Reverse process of usual optical analysis of boson-exchange superconductors: impurity effects on s- and d-wave superconductors

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Abstract
We performed a reverse process of the usual optical data analysis of boson-exchange superconductors. We calculated the optical self-energy from two (MMP and MMP + peak) input model electron-boson spectral density functions using Allen’s formula for one normal and two (s- and d-wave) superconducting cases. We obtained the optical constants including the optical conductivity and the dynamic dielectric function from the optical self-energy using an extended Drude model, and finally calculated the reflectance spectrum. Furthermore, to investigate impurity effects on optical quantities we added various levels of impurities (from the clean to the dirty limit) in the optical self-energy and performed the same reverse process to obtain the optical conductivity, the dielectric function, and reflectance. From these optical constants obtained from the reverse process we extracted the impurity-dependent superfluid densities for two superconducting cases using two independent methods (the Ferrel–Glover–Tinkham sum rule and the extrapolation to zero frequency of $-\epsilon_1(\omega)\omega^2$); we found that a certain level of impurities is necessary to get a good agreement on results obtained by the two methods. We observed that impurities give similar effects on various optical constants of s- and d-wave superconductors; the greater the impurities the more distinct the gap feature and the lower the superfluid density. However, the s-wave superconductor gives the superconducting gap feature more clearly than the d-wave superconductor because in the d-wave superconductors the optical quantities are averaged over the anisotropic Fermi surface. Our results supply helpful information to see how characteristic features of the electron-boson spectral function and the s- and d-wave superconducting gaps appear in various optical constants including raw reflectance spectrum. Our study may help with a thorough understanding of the usual optical analysis process. Further systematic study of experimental data collected at various conditions using the optical analysis process will help to reveal the origin of the mediated boson in the boson-exchange superconductors.

Keywords: boson-exchange superconductors, optical analysis, impurity effects

(Some figures may appear in colour only in the online journal)
systems including boson-exchange superconductors [4] can be analyzed as follows: first, a Kramers–Kronig analysis [5] is performed to obtain the optical constants including the optical conductivity. Then an extended Drude model is applied to get the optical self-energy [6] which can carry information of the correlations and is in one-to-one correspondence with the well-known quasiparticle self-energy [7–9]. Extended Allen’s formulas [10–13] are used for getting more fundamental quantity, the electron-boson spectral density function, from the optical self-energy. The Allen’s formulas relate linearly the optical self-energy to the electron-boson spectral density function. The electron-boson spectral density function can be obtained usually by solving numerically [14–16] the extended Allen’s formula which is an integral equation. Further systematic optical studies provide temperature and doping-dependent properties of the electron-boson spectral density function of high temperature superconductors [17, 18]. It has been known that the electron-boson spectral functions of cuprates obtained from various spectroscopic experimental (angle resolved photoemission (ARPES) [19], (scanning) tunneling (STS) [20, 21], inelastic neutron scattering (INS), Raman [22], and infrared (IR) [17, 18, 23]) techniques consist of two components: one broad background and a sharp mode. While the background shows small doping dependence the sharp mode shows strong doping and temperature dependencies [2]. The sharp mode appears and grows with decreasing temperature by consuming the spectral weight of the high temperature broad background [2, 6, 17, 18, 20–22, 24–29]. The sharp mode is known to be associated with the well-known magnetic resonance mode [30]. As the sample temperature reduces the sharp mode starts to appear above the superconducting transition temperature ($T_c$) in underdoped cuprates and at $T_c$ in the optimally and overdoped cuprates [2, 6, 24–26]. Many researchers believe that the high temperature superconductors including cuprates are boson-exchange superconductors as the conventional phonon-mediated superconductors and the electron-boson spectral functions can carry information of the bonding force of Cooper pairs in the high temperature superconductors. So the electron-boson spectral density function observed in cuprates has been known as the superconducting pairing glue function [6, 16, 20, 23, 31–34]. Figuring out the microscopic origin of the boson involved in the bonding force is one of the most important problems in contemporary condensed matter physics. We believe that the electron-boson density functions obtained by various experimental techniques will play a very important role in solving the problem.

In this paper, we performed a reverse process of the usual optical analysis process described above to better understand the usual process and investigate impurity effects on optical quantities. We started from an impurity-free pure (or ideal) system, and then introduced elastic impurities into the system, and finally examined the impurity effects on the optical constants including reflectance. To achieve this result we introduced two input model electron-boson spectral density functions, which are modeled with general shapes of the electron-boson spectral density functions observed by various spectroscopic experiments [2], and then calculated the imaginary part of the optical self-energy (or the optical scattering rate) from the input spectral density functions using the Allen’s formulas [10, 15]. One of the two input model spectral density functions is the phenomenological antiferromagnetic spin fluctuation [35], which is proposed by Millis, Monien, and Pines (MMP) and is also known as an MMP mode. The other is a combination of the MMP mode and a sharp Gaussian mode which is modeled on an observed electron-boson spectral function in a cuprate system at low temperature below the superconducting transition temperature [2, 17]. We considered three different cases: one normal and two different ($s$- and $d$-wave) types of superconducting states to investigate superconducting gap symmetry effects. Furthermore, we used a Kramers–Kronig relation to obtain the real part of the optical self-energy from the imaginary part (or the optical scattering rate). We calculated the optical conductivity using the extended Drude formalism [6, 36]. We calculated the dynamic dielectric function using the relation between optical constants and then finally obtained the normal incident reflectance spectrum using the Fresnel equations.

Impurities are not avoidable experimentally, especially for doped materials with substitution. The impurity effect on physical quantities is an important physical issue especially for unconventional superconductors including $d$-wave superconductors [37, 38]. Most experimental results may be contaminated by the impurities in the material systems or sometimes impurities are introduced experimentally to study their effects on the physical quantities [39]. There may be physical issues of which one may need to be aware, such as impurity effects, for the analysis of optical spectra. For example, violation of the Ferrel–Glover–Tinkham (FGT) sum rule [40, 41] in certain superconductors can be interpreted as the lowering kinetic energy which comes from contributions of both the condensation energy and the potential energy increase due to larger Coulomb repulsion in the Cooper pairs [42–44]. So we added several different impurity scattering rates (from the clean to the dirty limit) to the impurity-free optical scattering rate. We performed the same reverse procedure to obtain the optical conductivities, the dynamic dielectric constants and reflectance spectra from the optical self-energies which contain impurities. We discuss impurity effects on other optical constants including reflectance. Our results show that the measured reflectance spectrum and other optical constants clearly show important characteristic features of the input electron-boson spectral function and the superconducting gap feature. This may be quite useful because one can see important features even in raw reflectance spectra without going through a full optical analysis process. And then we investigate impurity effects on the physical quantities including the partial sum, spectral weight redistribution by the Holstein process, and the superfluid density which can be obtained from the optical conductivity and the dielectric function. Our results show that impurities may have an affect on the FGT sum rule; one may need a high enough level of impurities in the material systems to hold the FGT sum rule. We observed that the absolute superfluid density depends on the impurity level; the greater the impurities the lower the superfluid density. We
compared our results obtained by the reverse process with experimental data of optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ and observed good agreements for all optical constants considered including reflectance. These good agreements confirm that our reverse process is reliable. We could thoroughly understand the usual optical process through this study. We believe that further study in this direction may help to reveal the microscopic origin of the exchange boson in the high temperature superconductors as in the conventional superconductors by collecting more experimental data and applying the optical analysis process to them to obtain various physical properties of the exchange boson.

This paper is structured with the following sections. In section 2 we introduce general theoretical formalisms which we used in this paper. In section 3 we show and discuss our results obtained using the formalisms. In section 4 we summarize our results with some useful comments.

2. Theoretical formalisms

Theoretical analysis methods of measured optical data of s-wave and d-wave superconductors have been considerably developed [2, 4]. Important progress, which has been successful for conventional superconductors [45, 46], is the boson-exchange model approach to study unconventional superconductors [2]. One can extract the electron-boson spectral density function from measured optical self-energy [17, 18, 47, 48]. The optical self-energy is related to the optical scattering rate [1 -wave SC]

\[
\Sigma_{\text{opt}}(\omega) = \frac{1}{\tau_{\text{opt}}(\omega)} = \int_0^\infty d\Omega I^2(\omega) K(\omega, \Omega) + \frac{1}{\tau_{\text{imp}}(\omega)}
\]

where \(1/\tau_{\text{opt}}(\omega)\) is the optical scattering rate, \(K(\omega, \Omega)\) is the kernel for the Allen’s integral equation and \(1/\tau_{\text{imp}}(\omega)\) is the impurity scattering rate. We have different kernels for the normal state (here \(T = 0\) case) and s- and d-wave superconducting states. The kernels can be written as follows:

\[
K(\omega, \Omega) = 2\pi \left( 1 - \frac{\Omega}{\omega} \right) \theta(\omega - \Omega) \quad \text{(for normal state)}
\]

\[
= 2\pi \left( 1 - \frac{\Omega}{\omega} \right) \theta(\omega - 2\Delta_0 - \Omega)
\]

\[
\times E \left( 1 - \frac{4\Delta_0^2}{(\omega - \Omega)^2} \right) \quad \text{(for s-wave SC)}
\]

\[
\tau_{\text{imp}}(\omega) = \frac{1}{\tau_{\text{imp}}(\omega)} = \int_0^\infty d\Omega I^2(\omega) \chi(\omega) \pi K(\omega, \Omega) \quad \text{(for normal state)}
\]

\[
= 2\pi \left( \frac{\Omega}{\omega} \right) \theta(\omega - 2\Delta_0(\theta) - \Omega)
\]

\[
\times E \left( 1 - \frac{4\Delta_0^2(\theta)^2}{(\omega - \Omega)^2} \right) \quad \text{(for d-wave SC)}
\]

where \(\theta(x)\) is the Heaviside step function (i.e. 1 for \(x \geq 0\) and 0 for \(x < 0\)), \(E(x)\) is the complete elliptic integral of the second kind, and \((\cdot)\) stands for the angular average over \([0, \pi/4]\). \(\Delta_0\) and \(\Delta_0(\theta)\) are the superconducting gaps for s- and d-wave symmetry cases, respectively.

The impurity scattering rates \(1/\tau_{\text{imp}}(\omega)\) for normal and s- and d-wave superconducting states can be described as follows [10, 15]:

\[
\frac{1}{\tau_{\text{imp}}(\omega)} = \frac{1}{\tau_{\text{imp}}(\omega)} \quad \text{(for normal state)}
\]

\[
= \frac{1}{\tau_{\text{imp}}(\omega)} E \left( 1 - \frac{4\Delta_0^2}{\omega^2} \right) \quad \text{(for s-wave SC)}
\]

\[
= \frac{1}{\tau_{\text{imp}}(\omega)} \left( E \left( 1 - \frac{4\Delta_0^2(\theta)^2}{\omega^2} \right) \right) \quad \text{(for d-wave SC)}
\]

(3)

where \(1/\tau_{\text{imp}}\) is the impurity scattering rate, which is a constant. We note that for the s-wave superconductors the impurity scattering rates are frequency dependent.

In the extended Drude model formalism [6], which can describe correlated charge carriers, we can relate the optical conductivity, \(\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)\) to the optical self-energy, \(\Sigma_{\text{opt}}(\omega) = \Sigma_1(\omega) + i\Sigma_2(\omega)\) as follows [6]:

\[
\sigma(\omega) = \frac{\Omega_p}{4\pi} \frac{1}{\omega} \quad \text{or}
\]

\[
-2\Sigma_{\text{opt}}(\omega) = \frac{\Omega_p}{4\pi} \frac{1}{\sigma(\omega) - \omega}
\]

(4)

where \(\Omega_p\) is the plasma frequency of charge carriers. The imaginary and real parts of the optical self-energy can be related respectively to the optical scattering rate \(1/\tau_{\text{opt}}(\omega)\) and the optical mass enhancement factor \(\lambda_{\text{opt}}(\omega)\) as \(-2\Sigma_2(\omega) = 1/\tau_{\text{opt}}(\omega)\) and \(-2\Sigma_1(\omega) = \lambda_{\text{opt}}(\omega)\equiv [m^*(\omega)/m_e - 1]\omega\), where \(m^*(\omega)\) and \(m_e\) are the enhanced mass from the correlation and the electron mass, respectively. We note that the real and imaginary parts of the optical self-energy form a Kramers–Kronig pair. Therefore, if we know one of them we can get the other using the Kramers–Kronig relation between them.
In normal state at \( T = 0 \), \(-2\Sigma_1^{op}(\omega)\) can be written analytically as follows [8, 10, 49]:

\[
-2\Sigma_1^{op}(\omega) = 2 \int_0^\infty \text{d}\Omega I^2(\Omega) \left[ \frac{\Omega}{\omega} \ln \left| \frac{\Omega^2 - \omega^2}{\Omega \omega} \right| + \ln \left| \frac{\Omega + \omega}{\Omega - \omega} \right| \right].
\]

We introduce an interesting relation at zero frequency as follows:

\[
\lambda^{op}(0) = \lim_{\omega \to 0} \frac{-2\Sigma_1^{op}(\omega)}{\omega} = \lim_{\omega \to 0} \frac{\text{d}[-2\Sigma_1^{op}(\omega)]}{\text{d}\omega} = 2 \int_0^\infty \text{d}\Omega I^2(\Omega) \frac{\Omega}{\Omega} \equiv \lambda.
\]

The second step in the first equation is obtained by applying the L'Hopital's rule. The last equation is called the coupling constant which we denote as \( \lambda \) (see figure 5) and \( \omega_0 \) is the cutoff frequency.

The dynamic dielectric function \( \epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) \) can be related to the optical conductivity as follows:

\[
\epsilon(\omega) = \epsilon_{H} + 1 + \frac{4\pi}{\omega} \bar{\sigma}(\omega)
\]

where \( \epsilon_{H} \) is the high frequency background dielectric constant.

Finally, one can calculate the single bounce reflectance \([R(\omega)]\) at normal incidence from the dynamic dielectric function using the Fresnel equations and the relation between optical constants [5]. The reflectance can be described as follows:

\[
R(\omega) = \left| \frac{\tilde{N}(\omega) - 1}{\tilde{N}(\omega) + 1} \right|^2 = \left| \frac{\sqrt{\epsilon(\omega) - 1}}{\sqrt{\epsilon(\omega) + 1}} \right|^2 = \sqrt{\epsilon_1^2 + \epsilon_2^2} - \sqrt{2(\epsilon_1 + \sqrt{\epsilon_1^2 + \epsilon_2^2}) + 1} = \frac{\epsilon_1^2 + \epsilon_2^2 + \sqrt{2(\epsilon_1 + \sqrt{\epsilon_1^2 + \epsilon_2^2}) + 1}}{\epsilon_1^2 + \epsilon_2^2 + \sqrt{2(\epsilon_1 + \sqrt{\epsilon_1^2 + \epsilon_2^2}) + 1}}.
\]

where \( \tilde{N} \) is the complex index of refraction. \( \tilde{N} = n + ik = \sqrt{\epsilon} \), where \( n \) and \( k \) are called the index of refraction and the extinction coefficient, respectively. We note that if a sample is not transparent its reflectance is the single bounce one. Here \( \epsilon_0 \) is the dielectric constant of the vacuum or air. In the following section we will show and discuss the results of our calculations using the formulas of the reverse process.

3. Results and discussions

3.1. Model electron-boson spectral density, \( I^2\chi(\omega) \)

For our calculations of the reverse process we started with two input model electron-boson spectral density functions, \( I^2\chi(\omega) \), which are based on experimental results of hole-doped cuprates [2]. One model function consists of a broad mode, of which shape is a phenomenological antiferromagnetic spin fluctuation proposed by Millis, Monien, and Pines [35]. This is called the MMP model and described as \( I^2\chi(\omega) = \frac{\Delta_{\omega}}{\omega^{2+\alpha_{\omega_{0}}} + \frac{\Lambda_\rho}{\sqrt{2\pi}(d/2.35)^{2}}\exp\left[-(\omega-\omega_0)^2/4\right]} \), where \( \Delta_\omega \) (= 50 meV) and \( \omega_{0_{\omega}} \) (= 60 meV) are the amplitude and the characteristic frequency of the spin fluctuation mode, respectively. The MMP model has a maximum at \( \omega_{0_{\omega}} \) and is displayed in the upper frame (red solid line) of figure 1. The other model spectral density function consists of two components: the MMP and a relatively sharp Gaussian peak. The Gaussian peak is modeled as the magnetic resonance mode observed by an inelastic neutron scattering [24, 30] and is called the optical resonance mode [6, 18]. We denote this model as an MMP + peak model and describe it as \( I^2\chi(\omega) = \frac{\Delta_{\omega}}{\omega^{2+\alpha_{\omega_{0}}} + \frac{\Lambda_\rho}{\sqrt{2\pi}(d/2.35)^{2}}\exp\left[-(\omega-\omega_0)^2/4\right]} \), where \( \Lambda_\rho \) (= 50 meV), \( \omega_{0_{\rho}} \) (= 30 meV), and \( d \) (= 10 meV) are the amplitude, the peak frequency, and the width of the Gaussian mode, respectively. The MMP + peak model is displayed in the upper frame (blue dashed line) of figure 1 along with the MMP model (red solid line).

The physical quantities related to the electron-boson spectral density function are the coupling constant \( \lambda \equiv 2 \int_0^\infty \frac{I^2\chi(\Omega)/\Omega}{\Omega} \text{d}\Omega \), see also in equation (6)), the average electron-boson frequency \( \langle \omega_{0_{\omega}} \rangle \), and the maximum superconducting transition temperature \( T_{c}\text{max} \). The maximum superconducting transition temperature can be calculated in a generalized McMillan formalism [4, 23], which can be}

![Figure 1. Two input model electron-boson spectral density functions (MMP and MMP + peak) in the upper frame, the calculated optical scattering rates for the three cases (one normal and two SC cases) in the lower frame, and impurity scattering rates for the three cases in the inset (see in the text).](image-url)
Table 1. The calculated coupling constant ($\lambda$), the average frequency ($\omega_{\text{th}}$), and the maximum superconducting temperature ($T_{\text{max}}$) of our two model input electron-boson spectral density function (see in the text).

| Physical quantities | $\lambda$ | $\omega_{\text{th}}$ (meV) | $T_{\text{max}}$ (K) |
|--------------------|-----------|-----------------------------|-----------------------|
| MMP model          | 2.424     | 50.67                       | 161.8                 |
| MMP + peak model   | 5.830     | 36.61                       | 148.8                 |

described as follows:

$$k_B T_{\text{c max}} \simeq 1.13 \hbar \omega_{\text{th}} \exp \left[-\frac{1 + \lambda}{\lambda}\right]$$  \hspace{1cm} (9)

where $k_B$ is the Boltzmann constant, $\hbar$ is the reduced Planck’s constant, and $\omega_{\text{th}}$ is the logarithmically averaged electron-boson frequency which is defined as $\omega_{\text{th}} = \exp \left\{ (2/\lambda) \int_{0}^{\infty} \ln \Omega \, I^2 \chi(\Omega) / \Omega \, d\Omega \right\}$ where $\omega_c = 600 \text{ meV}$. In table 1 we show the calculated values of the coupling constant, the average electron-boson frequency, and the maximum superconducting transition temperature. We note that the superconducting transition temperature is influenced mostly by the average frequency. We note that these values in the table are comparable to reported ones for cuprates [17, 18].

3.2. Reverse process

Then we performed the reverse process starting from the two input electron-boson spectral density functions, $I^2 \chi(\omega)$. We obtained the imaginary part of the optical self-energy for the MMP and the MMP + peak, respectively) with the fractions $[\lambda/(1 + \lambda)] = 0.708$ and 0.854 for the MMP and the MMP + peak, respectively) of the total spectral weight, where $\lambda$ is the coupling constant (see table 1). The total spectral weight ($W_{\text{t total}}$) is $\pi/120$ times the plasma frequency squared, i.e. $W_{\text{t total}} = \int_{0}^{\infty} \sigma_1(\omega) \, d\omega = (\pi/120) \Omega_p^2$, where $\sigma_1(\omega)$ is in units of $\Omega^{-1} \text{ cm}^{-1}$ and $\Omega_p$ in units of $\text{ cm}^{-1}$. The total spectral weights for all three cases should be the same since we used the same plasma frequency for the three cases in the extended Drude model. We compared the incoherent Holstein boson-assisted absorption spectral weights ($\equiv 4.6 \times 10^6$ and $5.6 \times 10^6 \text{ cm}^{-1}$) obtained from the integration of the optical conductivity for the MMP and the MMP + peak, respectively) with the fractions $[\lambda/(1 + \lambda)] = 0.708$ and 0.854 for the MMP and the MMP + peak, respectively. Here we took the coupling constants ($\lambda$) for the MMP and MMP + peak from table 1. The resulting incoherent spectral weights obtained from two different ways show good agreements for both input $I^2 \chi(\omega)$ cases. In $\sigma_2(\omega)$ we can see that the sharp Gaussian peak in the MMP + peak model appears as very prominent kinks (abrupt slope changes) near $\omega_p + 2\Delta_0$ (i.e. 90 meV) for two SC states and a kink near $\omega_p$ (i.e. 30 meV) for the normal state. At the same frequencies where the kinks are, we can see sharp rises in the real part of the optical conductivity, $\sigma_2(\omega)$. So we can clearly observe the characteristic features of $I^2 \chi(\omega)$ in the optical conductivity.

3.3. Impurity effects

Then we added various impurity scattering rates (1, 5, 15, and 30 meV) to the impurity-free optical scattering rates as in equations (1)–(3) and used the same Kramers–Kronig relation to obtain the real parts of the optical self-energy. In figure 2 we display the optical self-energy for two representative impurity scattering rates, $1/\tau_{\text{imp}} = 1.0$ and 30.0 meV, which can be the clean ($1/\tau_{\text{imp}} \ll 2\Delta_0$) and the dirty ($1/\tau_{\text{imp}} \leq 2\Delta_0$) limit for $s$-wave and approximately $d$-wave superconductors, respectively. We clearly observe a very sharp peak (marked
Figure 2. The real (lower left frame) and imaginary (upper left frame) parts of the optical self-energy for all three cases are shown in the left frames. The real parts are obtained from corresponding imaginary parts using a Kramers–Kronig relation. The real (upper right frame) and imaginary (lower right frame) parts of the optical conductivity are obtained using the extended Drude formalism for all three cases and displayed in the right frames.

with a red arrow in the inset of the right lower frame) in the real part of the optical self-energy for the dirty limit case (1/τ\text{imp} = 30.0 meV) at 2Δ₀ (i.e. 60 meV) for s-wave SC case. At the same energy there is a sharp rise in the imaginary part of the optical self-energy as shown in the inset of the right upper frame. The sharp features seem to exist in the d-wave SC case but they are significantly suppressed; we can see it if we look very carefully near 2Δ₀ (i.e. 60 meV). This sharp feature gets more pronounced as the impurity level increases, i.e. this feature can be induced by impurities. The sharp feature may not be observed in d-wave superconductors by the infrared spectroscopic technique, which measures the averaged response over the anisotropic Fermi surface (or the k space). But a similar impurity-induced sharp feature was observed in Bi₂Sr₂CaCu₂O₈⁺δ (a d-wave superconductor) by high-resolution ARPES [28, 51, 52]. This feature showed strong temperature and momentum dependencies. It was interpreted theoretically as a result due to forward scattering in the d-wave cuprates [53].

We calculate the optical conductivity from the optical self-energy using the extended Drude formula [see equation (5)] with the same plasma frequency (Ωₚ = 2.0 eV) at various impurity scattering rates (1, 5, 15, and 30 meV). In figure 4 we display the calculated real parts of the optical conductivity and the real parts of the dynamic dielectric function for two representative impurity scattering rates, 1/τ\text{imp} = 1.0 and 30.0 meV. We display the real parts (dot–dashed black lines) of the corresponding Drude optical conductivity in the upper frames. The Drude conductivity is completely coherent; there is no incoherent Holstein boson-assisted absorption since the charge carriers are essential free (or λ = 0). In other words the optical self-energy is zero, i.e. Σ^{\text{op}}(ω) = 0, only elastic impurity scattering exists. For the normal cases (red solid and red dashed lines) we can see that the additional spectral weights appear at the low frequency region in the optical conductivity compared with corresponding spectra for 1/τ\text{imp} = 0 (see in the upper right frame of figure 2). Now the coherent portion of the total spectral weight (i.e. W_{\text{s, total}}/(1 + λ)) also shows up in the conductivity spectra in a finite frequency range; the coherent spectral weight was confined at zero frequency for 1/τ\text{imp} = 0. For 1/τ\text{imp} = 30.0 meV (or the dirty limit) case we can see the gap features (i.e. sharp rises) at 2Δ₀ (i.e. 60 meV) in σ₁(ω) of the s-wave superconductors. For the d-wave SC cases we can see the gap features (i.e. sharp rises) at 2Δ₀ but the features are suppressed significantly by the anisotropic SC gap. For 1/τ\text{imp} = 1.0 meV (or the clean limit) case those SC gap features cannot be seen very clearly.

In the optical conductivity calculated by the reverse process we can observe the Gaussian peak in I²χ(ω) which appears as a dip near ωₚ + 2Δ₀ (i.e. 90 meV) for both SC cases and near ωₚ (i.e. 30 meV) for the normal case. In the lower frame of figure 4 we display −ε₁(ω)ω^2 for all three cases. In principle this quantity at zero frequency gives the superfluid plasma frequency squared
Figure 3. The real and imaginary parts of the optical self-energy with two representative impurity scattering rates ($1/\tau_{\text{imp}}$), 1.0 meV (a clean limit) and 30.0 meV (a dirty limit). In the insets magnified views of the optical self-energy for the dirty limit case in the low energy region are displayed. The red arrow indicates a sharp peak in the real part of the optical self-energy which is induced by the impurities.

$(\omega_{\text{sp}}^2)$, i.e. $\lim_{\omega \rightarrow 0} [-\varepsilon_1(\omega)\omega^2] = \omega_{\text{sp}}^2$. We can clearly see the superfluid plasma frequency decreases as the impurity scattering rate increases for both superconducting cases; this result is expected for a superconductor moving into the dirty limit [37, 38]. The resulting superfluid plasma frequencies for various levels of impurities are calculated and shown in figure 6. For the normal case this quantity should be zero i.e. $\lim_{\omega \rightarrow 0} [-\varepsilon_1(\omega)\omega^2] = 0$ since there is no superfluid current. In $-\varepsilon_1(\omega)\omega^2$ the SC gap feature appears as a very sharp dip at $2\Delta_0$ (i.e. 60 meV). We can clearly see the sharp Gaussian peak feature in the electron-boson spectral function near $\omega_p + 2\Delta_0$ (90 meV) for both superconducting states and near $\omega_p$ (i.e. 30 meV) for the normal state, which appears as broad valleys.

Then we extract the superfluid plasma frequency with another method. In this method we monitor the spectral weight redistribution (or the missing spectral weight) when the system experiences a phase transition from normal to superconducting states. This method originated from the Ferrel–Glover–Tinkham (FGT) sum rule [40, 41]. We denote the superfluid plasma frequency extracted using this method as $\omega_{\text{sp, FGT}}$ and call it the FGT superfluid plasma frequency. We can describe $\omega_{\text{sp, FGT}}$ in the FGT sum rule formalism as follows:

$$\omega_{\text{sp, FGT}}^2 = \frac{120}{\pi} \left[ W_{s,N}(\omega) - W_{s,SC}(\omega) \right]$$  \hspace{1cm} (10)

where $W_{s,N}(\omega)$ and $W_{s,SC}(\omega)$ are the spectral weights of normal and superconducting states, respectively. We note that $\omega_{\text{sp, FGT}}^2(\omega)$ is in units of cm$^{-1}$ and $W_{s}(\omega)$ in units of $\Omega^{-1}$. For both normal and superconducting states the spectral weight is defined as $W_{s}(\omega) = \int_{-\infty}^{\infty} \sigma_1(\omega') d\omega'$. In the upper frames of figure 5 we display the spectral weights ($W_s(\omega)$) for one normal and the two SC cases with two input model $I^2\chi(\omega)$ and three representative impurity scattering rates (0.0, 1.0, and 30.0 meV) in an extended spectral range (up to 6.0 eV). The corresponding $\omega_{\text{sp, FGT}}(\omega)$ for the three representative impurity scattering rates are calculated and displayed in the lower frames. Interestingly, we have a finite superfluid plasma frequency for $1/\tau_{\text{imp}} = 0.0$ meV case, which indicates that some portion of the incoherent Holstein boson-assisted absorption is condensed into the superfluid state. At the same time we can see that the total coherent portion of the spectral weight is smaller than the superfluid spectral weight for $1/\tau_{\text{imp}} = 0.0$ meV case, i.e. $W_{s, \text{total}}[1/(1+\lambda)] < W_{s, \text{FGT}} = (\pi/120) \Omega_{\text{sp, FGT}}^2$ for both input $I^2\chi(\omega)$. This supports the idea that some incoherent Holstein spectral weight was condensed into the superfluid density. Since there is an overshot in the FGT superfluid plasma frequency which extends up to around 2000 cm$^{-1}$ a reasonable estimate for the cutoff frequency for the FGT plasma frequency can be around 2000 cm$^{-1}$.

In figure 6 we display the superfluid plasma frequencies obtained with two different methods as a function of the
Figure 4. Calculated real parts of the optical conductivity $[\sigma_1(\omega)]$ and real parts of the dynamic dielectric function $[\epsilon_1(\omega)]$ times-\(\omega^2\) for all three cases with two different input $I^2\chi(\omega)$ with two representative impurity scattering rates ($1/\tau_{\text{imp}}$), 1.0 meV and 30.0 meV. We show the real part of the optical conductivity spectra of the Drude modes (black dash–dotted lines) with corresponding impurity scattering rates.

Figure 5. The partial sum $[W_s(\omega)]$ and the difference between normal and superconducting states, $W_{s,N}(\omega) - W_{s,\text{SC}}(\omega)$, for all three cases with two different input $I^2\chi(\omega)$ with three representative impurity scattering rates ($1/\tau_{\text{imp}}$), 0.0, 1.0 and 30.0 meV. We show the partial sums of the Drude modes (black dash–dotted lines) with corresponding impurity scattering rate. We note that for $1/\tau_{\text{imp}} = 0$ meV there is no spectral weight at the finite frequency region.
Figure 6. Impurity-dependent superfluid plasma frequencies obtained by two different methods (see in the text) for two different superconducting gap types (s-wave: upper frame and d-wave: lower frame) with the MMP and MMP + peak input $I^2\chi(\omega)$. 

The plasma frequencies obtained using $\Omega^{2}_{sp} = \lim_{\omega \to 0}[-\epsilon_1(\omega)\omega^2]$ are shown with solid symbols and those obtained using $\Omega^{2}_{FGT}(\omega) = \frac{120}{\pi}[W_{s,N}(\omega) - W_{s,SC}(\omega)]$ are displayed with open symbols. In low impurity scattering rates (or in the clean limit) below $1/\tau_{imp} = 5.0$ meV $\Omega^{2}_{FGT}(\omega)$ decreases very quickly with reducing the impurity scattering rate because the coherent portion is too narrow to be taken into account completely. This means that to get a good agreement between the two methods the system should contain a high enough level of impurities in order to make the coherent portion broad enough. But in high impurity scattering rates (or in the dirty limit) above 15.0 meV results from both methods agree quite well with each other. We observe that the superfluid plasma frequency depends on the impurity scattering rate; as the impurity scattering rate increases the superfluid plasma frequency gradually decreases. The difference between the two superfluid plasma frequencies obtained by the two methods can be considered as an uncertainty for the FGT superfluid plasma frequency. We observe that the superfluid plasma frequency of a system with the MMP + peak in $I^2\chi(\omega)$ is more robust against the impurities than that with the MMP alone in $I^2\chi(\omega)$. Interestingly, the superfluid plasma frequencies of s-wave superconductors seem to be more robust against the impurities than d-wave ones.

Eventually, we calculated reflectance spectra $|R(\omega)|$ using the Fresnel equation with the dynamic dielectric functions [see equation (8)] with $\epsilon_H = 1.0$. We note that the calculated reflectance spectrum is at normal incidence. In figure 7 we display the calculated reflectance spectra for two representative impurity scattering rates ($1/\tau_{imp} = 1.0$ and 30.0 meV). We also display Drude reflectance spectra (dash–dotted lines) with corresponding impurity scattering rates. We can see that correlated electron systems show much suppressed reflectance below the plasma frequency ($\Omega_p = 2.0$ eV) compared with the free electron (or simple Drude) system. In the insets we show magnified views of reflectance spectra in the low frequency region. For $1/\tau_{imp} = 30.0$ meV the reflectance spectra of the s-wave SC case show clearly the superconducting gap feature at $2\Delta_0$ (i.e. 60 meV); below the energy the reflectance becomes essentially 1.0. For the d-wave SC case the gap feature is significantly suppressed; the reflectance becomes 1.0 at $\omega = 0$. We can see characteristic features which are caused by the input $I^2\chi(\omega)$. To see those features more clearly we compare reflectance spectra with the corresponding optical scattering rates; we display $1 - R(\omega)$ and $1/\tau_{opt}(\omega)$ in figure 8. Those two spectra look quite similar to each other. To show the similarity explicitly is not trivial since the reflectance is quite a complicated quantity theoretically. However, the
similarity can be understood roughly as follows: in general at the low frequency region a low scattering rate gives high conductivity which results in high $R(\omega)$ (or low $1 - R(\omega)$) and vice versa for a high scattering rate. So roughly one can say that $1/\tau_{\text{op}}(\omega) \propto 1 - R(\omega)$. Therefore, one may be able to see characteristic features of $I^2\chi(\omega)$ as well as the gap features in the raw measured reflectance spectrum as can be seen in the optical scattering rate. We note that thermal excitations may smear the distinction of the features and/or shift the position of the SC gap features.

3.4. Comparison with experimental data

We compared measured experimental data with the corresponding optical data obtained by the reverse process. In figure 9 we display measured reflectance data of a $d$-wave superconductor, optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi-2212) with $T_c = 96$ K, at $T = 27$ K (superconducting state) and 102 K (normal state) and optical constants obtained using the usual optical data analysis \[27\] in (a)-(f) frames and the corresponding optical constants including reflectance obtained from the reverse process for $d$-wave SC case with the MMP + peak model $I^2\chi(\omega)$ for $1/\tau_{\text{imp}} = 1.0$ and 30.0 meV in (g)-(l) frames. In (b) and (h) frames we can see that the results with $1/\tau_{\text{imp}} = 30.0$ meV show better agreements to the experimental data, which indicate that certain impurities caused by defects and/or thermal excitations exist in the experimental data. The experimental data would show temperature smearing effects from thermal excitations. Overall, all optical data displayed show quite good agreements even though experimental data are at finite temperatures while our calculations are done at zero temperature. We note that the electron-boson spectral function of Bi-2212 shows an additional intrinsic temperature-dependent evolution \[2, 18\]. We note that in the calculations we used the same input $I^2\chi(\omega)$ for both normal and superconducting states and for $1/\tau_{\text{imp}} = 1.0$ and 30.0 meV. We note that the real part of the optical self-energy shows relatively small impurity dependence. Actually, for the normal case $-2\Sigma_{i\omega n}^\text{op}(\omega)$ should not depend on the impurity level at all since a frequency-independent impurity scattering rate is added and its Kramers–Kronig counterpart is essentially zero. However, for superconducting cases since the impurity scattering rates show frequency dependence near $2\Delta_0$ their Kramers–Kronig counterparts are not zero any more. This gives the difference between $-2\Sigma_{i\omega n}^\text{op}(\omega)$ obtained with different impurity scattering rates near $2\Delta_0$. While the positions of the peaks of calculated and measured $-2\Sigma_{i\omega n}^\text{op}(\omega)$ have similar energies (i.e. 100 meV in frame (e) and 90 meV in frame (k)) the peaks of two (experimentally obtained and the input) $I^2\chi(\omega)$ are located at quite different energies (i.e. 60 meV in frame (f) and 30 meV in frame (l)). This difference comes from different superconducting energy gaps (i.e. $\Delta_0 \simeq 20$ meV for experimental data and $\Delta_0 = 30$ meV for the calculated ones). As mentioned in section 3.2 the peak in $-2\Sigma_{i\omega n}^\text{op}(\omega)$ is located at $\omega_p + 2\Delta_0$. So we can understand that 100 meV $\simeq 60$ meV+$2\times20$ meV for the peak in experimental data (frame (e)) and 90 meV = $30$ meV + $2 \times 30$ meV for the peak in the calculated one (frame (k)). These good agreements confirm that our reverse process is quite reliable.

![Figure 8. Comparison of the optical scattering rate (1/τ_{op}(ω)) and 1 - R(ω).](image-url)
4. Conclusions

In this study we have performed a reverse process of the usual process for optical data analysis. The reverse process is as follows: we started with the input model electron-boson spectral function, $I^2 \chi(\omega)$. We obtained the imaginary part of the optical self-energy using Allen’s formulas, the real part of the optical self-energy using a Kramers–Kronig relation, the optical conductivity using the extended Drude model, other optical constants using well-known relations between optical constants, and eventually reflectance using the Fresnel equations. We applied this reverse process to three cases (one normal and $s$- and $d$-superconducting cases with the superconducting gap $\Delta_0 = 30$ meV) with two (MMP and MMP + peak) input model $I^2 \chi(\omega)$ which are based on the reported experimental results. Since impurities are not avoidable experimentally we included various levels of impurities (from the clean to the dirty limit: $1/\tau_{\text{imp}} = 0 ~ 30.0$ meV) in the optical scattering rate and performed the same reverse process to investigate impurity-dependent optical properties. In the clean limit (for example, $1/\tau_{\text{imp}} = 1.0$ meV) for the both superconducting cases we do not observe the superconducting gaps clearly but still the characteristic feature (i.e. the sharp Gaussian peak and the MMP model) of $I^2 \chi(\omega)$ appears definitely in all optical constants including reflectance. For the normal case we are able to see the feature of $I^2 \chi(\omega)$ in the optical constants including reflectance. In the dirty limit (for example, $1/\tau_{\text{imp}} = 30.0$ meV) the superconducting gap appears definitely in $s$-wave superconductors but the gap feature is suppressed significantly in the $d$-wave one. In $d$-wave superconductors the optical constants are averaged response signals over the anisotropic Fermi surface which causes the suppression of those features. Furthermore, in the dirty limit the characteristic features (the Gaussian peak and the MMP model) of $I^2 \chi(\omega)$ can be seen clearly in the optical constants and measured reflectance spectrum. We find that in the clean limit the superfluid density obtained by the FGT sum rule cannot capture whole coherent electrons which participate in the superconductivity because the coherent absorption peak is too narrow. To get accurate superfluid density the SC system should be in a dirty limit. Our study shows that the superfluid density obtained by the FGT sum rule becomes quite accurate when $1/\tau_{\text{imp}}$ is large enough, above 15 meV, which is comparable to the superconducting gap, $\Delta_0$ (30.0 meV). We observe that the superfluid density decreases as the impurity level increases for both SC cases. We also observe that the $s$-wave superconductor is more robust against the impurities than the $d$-wave one. Our results will help to understand the usual optical analysis process thoroughly. Since the optical spectra clearly show the mediated boson features of the boson-exchange superconductors collecting experimental data at various (temperature, doping, magnetic field and so on) conditions and obtaining $I^2 \chi(\omega)$ applying the usual process can be a first step to revealing the microscopic origin of the exchange boson.

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