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Quasiparticle relaxation in Heavy Fermions studied using Inverse Fourier Transform of optical conductivity

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ABSTRACT

Inverse Fourier Transform of optical conductivity is used for studies of quasiparticle relaxation in Heavy Fermions in time domain. We demonstrate the usefulness of the procedure on model spectra and then use it to study quasiparticle relaxation in two Heavy Fermions $YbFe_4Sb_{12}$ and $CeRu_4Sb_{12}$. Optical conductivity in time domain reveals details of quasiparticle relaxation close to the Fermi level, not readily accessible from the spectra in the frequency domain. In particular, we find that the relaxation of heavy quasiparticles does not start instantaneously, but typically after a few hundred femto-seconds.

1. Introduction

Relaxation of quasiparticles is of central interest in condensed matter physics [1–5]. Numerous experimental techniques have been employed and various theoretical models have been developed over the years. Infrared spectroscopy (IR) is one of these techniques that can probe charge dynamics close to the Fermi level most directly. The physical quantity of interest is the complex optical conductivity $\tilde{\sigma}(\omega)=\sigma_1(\omega)+i\sigma_2(\omega)$, in particular its real, dissipative part $\sigma_1(\omega)$. Optical conductivity $\tilde{\sigma}(\omega)$ is usually obtained from IR spectroscopy via Kramers–Kronig transformation of raw reflectance spectra [3].

In this paper we use Inverse Fourier Transform (IFT) to convert optical conductivity from frequency to time domain, with the goal of studying quasiparticle (QP) relaxation in Heavy Fermions (HF). Heavy Fermions are materials that behave like normal metals at high temperature, but at low temperatures develop coherent Fermi liquid, with large effective mass of its QP [6]. The procedure we propose here is completely *model-independent*, and will allows us to study temporal relaxation of these heavy QP with femtosecond resolution. Moreover, the low intensity of IR sources (mercury lamp and globar) used to collect the raw data guaranties that the studied system is always in the linear regime. Non-linear effects, a common problem with laser based time-domain spectroscopies, are not playing any role.

We define *time-domain conductivity* $\sigma(t)$ as the IFT of $\tilde{\sigma}(\omega)$ (Ref. [7,8]):

$$\sigma(t)=F^{-1}[\tilde{\sigma}(\omega)]=\int_{-\infty}^{\infty}\tilde{\sigma}(\omega)e^{-i\omega t}\,d\omega. \tag{1}$$

Similarly defined function is sometimes referred to as the conductivity memory function [9,10]. The transform is evaluated numerically in discrete form, using the well known fast Fourier transform (FFT) algorithm [11]. Before the algorithm can be applied, optical conductivity data must be extended to negative frequencies, using the causality property of optical conductivity [12]: $\tilde{\sigma}(-\omega)=\tilde{\sigma}(\omega)^*$. Other issues with the transform include aliasing, filtering, frequency and time resolution, numerical precision, etc., and they have been discussed before [11]. In this paper we first apply the transform to several model spectra and then to two HF: $YbFe_4Sb_{12}$ and $CeRu_4Sb_{12}$.

2. Drude–Lorentz model

Drude model is the oldest [13,14] but ironically even today the most popular model of QP relaxation in solids. It is based on the assumption that successive QP collisions that give rise to electrical resistance are independent from each other [1]. The central parameter of the model is the so-called QP relaxation time τ, which is (twice) the average time between collisions [1,3]. The reciprocal of relaxation time, $1/\tau$ is commonly referred to as the scattering rate. The optical conductivity within Drude model is [1–5]:

$$\tilde{\sigma}_D(\omega)=\frac{1}{4\pi}\frac{\omega_p^2\tau}{1-i\tau\omega}, \tag{2}$$

where ω_p is the plasma frequency $\omega_p^2=4\pi e^2 n/m_b$, with n being the carrier density and m_b their band mass. The IFT of $\tilde{\sigma}_D(\omega)$ can

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be calculated in analytic form using elementary complex integration [7]:

$$\sigma_D(t) = F^{-1}[\tilde{\sigma}_D(\omega)] = \frac{\omega_p^2}{2} e^{-t/\tau}, \quad (3)$$

for $t > 0$ and zero for $t < 0$. Therefore, in time domain Drude conductivity is represented by an exponential decay whose time constant is the relaxation time τ. Note also that the IFT of a complex $\tilde{\sigma}_D(\omega)$ is a real function $\sigma_D(t)$ which is identically zero for negative time and positively definite for positive time.

Fig. 1 shows examples of model calculations. The top panel displays $\tilde{\sigma}_D(\omega)$ with three different relaxation times (or scattering rates), and the same plasma frequency ω_p. The bottom panel displays corresponding $\sigma(t)$, and as expected all three curves are exponential functions (note the log scale), with the slope being determined solely by the relaxation time (Eq. (3)). Fig. 1 also illustrates that larger relaxation times correspond to smaller slopes, and vice versa. We also note that since all three model spectra were generated with the same plasma frequency, they all start from the same $\sigma(t = 0)$, as follows from Eq. (3).

In correlated electron systems quite often more than one scattering mechanisms is present. IR spectroscopy is a momentum averaging technique and cannot discern them. In spite of that, optical conductivity is frequently decomposed into different modes, and various contribution are then phenomenologically assigned to different scattering channels. The method we propose here can also be used to address this situation. Fig. 2(a) displays model conductivity consisting of two Drude modes with different scattering rates. Time-domain conductivity is now more complicated (Fig. 2(b)), but again we can easily identify two straight segments, i.e. two relaxation channels. Calculations show that the IFT method can resolve relaxation processes with relaxation times that differ by only a factor of two.

In addition to intraband quasiparticle relaxation, various other contributions show up in the optical conductivity. To account for these finite energy excitations Drude model is usually supplemented with a finite number of Lorentz oscillators, whose

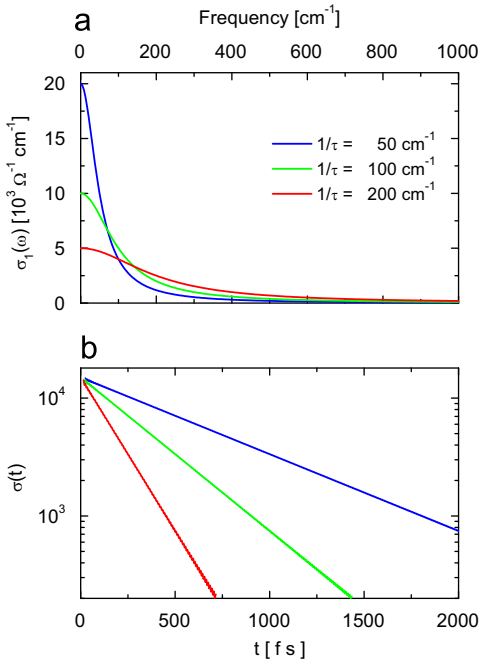

Fig. 1. (a) Drude conductivity in frequency domain for three different values of scattering rate. (b) Drude conductivity in time domain, calculated using Inverse Fourier Transform (Eq. (1)).

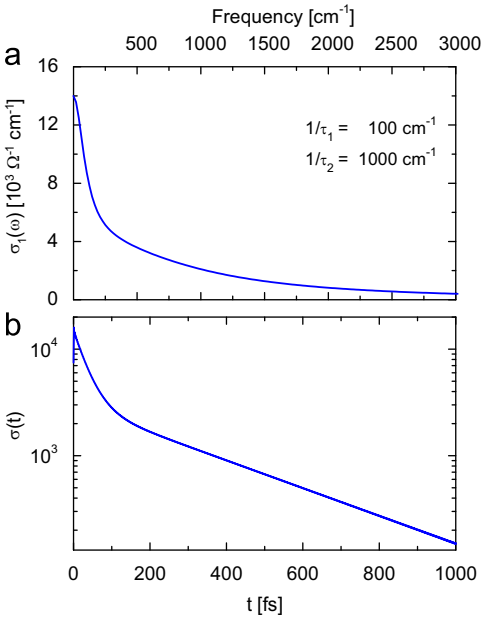

Fig. 2. (a) Optical conductivity in frequency domain consisting of two Drude modes with different relaxation times τ_1 and τ_2. (b) Corresponding time-domain conductivity. Two straight segments can easily be identified.

complex optical conductivity is given as [1–5]:

$$\tilde{\sigma}_L(\omega) = \frac{1}{4\pi} \frac{i\omega\omega_p^2}{\omega^2 - \omega_0^2 + i\gamma\omega}, \quad (4)$$

where ω_p is the oscillator strength of the mode, ω_0 its position and γ its width. The IFT of this complex function can also be calculated analytically [7]:

$$\sigma_L(t) = F^{-1}[\tilde{\sigma}_L(\omega)] = \frac{\omega_p^2}{2\omega_\gamma} e^{-t\gamma/2} \left(\omega_\gamma \cos\left(\frac{t\omega_\gamma}{2}\right) - \gamma \sin\left(\frac{t\omega_\gamma}{2}\right) \right), \quad (5)$$

for $t > 0$ and zero for $t < 0$. In Eq. (5), $\omega_\gamma = \sqrt{4\omega_0^2 - \gamma^2}$. In addition to exponential decay governed by γ, time-domain conductivity is now proportional to a linear combination of trigonometrical functions. Fig. 3(a) displays a model conductivity with a Drude mode and a single Lorentzian. For the purpose of comparison, the same Drude mode is also shown and analyzed without the Lorentzian. As expected from Eq. (5) the contribution from the Lorentzian shows up as oscillations in time domain. It is obvious from Fig. 3(b) that QP relaxation at short time scales is not affected by this Lorentzian. In the physical sense, finite energy excitations are far away from the Fermi level ($\hbar\omega_0$ in energy), and they need longer times to relax back to equilibrium, i.e. they begin to contribute to $\sigma(t)$ later (approximately 1000 fs in this example). Therefore the IFT method is primarily sensitive to relaxation process close to the Fermi level, and predominantly contributions at low frequencies in $\sigma(\omega)$ are probed.

3. Heavy Fermions

Numerical calculations on model spectra presented in the previous section revealed great potential of IFT method. In this section we demonstrate its usefulness on two HF metals, $YbFe_4Sb_{12}$ and $CeRu_4Sb_{12}$, which have been previously studied using IR spectroscopy and their frequency domain conductivities are available [15].

Infrared spectra of $YbFe_4Sb_{12}$ in frequency domain are shown in Fig. 4(a) at several selected temperatures between 300 and 10 K. Optical conductivity $\sigma_1(\omega)$ reveals that at high temperatures