

It is easy to see that for $\tilde{N}(\omega) = N(0) = \text{const}$ the previous equation reduces to a more familiar expression^{2,17}

$$\begin{aligned} \text{Im} \Sigma(\omega) = -\frac{\pi}{2} \int_0^{\infty} d\Omega \alpha^2 F(\Omega) \left(2 \coth \frac{\Omega}{2T} - \tanh \frac{\omega + \Omega}{2T} \right. \\ \left. + \tanh \frac{\omega - \Omega}{2T} \right). \end{aligned} \quad (32)$$

V. OPTICAL SCATTERING RATE: BOSON CONTRIBUTION

Substituting the self-energy (31) in the expression (24) and doing simple replacements of the variables, we arrive at the main result of the present paper,

$$\begin{aligned} \frac{1}{\tau(\omega)} = \frac{\pi}{\omega} \int_0^{\infty} d\Omega \alpha^2 F(\Omega) \int_{-\infty}^{\infty} d\epsilon \left(\frac{\tilde{N}(\epsilon - \Omega)}{N(0)} + \frac{\tilde{N}(-\epsilon + \Omega)}{N(0)} \right) \\ \times [n_B(\Omega) + n_F(\Omega - \epsilon)] [n_F(\epsilon - \omega) - n_F(\epsilon + \omega)], \end{aligned} \quad (33)$$

which establishes a link between the optical scattering rate $1/\tau(\omega)$, the electron-boson interaction function $\alpha^2 F(\Omega)$ and the quasiparticle DOS $\tilde{N}(\omega)$. It is important to stress that in contrast to $N(\omega)$, the quasiparticle DOS $\tilde{N}(\omega)$ which enters Eqs. (31) and (33) is directly related to the spectral function $A(\omega, \mathbf{k})$ measured by ARPES experiments.¹⁹ Note that in Eq. (33) material parameters enter only as the electron-boson spectral density and the fully dressed electron DOS. Different mechanisms leading to the same $\tilde{N}(\omega)$ are differentiated in the optical scattering rate only through the size and shape of $\alpha^2 F(\Omega)$.

To understand better the rather lengthy Eq. (33) we consider limiting cases where one can establish a link with already known results.

(i) For $T=0$ the Bose distribution in Eq. (33) drops out and it reduces to Eq. (8) with the band DOS $N(\omega)$ replaced by the quasiparticle DOS $\tilde{N}(\omega)$. Note that it was pointed out in Ref. 11 that $N(\omega)$ in Eq. (8) should be interpreted as the quasiparticle DOS, but the golden rule approach of Allen¹ used in Ref. 11 does not allow to establish this fact directly. Comparing Eqs. (8) and (33) one can see that finite temperature brings an essential element, the Bose distribution $n_B(\Omega)$.

(ii) When $\tilde{N}(\omega) = \text{const}$ it becomes possible to integrate over ϵ in (33). Indeed using the integral

$$\int_{-\infty}^{\infty} dz n_F(z+a) n_F(-z-b) = (a-b) n_B(a-b) \quad (34)$$

we arrive at Eq. (7) obtained by Shulga *et al.* in Ref. 2. Obviously, Eq. (7) also follows directly from Eqs. (32) and (24).

(iii) At temperatures much higher than the boson spectrum upper-energy cutoff, $T \gg \Omega_c$, expression (33) reduces to

$$\lim_{T/\Omega_c \rightarrow \infty} \frac{1}{\tau(\omega)} = \frac{\pi T}{\omega} \int_0^\infty d\Omega \frac{\alpha^2 F(\Omega)}{\Omega} \int_{-\infty}^\infty d\epsilon \left(\frac{\tilde{N}(\epsilon - \Omega)}{N(0)} + \frac{\tilde{N}(-\epsilon + \Omega)}{N(0)} \right) [n_F(\epsilon - \omega) - n_F(\epsilon + \omega)]. \quad (35)$$

When $\tilde{N}(\epsilon) = \text{const}$ the last equation can be further simplified⁵

$$\lim_{T/\Omega_c \rightarrow \infty} \frac{1}{\tau(0)} = 4\pi T \int_0^\infty d\Omega \frac{\alpha^2 F(\Omega)}{\Omega}. \quad (36)$$

In the case when the electron-phonon interaction is the origin of $\alpha^2 F(\Omega)$, Eq. (36) reflects the familiar result that the high-temperature electron-phonon contribution to a dc resistivity is linear in temperature. This no longer strictly holds for Eq. (35) where there is an additional T dependence in the integral over ϵ .

VI. OPTICAL SCATTERING RATE: CONTRIBUTION OF IMPURITIES

While Eq. (33) represents the electron-boson contribution to the optical scattering rate, the total scattering rate

$$\frac{1}{\tau_{\text{tot}}(\omega)} = \frac{1}{\tau(\omega)} + \frac{1}{\tau_{\text{imp}}(\omega)} \quad (37)$$

consists of two parts, viz. the above-mentioned bosonic $1/\tau(\omega)$ and that caused by impurities $1/\tau_{\text{imp}}(\omega)$.

There is a simple way of obtaining $1/\tau_{\text{imp}}(\omega)$ by using the following expression for

$$\alpha^2 F_{\text{imp}}(\Omega) = \frac{1}{2\tau_{\text{imp}}} \frac{\Omega \delta(\Omega)}{\pi T} \quad (38)$$

and assuming that the integration of $\delta(\Omega)$ over Ω from 0 to ∞ gives $1/2$. $1/\tau_{\text{imp}}$ in Eq. (38) is the normal state impurity scattering rate and it is implied that the limit $\Omega \rightarrow 0$ in $\alpha^2 F_{\text{imp}}(\Omega)$ must be taken before doing the limit $T \rightarrow 0$. Substituting Eq. (38) in Eq. (33) we arrive at the expression

$$\frac{1}{\tau_{\text{imp}}(\omega)} = \frac{1}{\tau_{\text{imp}}} \frac{1}{4\omega} \int_{-\infty}^\infty d\epsilon [n_F(\epsilon - \omega) - n_F(\epsilon + \omega)] \times \left(\frac{\tilde{N}(\epsilon)}{N(0)} + \frac{\tilde{N}(-\epsilon)}{N(0)} \right). \quad (39)$$

Energy dependence in $\tilde{N}(\epsilon)$ implies an energy and temperature dependence in the impurity scattering rate. For $T=0$, Eq. (39) reduces to the result of Ref. 11,

$$\frac{1}{\tau_{\text{imp}}(\omega)} = \frac{1}{\tau_{\text{imp}}} \frac{1}{\omega} \int_0^\omega d\epsilon \frac{1}{2} \left(\frac{\tilde{N}(\epsilon)}{N(0)} + \frac{\tilde{N}(-\epsilon)}{N(0)} \right). \quad (40)$$

Note that due to the above-mentioned noncommutativity of the limits $\Omega \rightarrow 0$ and $T \rightarrow 0$ in Eq. (38), the last expression cannot be obtained simply by substituting Eq. (38) in Eq. (8).

It is very easy to see that for $\tilde{N}(\epsilon) = \text{const}$, Eq. (40) as well as

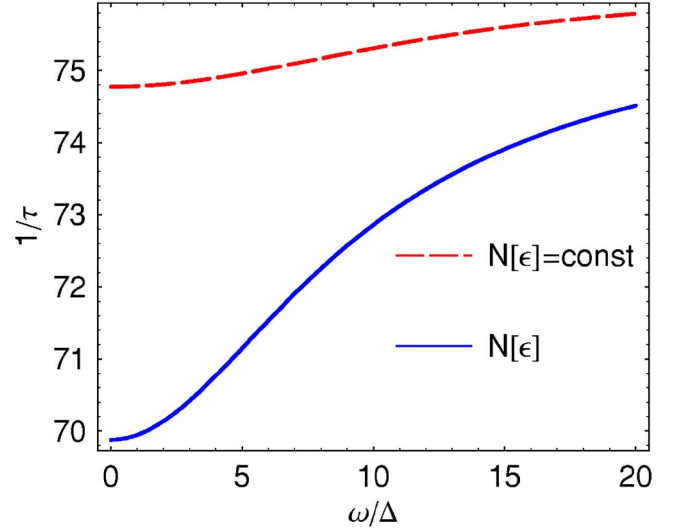


FIG. 1. (Color online) The dependence $1/\tau(\omega)$ (in arbitrary units) obtained from Eqs. (7) for $\tilde{N}(\epsilon) = \text{const}$ and (33) with $\tilde{N}(\epsilon)$ given by Eq. (41). We take the Einstein model for $\alpha^2 F(\Omega) = \alpha^2 \delta(\Omega - \Omega_E)$ with $\Omega_E = 2\Delta$ and $T = 2.5\Delta$.

Eq. (39) reduce to the trivial result $\tau_{\text{imp}}(\omega) = \tau_{\text{imp}}$. For a more extensive discussion of the impurity scattering problem when the DOS is energy dependent the reader is referred to Ref. 20. In the fits to data made in Ref. 3 residual scattering is small and not important. In that case $1/\tau_{\text{imp}}$ is estimated to be a few meV while the inelastic scattering rate rises to a value larger than 600 meV in the frequency range of interest in the fit. Under such circumstances any modulation of $1/\tau_{\text{imp}}(\omega)$ brought about by energy dependence in $\tilde{N}(\epsilon)$ is of no consequence when fitting to the inelastic scattering part. This would not be so if impurity scattering became large and of the order of the inelastic scattering in the important frequency range.

VII. DISCUSSION

To illustrate the effect of the opening of the pseudogap on $1/\tau(\omega)$ in Fig. 1 we plot $1/\tau(\omega)$ computed with and without pseudogap, but do not consider the contribution from impurities. The case without pseudogap which corresponds to $\tilde{N}(\epsilon) = N(0) = \text{const}$ was considered using Eq. (7), while to model a pseudogap we took³

$$\frac{\tilde{N}(\epsilon)}{N(0)} = \left[\frac{\tilde{N}(0)}{N(0)} + \left(1 - \frac{\tilde{N}(0)}{N(0)} \right) \frac{\epsilon^2}{\Delta^2} \right] \theta(\Delta - |\epsilon|) + \theta(|\epsilon| - \Delta) \quad (41)$$

and used Eq. (33). It is easy to see that the main effect of the opening of the pseudogap [e.g., $\tilde{N}(0) < N(0)$] is to reduce $1/\tau(\omega)$. This result implies that when there is a pseudogap one cannot use Eq. (6) to estimate $\alpha^2 F(\Omega)$, because the strength of the peaks of $\alpha^2 F(\Omega)$ would be underestimated. More importantly, the position of these peaks would be shifted depending on our assumptions about the absence or presence of the pseudogap.

Indeed by applying Eq. (33) in Ref. 3 to the analysis of the experimental data it was demonstrated that there is agreement between the sharp bosonic resonance observed in the infrared scattering rate and the properties of the (π, π) spin-flip neutron mode. Using the above-mentioned property that the decrease of $N(\epsilon)$ due to the opening of the pseudogap effectively reduces $1/\tau(\omega)$, one can choose the position of the bosonic resonance in $\alpha^2F(\Omega)$ at $\Omega=248\text{ cm}^{-1}$ and thus makes it agree with the frequency of the 31 meV neutron mode, measured by Stock *et al.*²¹ The use of Eq. (33) is crucial for this agreement and the conventional relationship (6) valid for $T=0$ and $N(\epsilon)=\text{const}$ would produce a peak in $\alpha^2F(\Omega)$ at $\Omega=350\text{ cm}^{-1}$. The possibility of achieving a reconciliation between the experimental results obtained from neutron scattering and optical conductivity is quite important in developing a coherent theoretical description of cuprate superconductors and shows the usefulness of Eq. (33).

We note that since this kind of analysis involves modeling the form of the pseudogap and its temperature dependence, the final results for $\alpha^2F(\Omega)$ are definitely not unique. However, one does not expect any qualitative change to the model for $\alpha^2F(\Omega)$ obtained in Ref. 3 which includes a very wide temperature-independent background and a sharp temperature-dependent peak. As a given sample is studied using several experimental techniques and the quality of the

data improves, the fit should become more unique. Also it would be interesting to repeat the analysis made in Ref. 10, but now based on Eq. (33) derived in this paper, rather than on Eq. (7) which is valid only for a constant density of states.

Finally we mention that in Ref. 10 data were analyzed not only in the normal or pseudogap state at finite T , but also in the superconducting state. This latter analysis is based on a relationship between $1/\tau(\omega)$ and $\alpha^2F(\Omega)$ derived in Ref. 1 for s -wave superconductor at $T=0$. In relation to the results obtained in the present paper it is worthwhile to ask the following question. Is it possible to distinguish the decrease of $1/\tau(\omega)$ caused by the pseudogap and by the superconducting s - or even d -wave gap? To address this question in detail there is a need to generalize the corresponding expression from Ref. 1 to d -wave symmetry of the superconducting gap and $T\neq 0$. Such considerations go beyond the scope of the present work.

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