Differential Sum Rule for the Relaxation Rate in the Cuprates

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Motivated by recent experiments by Basov et al., we study the differential sum rule for the effective relaxation rate \(1/\tau(\omega)\). We show that, in a dirty BCS superconductor, the area under \(1/\tau(\omega)\) does not change between the normal and the superconducting states. For magnetically mediated pairing, a similar result holds between \(T < T_c\) and \(T \geq T_c\), while, in the pseudogap phase, \(1/\tau(\omega)\) is just suppressed compared to \(1/\tau(\omega)\) in the normal state. We argue that this violation of the differential sum rule in the pseudogap phase is due to the absence of the feedback effects from the pairing.

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The analysis of the optical sum rules in condensed matter systems is a valuable tool that helps one to understand the key physics and relevant energy scales in the problem [1]. The focus of this Letter is the recent experimental results [2] for the effective relaxation rate \(\tau^{-1}(\omega) = (4\pi/\omega_p^2)\Re[1/\sigma(\omega)]\), where \(\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)\) is the optical conductivity, \(\omega_p^2 = 4\pi ne^2/m\) is the plasma frequency, and \(n\) is the density of particles. The data analysis for optimally doped YBa\(_2\)CuO\(_{6.95}\) [3] and Tl\(_2\)Ba\(_2\)CuO\(_{6.0+x}\) [4] and underdoped YBa\(_2\)CuO\(_x\) and Bi\(_2\)Sr\(_2\)CaCuO\(_{6+x}\) [2] revealed an approximate differential sum rule for \(\tau^{-1}(\omega)\) between \(T > T_c\) and \(T < T_c\): although \(\int d\omega \tau^{-1}(\omega)\) does not converge, it changes very little when the system enters into the superconducting state. This differential sum rule, however, is not satisfied between the normal and the pseudogap phases; \(1/\tau(\omega)\) in the pseudogap phase appears to be just suppressed.

The exact sum rules are generally related to conservation laws. The \(f\)-sum rule for the optical conductivity states that at a given density of particles, the total absorbing power of the solid characterized by \(\sigma_1\) does not depend on the details of the interactions and is determined only by the total number of particles in the system [5]. The total absorption power is given by \(\int_0^{\omega_p} d\omega \sigma_1(\omega)\). By applying the Kubo formula that relates \(\sigma(\omega)\) with the full retarded current-current correlator \(\Pi(\omega)\), \(\sigma(\omega) = (\omega_p^2/4\pi)\Pi(\omega)/(i\omega + \delta)\), separating the frequency integral into the integral over infinitesimally small \(\omega\) and the rest, and using the Kramers-Kronig relation for \(\Pi(\omega) - 1\) that vanishes at the highest frequencies, we obtain \(\int_0^{\omega_p} d\omega \sigma_1(\omega) = \omega_p^2/8\) independent of \(\Pi(\omega)\).

Is there an analogous sum rule for \(1/\tau(\omega)\)? Using \(1/\tau(\omega) = -\text{Im}\{\omega^2/\Pi(\omega)\}/\omega\) and applying the Kramers-Kronig relation, we find

\[
\int_0^{\infty} \frac{d\omega}{\tau(\omega)} = \frac{\pi}{2} \left[ \text{Re} \frac{\omega^2}{\Pi(\omega)_{\omega \to 0}} + C \right] = \frac{\pi}{2} C. \tag{1}
\]

The constant \(C\) again has to be chosen such that \(\omega^2/\Pi(\omega) + C\) vanishes at \(\omega \to \infty\). However, \(C\) turns out to be infinite as at high frequencies \(\Pi(\omega) = 1\), and \(\omega^2/\Pi(\omega)\) diverges. This divergence implies that there is no conservation law associated with the relaxation rate and hence no sum rule for \(1/\tau(\omega)\).

Marsiglio et al. [6] recently demonstrated that, at low frequencies, \(1/\tau(\omega)\) is numerically close to the effective \(1/\tau_{\text{eff}}(\omega) = -(\omega_p^2/4\pi)\text{Im}[1/\epsilon(\omega)]\) that obeys an exact sum rule \(\epsilon(\omega) = 1 + 4\pi i \sigma(\omega)/\omega\) is the dielectric function. They argued that one can introduce an approximate sum rule for \(1/\tau(\omega)\) by restricting the frequency integration to small frequencies. We follow a somewhat different route and consider whether one can get useful information by comparing \(1/\tau(\omega)\) for two different system parameters, e.g., temperatures, which do not affect the system behavior at high frequencies. Indeed, according to Eq. (1), if \(\omega^2/[\Pi(\omega, T_1) - 1/\Pi(\omega, T_2)]\) vanishes at high frequencies, then the area under \(1/\tau(\omega)\) does not change with \(T\). This would create a valuable tool to study the evolution of the spectral weight in \(1/\tau(\omega)\), e.g., the normal and superconducting states. This new differential sum rule, however, is not associated with a conservation law and therefore is not guaranteed to be satisfied—only explicit calculations can determine whether or not the temperature dependence in \(\Pi(\omega, T)\) is weak enough to ensure the convergence of the area under \(1/\tau(\omega)\).

In this Letter we study under which conditions the differential sum rule for \(1/\tau(\omega)\) is actually satisfied, and at which frequencies it is exhausted. We consider the magnetic scenario for the pairing in the cuprates, and argue that the differential sum is approximately satisfied and exhausted at frequencies comparable to the pairing gap if there is a strong feedback effect from the pairing on the fermionic propagator. Without feedback, \(1/\tau(\omega)\) appears to be just lost at these frequencies compared to the normal state. We associate the first regime with \(T < T_c\), and the second one with the pseudogap phase.

To put our analysis of the spin mediated pairing into perspective we first analyze the situation in a dirty BCS \(s\)-wave superconductor at \(T = 0\), when the pairing causes a strong feedback on the fermionic propagator, and in the toy model where there is no feedback from the pairing on the fermionic self-energy.

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The theory of a dirty superconductor is well developed [7,8]. In the normal state, the inelastic scattering by impurities yields a retarded fermionic self-energy $\Sigma(\omega) = i/2\tau$. In a superconducting state, this self-energy is modified due to a feedback from superconductivity and takes the form $\Sigma(\omega) = (i/2\tau)\omega/\sqrt{\omega^2 - \Delta^2}$, where $\Delta$ is the superconducting gap [8]. By substituting these forms into the current-current polarization bubble and performing the momentum integration, we obtain

$$\Pi(\omega) = \int_0^\infty d\Omega \frac{1}{\sqrt{\Omega_+^2 - \Delta^2 + \sqrt{\Omega_-^2 - \Delta^2} + i/\tau}} \times \frac{\sqrt{\Omega_+^2 - \Delta^2 \Omega_+^2 - \Delta^2 - \Omega_+ \Omega_-}}{\sqrt{\Omega_+^2 - \Delta^2 \Omega_+^2 - \Delta^2}}$$

where $\Omega_\pm = \Omega \pm \omega/2$. In the normal state, this reduces to a conventional Drude form $\Pi(\omega) = \omega/(\omega + i/\tau)$. In the superconducting state, the frequency integral in (2) can be evaluated analytically in the clean limit $\Delta \tau \gg 1$. After lengthy but straightforward calculations we found that both $\sigma_1(\omega)$ and $1/\tau(\omega)$ vanish at $\omega < 2\Delta$, while at larger frequencies

$$\sigma_1(\omega) = \frac{\omega_{pl}^2}{4\pi^2 \tau \omega^2} E\left(\sqrt{1 - 4\Delta^2/\omega^2}\right)$$

where $E(x)$ is the complete elliptic integral [9]. At $\omega = 2\Delta + 0$, $E = \pi/2$ and both $\sigma_1(\omega)$ and $1/\tau(\omega)$ jump to finite values. At high frequencies, $E(x = 1) \to 1$, $\sigma_1(\omega)$ vanishes as $\omega^{-2}$, and $1/\tau(\omega)$ approaches the normal state result $\tau(\omega) = \tau$. To the same order, we also have $\Pi(0) = 1 - \pi/(8\Delta \tau)$. We checked analytically that the f-sum rule $(8/\omega_{pl}^2) \int_0^\infty d\omega \sigma_1(\omega) = 1 - \Pi(0)$ is indeed satisfied.

Expanding $E(x)$ near $x = 1$, we find that at high frequencies $\tau^{-1}(\omega) - \tau^{-1} = (2\Delta^2/\omega^2)\left[\log(2\omega/\Delta) - 0.5\right]$, i.e., $\int d\omega [1/\tau(\omega) - 1/\tau]$ converges. The convergence implies that, for a dirty BCS superconductor, the differential sum rule for $1/\tau(\omega)$ is an exact one, and is exhausted at frequencies of the order of $\Delta$. The plots of $\sigma_1(\omega)$ and $1/\tau(\omega)$ are presented in Fig. 1 together with the results for $I_\rho(\omega) = (8/\omega_{pl}^2) \int_0^\infty d\omega \sigma_1(\omega)$ and $I_\tau(\omega) = (\pi/2\Delta) \int_0^\infty d\omega [1/\tau(\omega) - 1/\tau]$.

We next consider the behavior of $\sigma_1(\omega)$ and $1/\tau(\omega)$ in the toy model in which the pairing does not change the fermionic self-energy. This model makes sense if the normal state is not a Fermi liquid, i.e., fermionic self-energy at low frequencies behaves as $\Sigma(\omega) = (i\omega)^{\alpha} \omega^{1-\alpha}$ with $\alpha < 1$. Without the feedback effect on fermions, the fermionic density of states in the presence of the gap $N(\omega) = \text{Im}[\Sigma(\omega)/(\sqrt{\Delta^2 - \Sigma(\omega)^2})^{1/2}]$ has a maximum at $\omega = \tilde{\Delta} \sim \Delta^{1/\alpha} \omega^{(1-\alpha)/\alpha}$, but remains finite at $\omega < \tilde{\Delta}$ such that $\tilde{\Delta}$ is a pseudogap. For definiteness, we present the results for $\alpha = 1/2$, which is the normal state quantum-critical exponent in the spin-fermion theory [10], but the results are qualitatively the same for all $\alpha$ including the marginal Fermi liquid limit $\alpha \to 1$ [11].

For the frequency dependent self-energy $\Sigma(\omega)$, the current-current correlator $\Pi(\omega)$ is still given by Eq. (2), but with $\Omega_+ + \Sigma(\Omega_2)$ instead of $\Omega_2$. By evaluating $\Pi(\omega)$ and substituting it into $\sigma_1(\omega)$ and $1/\tau(\omega)$, we found that, in the normal state, $\sigma_1(\omega) \propto (\omega/\omega)^{-1/2}$ at $\omega \ll \omega$ and $\sigma_1(\omega) \propto (\omega/\omega)^{1/2}$ at $\omega \gg \omega$, while $1/\tau(n)(\omega) \propto (\omega/\omega)^{1/2}$ in both limits. For $\Delta \neq 0$, we found that, at $\omega \ll \Delta$, $\sigma_1(\omega) \propto (\omega/\omega)^{-1/2}(\omega/\Delta)^{1/2}$ and $1/\tau(\omega) \propto (\omega/\omega)^{1/2}(\omega/\Delta)^{1/2}$. We see that $\sigma_1(\omega)$ and $1/\tau(\omega)$ are reduced compared to their normal state values but are still finite. At larger $\Delta \ll \omega \ll \omega$, $\sigma_1(\omega) = 1.992(\omega_{pl}/4\pi)(\Delta^3/\omega^2)^{1/2}$ and $1/\tau(\omega) = 1/\tau(n)(\omega) = 3.51(\Delta/\omega)^{1/2}$. Finally, at $\omega \gg \omega$, $\sigma_1(\omega) - \sigma_1(\omega) \propto \omega^{-1/2} \omega^{3/2} \log \omega$, and $1/\tau(\omega) - 1/\tau(n)(\omega) \propto \omega^{3/2} \log \omega$.

We see that $\sigma_1(\omega)$ converges to its normal state value at frequencies of order $\tilde{\Delta}$, as in a dirty BCS superconductor; the sum rule for $\sigma_1(\omega)$ is then exhausted at $\omega \sim \Delta$. This behavior is illustrated in Fig. 2b, where we present the results of our numerical calculations. $I_\rho(\omega)$ converges to $I_\rho(\infty) = 1 - \Pi(0) = 0.67$ for our choice of $\omega = 2\Delta$ already at $\Delta \sim \Delta$. On the other hand, $\tau^{-1}(\omega) - \tau^{-1}(\omega)$
scales as $\omega^{-1/2}$ between $\omega \sim \Delta$ and $\omega \sim \omega_0$ such that, at these frequencies, $I_s(\omega) = \int d\omega [\tau^{-1}(\omega) - \tau^{-1}_n(\omega)]$ does not converge. Furthermore, at these frequencies, $1/\tau(\omega)$ is still smaller than $1/\tau_n(\omega)$. This result holds for all $\alpha < 1$ as one can straightforwardly verify. Only at $\omega > \omega_0$, $\tau^{-1}(\omega)$ finally becomes larger than $\tau^{-1}_n(\omega)$, and $I_s(\omega)$ converges. The convergence implies that the differential sum rule for $1/\tau(\omega)$ is again exactly satisfied; however it is exhausted only at frequencies that well exceed the pseudogap. We present the numerical results for $1/\tau(\omega)$ and $I_s(\omega)$ in Fig. 2a.

We now present the results for $\sigma_1(\omega)$ and $1/\tau(\omega)$ for spin-fluctuation mediated $d$-wave pairing. We obtained these results by solving a set of coupled Eliashberg equations for the spin-fermion model that describes the spin-fluctuation exchange at low energies [12]. We will demonstrate that, at low $T$, the behavior of the conductivity and the relaxation rate resembles that in a dirty BCS superconductor, while immediately below the pairing instability the system behavior is similar to that in the toy model for the pseudogap.

The spin-fermion model is characterized by a single dimensionless coupling constant $\lambda$ and a single overall energy $\omega_0$ that scales with the effective spin-fermion interaction [10]. We will also use a characteristic energy scale for the spin fluctuations $\omega_{sf} = \omega_0/4\lambda^2$. A fit to the NMR, angle-resolved photoemission spectroscopy, and neutron experiments yields $\lambda \sim 1-2$ near the optimal doping [10]. We refer the readers to Ref. [10] for the discussion of the applicability of the model to the cuprates and the justification of the Eliashberg approach at strong spin-fermion coupling despite the formal absence of the Migdal theorem. The application of this model to conductivity calculations requires extra care as $\lambda$ and $\omega_{sf}^{-1} = 4\lambda^2/\omega_0$ vary along the Fermi surface being the largest near hot spots. We, however, checked explicitly in earlier works that this variation is only relevant at low frequencies $\omega \sim \omega_{sf}$, while, at larger $\omega$, $\lambda$ and $\omega_{sf}$ appear only in a combination $\lambda^2 \omega_{sf}$ that is independent of the position at the Fermi surface. Furthermore, even at $\omega < \omega_{sf}$, the variation of $\lambda$ along the Fermi surface in optimally doped cuprates turns out to be modestly numerical ($\lambda$ changes by about a factor of 2 between hot and cold points [13]). This modest variation does not affect the physics and is within the uncertainty of $\lambda$. We neglect it in our analysis, present the results for both $\lambda = 1$ and $\lambda = 2$, and show that they are quite similar.

We begin with the normal state. In Fig. 3a we present our results for $1/\tau(\omega)$ and $I_s(\omega)$ at various $T$. For definiteness we set $\lambda = 2$. We see that $I_s(\omega)$ diverges at high frequencies, i.e., the differential sum rule is not satisfied. We checked analytically that this is caused by the $1/\omega$ behavior of the integrand in $I_s(\omega)$. In Fig. 3b we present the results for $\sigma_1(\omega)$ and $I_s(\omega)$ at various $T$. We see that $I_s(\omega)$ flattens at $\omega \approx 10\omega_{sf}$, but its value is still about 30% smaller than it should be for $\omega = \omega_0$. The full sum rule is exhausted only at unrealistically large $\omega \sim 10^3 \omega_{sf}$ (Ref. [10]), where the low-energy theory is clearly inapplicable. The weak convergence of $I_s(\omega)$ is related to the fact that over a wide frequency range $\sigma_1(\omega)$ is inversely proportional to $\omega$, and $I_s(\omega)$ increases as $\log \omega$ [10,14].

We next consider what happens below the pairing instability temperature $T_{ins} \sim 0.2\omega_0$ [15]. Earlier we and Schmalian found [12] that, at $T \leq T_{ins}$, the fermionic self-energy remains large at the smallest $\omega$ and smoothly evolves from its normal state value. It drops at the lowest $\omega$, due to a feedback from the pairing only below $T_c < T_{ins}$, and the difference between $T_{ins}$ and $T_c$ increases with increasing $\lambda$. This gradual behavior is qualitatively different from a dirty BCS superconductor; as in the latter the quasiparticle spectral function instantly drops to zero at frequencies below $\Delta$ due to a feedback from the pairing [7,8]. We conjectured that, at $T_c < T < T_{ins}$, fluctuations destroy coherent superconductivity, i.e., the system is in the pseudogap regime.

In Fig. 4 we present the results for $1/\tau(\omega)$ for two different $\lambda$ and three different temperatures: $T \ll T_c$, $T \approx T_c$, and $T = T_{ins}$, where $1/\tau(\omega)$ is the same as in the normal state. We see that, between $T_{ins}$ and $T_c$, $1/\tau(\omega)$ is nearly homogeneously suppressed, while between $T_c$ and $T \ll T_c$ it develops an overshoot at $\omega \approx 2\Delta$. The magnitude of the overshoot depends on the coupling and is larger at larger $\lambda$, when there is also a larger reduction of $1/\tau$ between $T_{ins}$ and $T_c$. Figure 4 also presents our results for the differential sum rule between $T \sim T_c$ and $T < T_c$ and between $T_{ins}$ and $T_c$. We see that between $T_{ins}$ and $T_c$ the spectral weight is just lost, while between $T_c$ and $T < T_c$ it is approximately conserved. The near conservation of the spectral weight particularly holds if the upper limit of the frequency integral is chosen close to $3-4\omega_0 \sim 10\Delta$. If the integration is extended to larger $\omega$, $I_s$ between $T_c$ and $T_c$ progressively increases, but Fig. 4 shows that the rate of variation of $I_s$ is very small compared to $I_s$ between $T_c$ and $T_{ins}$.

The conservation of the spectral weight between $T \ll T_c$ and $T \geq T_c$ and the loss of the spectral weight between $T_c$ and $T_{ins}$ are the main results of recent experimental analysis of optimally doped YBCO [2]. In these
The low frequency behavior of the pseudogap temperature is also consistent with this behavior with the strong feedback from the pairing quencies compared to the pairing gap, $D$. The temperatures between which $I_s$ was computed are indicated on the plots. Observe that the overshoot between the spectra of $1/\tau(\omega)$ develops only below $T_c$.

experiments, the frequency integration was performed up to 2500–3000 cm$^{-1}$ that is close to $10\Delta$. These results are reproduced in our analysis. For larger frequencies, the measured differential sum rule becomes less precise. This is also reproduced in our theory.

For completeness, in Fig. 5 we present the results for the conductivity. We see that $\sigma_1(\omega)$ keeps increasing at small $\omega$ between $T_{ins}$ and $T_c$. This indicates that the development of the pseudogap does not give rise to a suppression of the conductivity at the lowest frequencies. The latter is reduced only below $T_c$. To emphasize this point, we plot $\sigma_1(\omega)$ at a low $\omega$ vs $T$. The change of behavior at $T_c$ is clearly visible. The sensitivity of $\sigma_1(\omega = 0)$ to $T_c$ rather than to the pseudogap temperature is also consistent with the data [16]. The low frequency behavior of $\sigma_1(\omega = 0)$ well below $T_c$ is indeed not captured in our theory as it is predominantly determined by impurities [17]. Finally, we found both analytically and numerically that, at large $\omega$, $\sigma_1(\omega)$ again is sensitive to $T_c$ rather than $T_{ins}$ (the last panel in Fig. 5). This also agrees with the data [18].

To conclude, in this paper we considered the differential sum rule for the effective scattering rate $1/\tau(\omega)$ [the difference between the area under $1/\tau(\omega)$ for two different temperatures]. We argued that for spin-fluctuation mediated pairing, this sum rule is generally not an exact one, but is rather well satisfied below $T_c$ and is exhausted at frequencies compared to the pairing gap, $\Delta$. We identified this behavior with the strong feedback from the pairing on the fermionic self-energy. We found that in the pseudogap region, where feedback effects are small, $1/\tau(\omega)$ at $\omega = O(\Delta)$ is nearly homogeneously suppressed compared to the normal state, and the differential sum rule is not satisfied. We argued that this behavior as well as the behavior of $\sigma_1(\omega)$, is consistent with the experimental data for the cuprates.

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![Figure 4](https://example.com/fig4.png)

**FIG. 4.** The $1/\tau(\omega)$ and the differential sum rule $I_s$ for the spin-fermion model for $\lambda = 2$ ($\Delta \sim 0.3\omega$, $T_c \sim 0.3T_{ins}$) and $\lambda = 1$ ($\Delta \sim 0.2\omega$, $T_c \sim 0.5T_{ins}$). The temperatures between which $I_s$ was computed are indicated on the plots. Observe that the overshoot between the spectra of $1/\tau(\omega)$ develops only below $T_c$.

![Figure 5](https://example.com/fig5.png)

**FIG. 5.** The behavior of $\sigma_1(\omega)$ in the spin-fermion model below the pseudogap temperature $T_{ins}$ for $\lambda = 1$. The lower panels show the behavior of $\sigma_1(\omega) vs T$ at small and large frequencies for $\lambda = 1$. Observe that the changes in $\sigma_1$ are confined to $T_c$ rather than to $T_{ins}$. The behavior of $\sigma_1(\omega)$, is consistent with the experimental data for the cuprates.

[9] See also H. Westfahl and D. Morr, cond-mat/0002039.