Chapter-4

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Summary of the Thesis

CHAPTER- IV

SUMMARY OF THE THESIS

4.1 Summary of chapter-I

In chapter-I, we presented our review work on crystallographic features, electronic structure, theoretical modeling and recent existing work on dynamical conductivity of cuprate superconductors (CS). They are type-II superconductors. The CS show high transition temperature, weak isotope effect, extreme sensitive to oxygen deficiency and electronic anisotropy. In the different series of cuprates, the T_c varies with hole concentration. Some of the important properties of CS are the anisotropy in resistivity, specific heat, critical field, critical current, magnetic penetration depth and coherence length. The resistivity (o) of CS is found highly anistropic. The resistivity along *a-b* plane is of the nature of metallic, whereas resistivity along c-axis may or may not metallic. It is more than 3 order of magnitude larger than that of metallic Cu. The anisotropic ratio of the resistivity of different compounds is of the order of 10^2 to 10^5 at different temperature. Above T_c, the specific heat of HTSC follows the Deby's theory. The BCS theory which predicts that the electronic specific heat jumps abruptly at T_c from normal state value to the superconducting state value. The anisotropy in critical magnetic field is much smaller as compared that in resistivity. Measurements on penetration depth (λ) along *a*-*b* plane and *c*-axis indicates that it is linear T-dependent in a perticular temperature range. The coherence length is generally 10-30 A^0 in the *a-b* plane and around 3 A^0 perpendicular to the plane. As the CS possesses strongly interacting system of charge carrier, the

carrier density-(n) is of the order of 10^{21} - 10^{23} cm⁻³. In general current density (J_e) along *a-b* plane is much larger than it is along *c*-axis. The critical current in both polycrystalline and single crystal materials of all the cuprates is generally small (< 10^3 amp/cm²) due to presence of grain boundaries and weak flux pinning. Large current densities (10^5 - 10^6 amp/cm²) have been obtained in thin film only. The superconducting gap Δ in YBa₂Cu₃O₇ seems to be around (3-4) k_βT_e. It is found larger along *a-b* plane than that along *c*-axis. Microwave conductivity as a function of temperature shows a broad peak below T_c. The charge transport along c-axis is very different in nature than it is in *a-b* plane. There exists a definite pseudogap in underdoped CS above T_c. The flux quantization experiments exhibit that the charge carrier do form pairs below T_c in CS.

Superconductivity has intensive interest in engineers and technologists because of variety of applications in medical diagnostics using large superconducting materials, electronics, magnetic and microwave devices using superconducting materials and power transmission or energy storage using superconducting wires. The laviting trains using superconducting technology is marvelous achievement. All these have been done with materials which become superconducting at liquid helium temperature. There have many ceramic oxide materials which become superconducting well above liquid nitrogen temperature. Efforts have been made to discover superconductor at room temperature.

The different cuprates said to be consists of rock-salt type metal-oxygen (M-O) and defect pervoskite layers, in addition they have Cu-O chains. All of them have Cu-O planes essentially with a square pyramidal (or octahedral) coordination of Cu with an apical oxygen. The Cu-O band is quite covalent with an average distance of around 1.9 A^0 . They have charge reservoir in the 123

cuprates by removing the chain oxygen is not favorable for superconductivity. The superconducting cuprates generally have parent members, which are antiferromagnetic insulators e.g. La_2CuO_4 , $YBa_2Cu_3O_7$ and $Bi_2Ca Sr_2LnO_8$. The CS can be classified into five categories. The LSCO based materials with $T_c\sim 38$ K, materials related to YBCO with $T_c\sim 93$ K, cuprates bearing Bi with $T_c\sim 110$ K. Tl bearing cuprates with $T_c\sim 127$ K and cuprates bearing Hg with $T_c\sim 133$ K. The doping and oxygen deficiency leads to phase transition of the AF to paramagnet, the insulator to metal and the normal to superconductor. One common feature of all CS is the presence of one or several quasi 2D-CuO₂ conducting planes in the unit cell. Most of the CS are orthorhombic at room temperature. Studies on Hall coefficient measurements suggest that the charge carriers in CS are holes.

The CS are strongly correlated systems. Present theories can be divided into two categories: (i) BCS type and (ii) non-BCS type. BCS type theories believe that there exist strongly interacting carrier gas which has Fermi-liquid behavior and pairs are formed below T_c via exchange of phonons, plasmons, excitons, spinons etc. Theoretical calculations based on resonant valence bond and t-J coupling model come under non-BCS type theories. Transport properties of cuprates such as resistivity and Hall-effect are often described using Fermiliquid hypothesis. Anomalies of normal state properties ascribed to marginal Fermi-liquid theory. Anderson attributed the superconductivity of cuprates to break down of Fermi-liquid theory and suggested the applicability of what are called Luttinger liquids. Hubbard model, t-J model have also been applied to Fermi-liquid. Optimally doped cuprate superconductors possases Fermi surface and they are essentially metallic. Band structure calculations seem to predict shape of Fermi surface with considerable accuracy.

Surface impedance measurements probe the complex conductivity $(\sigma=\sigma_1-i\sigma_2)$ of a superconductor as a function of frequency- ω and temperature-T.

It is usual to interpret the complex conductivity in terms of two-fluid model and various authors discussed the validity of partitioning the conduction electron density in to normal and superfluid fraction n_n and n_s ($n_n+n_s=1$) and conclude that this is appropriate in London limit. Infra-red conductivity gives information about the properties of superconducting state. It contains interaction on the value of the energy gap as well as on the coupling of electrons to the low-lying excitations in which they are coupled. Infra-red studies of the classical low temperature superconductors provided the existence of the superconducting energy gap as well as information on the plasma mediated pairing interactions. The *a-b* plane conductivity, which avoids chain is believed to provide a probe of the properties of CuO₂ planes. It has been proposed that the behavior of the conductivity in normal state reflects a two component response consisting "free carriers" and "bound carriers". It was found that the pure and dirty limits are not suitable for the study of anisotropy in CS.

It has been reported that, for weak interlayer coupling, it is preferable for electrons to travel along the *c*-axis by making a series of interband transition rather than to stay within a single band. It was reported further that many of the properties of the normal state optical conductivity including the pseudogap can be explained by interband transitions. It is found that there is no clear signature of the symmetry of the superconducting order parameter. The frequency dependence of the conductivity below T_c, can be described by a narrow Drude-like peak with strongly temperature dependent transport relaxation rates. Measurements of the surface impedance of good quality optimized YBCO film, suggest below 40 K, the normal electrons enter the anomalous skin-effect regime. Microwave surface impedance measurements on a high quality single crystal of YBCO shows a linear increase of the penetration depth at low temperature. From recent measurements on microwave and infra-red conductivity of high quality single crystal films of YBCO, it has been found that

 σ_1 features a peak which increases with amplitude and shifts to lower temperature as frequency decreases. The real part of conductivity of YBa₂Cu₃O₇₋₈ and Bi₂Sr₂Cu₂O₈ crystals shows a broad frequency-dependent peak. Optical conductivity measurements shows that high temperature superconductor exhibits a number of anomalies when compared with the usual Drude like Fermi-liquid behavior, found in conventional metals. Experimental measurements shows that effective transport scattering rate, $1/\tau(\omega)$ exhibits linear-in- ω behavior over a wide frequency range. It seems likely that structural vibrations between the different compounds are affecting the superconductivity. The non monotonic T-dependence of *a*-*b* plane surface resistance R_s^{ab} observed by Bonn et.al. has been interpreted in terms of effective quasi-particle scattering rate (τ) that increases rapidly below T_c. Doping in small amount causes decrease in R_s^{ab} as increasing scattering.

The calculated in-plane and out-of plane longitudinal plasma frequencies in the long wavelength limit as a function of hole density and temperature shows that both of the in-plane and out-of plane results are unaffected by the anisotropy of the order parameter and almost do not depends on T. It has been found that the plasmon modes remains below the superconducting gap edge. The mode crosses the gap edge, either by increases the wave vector or tilting its direction with respect to the superlattice axis. It was found that if the tunneling rate is large enough, the plasma mode may all be lifted out of the gap. The plasma oscillations in a superconductor are investigated for the case when plasma energy is smaller than the superconducting gap. A pole analysis show that the coupling occur just below T_c . However, it was found that two different mode like peak structure can be still observed in spectra of the density-density correlation function and the structure function of the pair field susceptibility.

4.2 Summary of Chapter-II

In chapter-II, we present a model calculation of macroscopic dynamical conductivity, $\sigma^0(q, k_z, \omega, T)$ and microscopic dynamical conductivity, $\sigma(q, k_z, \omega, T)$, in long wavelength limit, for layer superconductors which consists of one or two conducting layers per unit cell. We modelled cuprate superconductor (CS) as layered structure which incorporates: (i) weak tunneling of current between conducting layers, (ii) strong electron-electron interactions which results in frequency and temperature dependent transport relaxation time and (iii) optical phonons which contribute to dynamical conductivity in infra-red frequency regime. We calculated $\sigma_1^0(q, k_z, \omega, T)$, $\sigma_2^0(q, k_z, \omega, T)$, $\sigma_1(q, k_z, \omega, T)$ and $\sigma_2(q, k_2, \omega, T)$ in terms of dielectric response function, $\varepsilon(q, k_2, \omega, T)$ and polarization function, $\alpha(q, k_z, \omega, T)$, where q and k_z are wave vector components along a-b plane and c-axis, respectively. The subscript represents CS having one conducting layer per unit cell such as La_{2-x}Sr_xCuO₄ (LSCO) and 2 represents CS with two conducting layer per unit cell such as YBa₂Cu₃O₇ (YBCO). Possible charge transfer between conducting layers in a CS is also introduced in $\alpha(q, k_z)$ ω, T) through single particle energy involving half-width of miniband (W) and the wave function. We assumed that our model CS is a one-dimensional (1D) periodic sequence of 2D conducting planes (2DCP) embedded in a dielectric host medium represented by $\varepsilon_1(\omega)$. A simple expression of damping constant, $\gamma(\omega, T)$ which very well describes asymtotic behavior in CS, have been used to calculate $\alpha(q, k_z, \omega, T)$. To estimate anisotropic ratio of the resistivity (ρ_c/ρ_{ab}), we deduced d. c. conductivity σ_d^{ab} (along *a-b* plane) and σ_d^{c} (along *c*-axis). The (ρ_c/ρ_{ab}) has been found reasonably high for CS.

The *a-b* plane conductivity, $\sigma^{0}_{1ab}(q, \omega, T)$ and $\sigma_{1ab}(q, \omega, T)$ are computed as a function of ω and T by modelling LSCO in terms of following value of parameter: $\omega_p=1.308 \text{ eV}$, $\omega_g=0.238 \text{ eV}$. $\varepsilon_{\infty}=5.0$, $\delta_{ab}=0.55$, $\lambda_{ab}=0.80 \text{ mev/K}$ and $d=13.25 \text{ A}^0$ (interplaner distance). We modelled YBCO to calculate $\sigma^0_{2ab}(q, \omega, T)$ and $\sigma_{2ab}(q, \omega, T)$ by taking $\omega_p=1.315 \text{ eV}$ and $\omega_g=0.239 \text{ eV}$, $\varepsilon_{\infty}=4.0$, $\delta_{ab}=0.55$, $\lambda_{ab}=0.4 \text{ meV/K}$, $d=11.67 \text{ A}^0$ and $d_1=d/3$. The γ_{ab} (ω , T) is given in terms of values δ_{ab} and β_{ab} . To compute $\varepsilon_i(\omega)$ for *a-b* plane, $\varepsilon_i^{ab}(\omega)$, for LSCO we used: $\omega_{L1}=81.80 \text{ meV}$, $\omega_{L2}=48.37 \text{ meV}$, $\omega_{L3}=18.69 \text{ meV}$, $\omega_{T1}=80.56 \text{ meV}$, $\omega_{T2}=44.62 \text{ meV}$ and $\omega_{T3}=16.73 \text{ meV}$. And to compute $\varepsilon_i^{ab}(\omega)$ for YBCO, we used $\omega_{L1}=67.35 \text{ meV}$, $\omega_{L2}=58.25 \text{ meV}$, $\omega_{L3}=42.38 \text{ meV}$, $\omega_{L4}=29.62 \text{ meV}$, $\omega_{T1}=67.42 \text{ meV}$, $\omega_{T2}=48.96 \text{ meV}$, $\omega_{T3}=35.94 \text{ meV}$ and $\omega_{T4}=29.50 \text{ meV}$. The damping constant for lattice vibrations, $\gamma_{ph}=0.2 \text{ meV}$ has been taken for both LSCO and YBCO.

Macroscopic conductivity for longitudinal and transverse field, $\sigma_{2L}^0(q, k_z, \omega, T)$ and $\sigma_{2T}^0(q, k_z, \omega, T)$, respectively are contributed by intralayer as well as interlayer interactions. L and T stand for longitudinal and transverse components of the external field, respectively. For $k_z \rightarrow 0$, contribution of interlayer interactions is roughly proportional to q^2 for ω close to zero and it is almost zero at higher ω -values for all q-values. It is found that the maximum contribution from interlayer interactions is less then 6% of intralayer interactions for long wavelength case. Our computed $\text{Res}_{1ab}^0(q, \omega, T)$, real part of $\sigma_{1ab}^0(q, \omega, T)$, has been computed as a function of ω for qd=0.005, for three different value of T. It is found that, increase in temperature reduces $\text{Res}_{1ab}^0(q, \omega, T)$, in lower range of ω ($\omega < \lambda_{ab} T$), whereas $\text{Res}_{1ab}^0(q, \omega, T)$ increases with T in middle range of ω and then it become independent, of T for $\lambda_{ab}T << \omega$. The variation of $\text{Res}_{1ab}^0(q, \omega, T)$ versus T at qd=0.005 for two values of ω (10 meV and 60 meV) is approximately proportional to 1/T for ω =10 meV. The general behavior of $\text{Res}_{2ab}^0(q, \omega, T)$ versus ω is found similar to that of $\operatorname{Res}_{1ab}^{0}(q, \omega, T)$. The over all nature of our computed $\operatorname{Res}_{2ab}^{0}(q, \omega, T)$ as a function of ω at different temperatures agrees with the experimentally measured real part of macroscopic conductivity as a function of ω at different T. This supports our choice of γ . A small peak in lower frequency regime, which belongs to phonon modes, has been observed in our calculations. Our computed $\operatorname{Res}_{2ab}^{0}(q, \omega, T)$ shows very good agreement with experimental data for 25 meV $\leq \omega \leq 60$ meV.

The *a-b* plane microscopic conductivity is calculated by taking $k_z \rightarrow 0$ limit of $\sigma_{mL}(q, k_{zs}, \omega, T)$ and $\sigma_{mT}(q, k_{zs}, \omega, T)$. m takes value 1 for CS like LSCO and 2 for CS like YBCO. $\sigma_{mL}(q, \omega, T)$ describes optical conductivity in *a-b* plane when qd<<1. We find that for $\omega < \omega_{ps}$, $\sigma_{mT}(q, \omega, T) \cong \sigma_{mT}^{0}(q, \omega, T)$, whereas $\sigma_{mL}(q, \omega, T) < < \sigma_{pL}^{0}(q, \omega, T)$. This is because of the severe screening of longitudinal component of field and no screening of transverse component of field for $\omega < \omega_{p}$. The propagation of plasma oscillations (also known as transverse magnetic TM modes) in *a-b* plane are studied by calculating complex zeros of $\varepsilon_{m}(q, \omega, T)$. Whereas, propagation of transverse electric (TE) modes in *a-b* plane studied by calculating complex zeros of transverse response function, $F_m(q, \omega, T)$. The solution of the $\varepsilon_1(q, \omega, T) = 0$ for ω , when ω is much larger than any of $\omega_{Li}(\omega_{Ti})$ and it is comparable with ω_p . For qd <<1, $\omega_0 \cong \{\omega_{pl}/\sqrt{\varepsilon_{\omega}}\}$, which is much larger than $\delta_{ab}\beta_{ab}$ when T<100 K.

The $\text{Re}\omega_{1p}^{ab}(q)$ gives the real part of frequency of plasma oscillations, whereas $-\text{Im}\omega_{1p}^{ab}(q)$, imaginary part of frequency of plasma oscillations, is the measure of damping of plasma oscillations. $-\text{Im}\omega_{1p}^{ab}(q)$ is not very small, as compare to Re $\omega_{1p}^{ab}(q)$, it is 27% of Re $\omega_{1p}^{ab}(q)$ for $\delta_{ab}=0.55$ and $\beta_{ab}=32.0$. This results in a broad peak in Re $\sigma_{1L}(q, \omega, T)$. It is important to notice that ω and T

dependence of γ_{ab} and above mentioned values of δ_{ab} and β_{ab} are needed to explain experimentally observed behavior of normal state macroscopic conductivity as the function of ω and T, within our formalism. Further, we relate δ_{ab} and λ_{ab} to electron-electron interactions in our model calculation. We therefore conclude that larger value of $-\text{Im }\omega_{1p}^{ab}(q)$ is manifestation of electronelectron interactions. Increase of $[-Im\omega_{1p}^{ab}]/[Re\omega_{1p}^{ab}]$ with T suggests that at very high temperatures plasma oscillations may not remain well behaved and the peak in -Im $[1/\epsilon_1(q, \omega, T)]$ will disappear. Our computed -Im $[1/\epsilon_1(q, \omega, T)]$ as a function of ω at qd=0.005, for different values of of T, shows that peak position which appears at $\omega = \operatorname{Re}_{1p}^{ab}$, remains almost unchanged, whereas peak height decreases marginally on increasing T. Peaks which correspond to phonon frequencies are not seen here because of their suppression due to the screening of longitudinal component of field. In order to see how plasma oscillations in CS like YBCO differ from those in CS like LSCO, we solve $\varepsilon_2(q, \omega, T) = 0$ for qd << 1, when $\varepsilon_1(\omega)$ is replaced by ε_{∞} . We obtain two values of ω for which $\epsilon_2(q, \omega, T)=0, \omega_{2p}^+(q, T)$ and $\omega_{2p}^-(q, T)$. The real and imaginary parts of $\omega_{2p}^+(q)$ behaves like that of $\omega_{1p}^{ab}(q)$ and the magnitude are larger than those of $\omega_{1p}^{ab}(q)$. We also found that imaginary part of $\omega_{2p}^{+}(q)$ is approximately 27% of its real part in our model calculation. The $\omega_{2p}(q)$ is caused by interlayer interactions in YBCO. The non-zero real part of $\omega_{2p}(q)$ suggests that there exists a cut-off q-values, $q_c=1.25\times10^5$ cm⁻¹. For q<q_c, plasma mode of frequency ω_{2p} (q) does not propagate. We further found that for $q > q_c$, $\omega_{2p}(q)$ is roughly proportional to $(q^2-q_c^2)^{1/2}$ which suggests that there is no possibility of observing soft acoustic plasma modes in any of CS. The behavior of $-Im[1/\epsilon_2(q, \omega, T)]$ as a function of ω at given value of qd and T is almost similar to that of $-Im[1/\epsilon_1(q, \omega, T)]$ versus ω for $q > q_c$ and shows a peak which corresponds to $\omega_{2p}^+(q)$, for $qd \le 1.0$, However, for qd>1.0, two peaks in $-Im[1/\epsilon_2(q, \omega, T)]$ can clearly be seen.

Solution of $F_1(q, \omega, T)=0$ for ω as a function of q and T gives the complex frequency of a TE mode which can propagate in normal state of a CS like LSCO. Computation of $-Im[1/F_1(q, \omega, T)]$ as a function of ω at qd=0.005 for different values of T gives a broad peak which represents the frequency of smallest frequency TE mode of LSCO. The position and half width of the peak can roughly be obtained by solving $F_1(q, \omega, T) = 0$. It is found that like TM modes, TE modes have large damping constant. However, q-dependence of a TE modes is very different than that of a TM modes. It also exhibits small peaks in low frequency regime belongs to phonon modes because of almost no screening of transverse field for $\omega < \omega_p$. Solution of $F_2(q, \omega, T) = 0$ for ω as a function of q and T gives complex frequency of TE modes which can propagate in normal state of YBCO. Real and imaginary part of frequency of smallest TEmode ($\operatorname{Re}_{2t}^{s}(q)$ and $\operatorname{Im}_{2t}^{s}(q)$) as a function of q at T=100 K vary almost linearly with q and $\{Im\omega_{2t}^{s}(q)/Re \omega_{2t}^{s}(q)\} \cong 26\%$ at all q-values. For qd < 0.001, both $\operatorname{Re}\omega_{at}^{s}(q)$ and $\operatorname{Im}\omega_{at}^{s}(q)$ become almost independent of q. Other TE modes exist at very high o-values.

The c-axis conductivities, $\sigma_{1c}^{0}(q, k_{z}, \omega, T)$, $\sigma_{1c}(q, K_{z}, \omega, T)$, $\sigma_{02c}^{0}(q, k_{z}, \omega, T)$ and $\sigma_{2c}(q, k_{z}, \omega, T)$ are calculated by taking $q \rightarrow 0$ limit. γ_{c} is estimated by taking $\delta_{c} = 0.11$ and $\lambda_{c} = 1280$ mevK for LSCO and $\delta_{c} = 0.11$ and $\lambda_{c} = 4000$ meVK for YBCO. Values of phonon frequencies to compute $\varepsilon_{l}(\omega)$ along c-axis, $\varepsilon_{l}^{c}(\omega)$, are taken to be $\omega_{L1} = 52.43$ meV, $\omega_{L2} = 25.78$ meV, $\omega_{13} = 18.59$ meV, $\omega_{T1} = 46.48$ meV, $\omega_{T2} = 19.95$ meV, $\omega_{T3} = 13.50$ meV for YBCO and $\omega_{L1} = 76.74$ meV, $\omega_{L2} = 57.63$ meV, $\omega_{T1} = 61.22$ meV, $\omega_{T2} = 30.00$ meV for LSCO. The $\varepsilon_{l}^{c}(\omega)$ is needed to calculate macroscopic and microscopic conductivity along c-axis.

The c-axis macroscopic conductivity for LSCO, $\sigma_{1c}^{0}(\omega, T)$ is found independent of k_z , whereas that of YBCO $\sigma_{2c}^{0}(k_z, \omega, T)$ depends on k_z . Our computed Re $\sigma_{1c}^{0}(\omega, T)$ as a function of ω for different values of T decreases on increasing ω not close to phonon frequency. However, it shows: (i) linear T-dependent for ω close to zero, (ii) magnitude of $\text{Res}_{1c}^{0}(\omega, T)$ is smaller than that of Re $_{1ab}^{0}(q, \omega, T)$ for ω smaller then phonon frequency and (iii) large height peaks which correspond to lattice vibrations , because of $\gamma_c < \gamma_{ab}$. The behavior of our computed $\text{Res}_{2c}^{0}(k_z, \omega, T)$ versus ω and T at given k_z value is found similar to that of $\text{Res}_{1c}^{0}(\omega, T)$ with ω and T.

The microscopic conductivity, $\sigma_{1c}(q, k_z, \omega, T)$ and $\sigma_{2c}(q, k_z, \omega, T)$ along c-axis are obtained by taking $q \rightarrow 0$ limit. As is obvious, a transverse field can not be confined to a single direction, c-axis conductivity can therefore not be defined. Therefore, we computed, $\sigma_{1L}^{c}(\omega, T)$ and $\sigma_{2L}^{c}(k_z, \omega, T)$ for LSCO and YBCO, respectively. $\sigma_{1L}^{c}(k_z, \omega, T)$ is independent of k_z , whereas $\sigma_{2L}^{c}(k_z, \omega, T)$ depends on k_z because of contribution of interlayer interactions to $\sigma_{2L}^{c}(k_z, \omega, T)$. We obtain two plasma frequency on solving $\varepsilon_2(k_z, \omega, T)=0$ for ω as a function of k_z which suggests that lower c-axis plasma mode can exist for $k_z \ge k_{zc}$. On substituting values of δ_c , β_c , ϵ_{∞} and ω_g , we found that lower c-axis plasma frequency is non-zero for $k_z d \ge 0.11$. Our computed Re $\sigma_{2L}^{c}(k_z, \omega, T)$ as a function of ω for different k_zd at T=100 K shows large and broad peak which represents the upper c-axis plasma mode, whereas one of the small peaks in low frequency regime ($\omega \le 500 \text{ cm}^{-1}$) belong to lower c-axis plasma mode. Position of peak representing lower plasma mode, shifts towards higher ω -value and its size increases on increasing $k_z d$. Whereas, size of peak representing upper plasma mode reduces and its position shifts towards lower ω -value on increasing k_zd. Broad peak in our computed Re $\sigma_{2L}^{c}(k_z, \omega, T)$ is originated from charge transfer

along *c*-axis which is represented by ω_g and the ω -and T-dependent ρ_c . Our simple model calculation qualitatively agrees with detail numerical calculation of *c*-axis optical conductivity reported in past. It can therefore be said that our simple model calculation qualitatively described broad feature of normal state dynamical conductivity of a CS

4.3 Summary of chapter-III

In chapter-III, we present a model calculation of frequency and temperature dependent conductivity for temperature below T_c. Calculation has been performed for cuprate superconductors with one and two conducting Cu-O layers per unit cell. However, our results are mainly discussed for YBCO, which consists of two conducting layers per unit cell. We explained some of the features of the experimental data on ω -and T-dependent dynamical conductivity of CS below T_c, using a simple model. A CS has seen modeled to be layered structure of Cu-O conducting layer (COCL) embedded into an anisotropic dielectric medium of back ground dielectric function, $\varepsilon_{a-b}(\omega)$ along a-b plane and $\varepsilon_c(\omega)$ along c-axis in terms of a phonon frequencies. A coupling between the COCL is taken into consideration for calculating polarization function, $\prod(q, k_z, \omega, T)$ of a COCL. The ω -and T-dependence of $\tau(\omega, T)$ is taken in a phenomenological manner and nature of ω -and T-dependent $\tau(\omega, T)$ has been chosen to be same for both the cases of $T \ge T_c$ and $T < T_c$. Also, ω -dependence of effective mass of an electron has been introduced in our model calculation to obtain good agreement between experimental data and our calculation. Our calculated macroscopic conductivity, $\sigma^0_{\rho}(q, k_z, \omega, T)$ and microscopic conductivity, $\sigma_{\rho}(q, k_z, \omega, T)$ (ρ represents number of COCL in a unit cell) depends on calculation of $\prod(q, k_z, \omega, T)$. Our calculation incorporate X_s , $X_n \gamma_n$, γ_s , m^{*}, v_F and ω_g . X_s(= n_s/n) and X_n(= n_n/n) which are superfluid and normal fluid fractions, respectively. γ_n and γ_s , are inverse of scattering rate for normal

and superconducting state, respectively. v_F is 2D Fermi velocity. v_0 is attractive potential within a layer and m^{*} is effective mass of an electron. ω_g is measure of coupling between COCLs. Recent experiments on the measurements of surface resistance and optical properties of CS suggest that quasi-particle transport scattering rate, for both the cases of T>T_c and T<T_c, depends on ω and T.

We applied our calculation to $YBa_2Cu_3O_{7-\delta}$ (YBCO) for which maximum. experimental data is available. To calculate macroscopic and microscopic conductivity, we modeled YBCO in terms of following value of parameter: ε_{∞} =4.0, d=11.67 A⁰, d₁=d/3 and n=17×10²¹ cm⁻³. To compute dominant ω -dependent behavior of $\varepsilon_{i}(\omega)$ in a simple manner, we incorporated contribution from optical phonons in $\varepsilon_{ab}(\omega)$ and $\varepsilon_{c}(\omega)$. The phonon frequencies are taken same as those used in chapter-II. The ω -dependent of $\alpha_s(\omega)$ has been determined by keeping in mind; (i) almost linear ω -dependence of γ_s and (ii) to obtain a best possible agreement between our calculation and experimental results on macroscopic conductivity. Existing theoretical and experimental work on $\gamma_s(\omega)$ suggests that $\gamma_s(\omega)$ almost linearly depends on ω for all values of ω , covering microwave to optical frequency regime. We interpolated values of X_s along a-b plane using experimental data. To compare our theoretical results with experimental data, we computed $\text{Re}\sigma_2^{0}(q, k_z, \omega, T)$ (real part of $\sigma_2^{0}(q, k_z, \omega, T)$) as a function of T for different values of ω for fixed qd and k_zd and then as a function of ω for fixed T, qd and k_zd . The behavior of α_s and m^* as a function of ω , deduced from experimental data on dynamical conductivity suggested that α_s and m[•] depend on ω for $\omega \le \omega_c$, where ω_c (=0.15meV) is a cut-off frequency. We also used $\alpha_s=0.0045$ and $m^*/m_c=2.0$ for $\omega>0.15$ meV. Computed $\alpha_s^{ab}(\omega)$ and m^{*}/m_e for *a-b* plane conduction as a function of ω shows that m^{*}/m_e has a strong ω -dependence for $\omega < 0.02$ meV and it becomes almost independent of ω for ω close to 0.15 meV. The computed α_s versus ω becomes almost independent of ω approaching to 0.15 meV. The behavior of our computed $\gamma_{s}(\omega, T)$ agrees with the behavior of $\gamma_{s}(\omega, T)$ deduced from the experimental data on dynamical conductivity.

To compute $\operatorname{Re\sigma}_{2ab}^{0}(q, \omega, T)$, value of $\operatorname{Re\sigma}_{2}^{0}(q, k_z, \omega, T)$ for a-b plane, as a function of T for three values of ω we used $\beta_n^{ab} = 0.4 \text{ meV/K}, \beta_s^{ab} = 0.5$ meV/K, $\alpha_n^{ab}=0.55$. We found that T-dependence of Re $\sigma_{2ab}^0(q, \omega, T)$ mainly comes from the T-dependence of $\gamma_s^{ab}(\omega, T)$, $\gamma_n^{ab}(\omega, T)$ and of X_s. It has further been found that the peak in our computed $\operatorname{Res}_{2ab}^{0}(q, \omega, T)$ cannot be seen on taking; (i) T-independent value of γ_s^{ab} and (ii) qv_F close to $|\omega+i\gamma_S^{ab}|$. This suggests that to understand the experimentally observed peak in microwave conductivity (as a function of temperature below T_c) within the frame-work of Fermi-liquid theory, one has to take ω -and T-dependent transport relaxation time. During the computation of our results, we found that; (i) height of peak in $\operatorname{Re\sigma}_{2ab}^{0}(q, \omega, T)$ is basically governed by ω_{p} and (ii) position and shape of peak is controlled by the choice of values of β_s^{ab} and α_s^{ab} . We further found that the T-dependence of $\text{Res}^{0}_{2ab}(q, \omega, T)$ for T≤peak position remains almost unchanged whereas, $\operatorname{Re\sigma}^{0}_{2ab}(q, \omega, T)$ exhibits stronger T-dependence for T>peak position, on increasing β_{s}^{ab} . Our model calculation gives a very good agreement with experimental results for appropriate choice of values of parameters used in our calculation.

We computed $\text{Res}_{2c}^{0}(k_{z}, \omega, T)$, real part of $\sigma_{2c}^{0}(q, k_{z}, \omega, T)$ along *c*-axis as a function of T for fixed ω and $k_{z}d$. We took; $\beta_{s}^{c}=5000.0 \text{ meVK}$, $\alpha_{s}^{c}=0.00027$, $\beta_{n}^{c}=4000.0 \text{ meVK}$, $\alpha_{n}^{c}=0.11$, $\omega_{g}=98.85 \text{ meV}$ and $\omega_{p}=312.62 \text{ meV}$. We found a broad peak which is in good agreement for T≤peak position as compared that for T>peak position. It has been suggested that ω -dependent and T-independent of m^{*} and γ_s along with right choice of other parameters can be used to improve further the agreement between theory and experiment. We also computed Re $\sigma^0_{2ab}(q, \omega, T)$ as a function of ω at fixed T and qd using α_s^{ab} and m^{*}/m_e for $\omega \le 0.15$ meV. For $\omega > 0.15$ meV, we used $\alpha_s^{ab} = 0.05$ and m^{*}/m_e=2.0. Our calculation shows a good agreement with experimental results for $\omega \le 400$ cm⁻¹.

Our computed $\sigma_2^{0}(q, k_z, \omega, T)$ is contributed by both intralayer as well as interlayer interactions, whereas $\sigma_1^{0}(q, k_z, \omega, T)$ is contributed by intralayer interactions only. We have computed intralayer contribution and interlayer contribution to $\operatorname{Re}\sigma_2^{0}(q, k_z, \omega, T)$ as a function of T at fixed ω -values and then as a function of ω at fixed value of T. We found that interlayer interaction contribution more for smaller value of ω and T and their contribution is positive. However, for qd<<1 and k_z d<<1, contribution from interlayer interactions to $\operatorname{Re}\sigma_2^{0}(q, k_z, \omega, T)$ is negligibly small as compared to that from intralayer interactions. The behavior of $\operatorname{Re}\sigma_{1ab}^{0}(q, \omega, T)$ and $\operatorname{Re}\sigma_{1c}^{0}(k_z, \omega, T)$ has been found very similar to that of $\operatorname{Re}\sigma_{2ab}^{0}(q, \omega, T)$ and $\operatorname{Re}\sigma_{2c}^{0}(k_z, \omega, T)$, respectively.

The real part of microsopic conductivity, $\operatorname{Res}_2(q, k_z, \omega, T)$ exhibits peaks which corresponds to zeros of the $\varepsilon_2(q, k_z, \omega, T)$. The solution of $\varepsilon_2(q, k_z, \omega, T)=0$ for ω as a function of q, k_z and T gives the frequency of collective excitation modes (plasmons) in the system which can also be determined by computing $\operatorname{Im}\{-1/\varepsilon_2(q, k_z, \omega, T)\}$ as a function of T for different values of q, k_z and ω . Our computed $\operatorname{Im}\{-1/\varepsilon_{2ab}(q, \omega, T)\}$ as a function of ω at fixed values of T and qd shows a broad peak for ω close to ω_p , because of large contribution from unpaired electrons. It has also been found that the change in temperature does affect much the frequency of a collective state. Our computed $\operatorname{Im}\{-1/\varepsilon_{2c}(q, \omega, T)\}$ as a function of ω for fixed T and k_z d shows one broader and large peak which appears at ω close to ω_g represents electronic collective excitations and two smaller peaks appearing in the range of ω for $\omega \leq 20$ meV which represents lattice vibrations. The collective state which corresponds to zeros of $\varepsilon_2(q, k_z, \omega, T)$ can also be studied by plotting Im{-1/ $\varepsilon_{2ab}(q, \omega, T)$ } as a function of T for fixed value of ω and qd. A doublet has been seen for T varying in the range of 82 K to 85 K. The position of the peaks does not change while height of the peak increases on increasing ω . Our computed frequency of an electronic collective excitations mode along an arbitrary vector direction is found smaller than superconducting gap ($2\Delta = 20.895$ meV) and it exhibits a linear dependence on qd.

We also made a calculation of $\sigma_{\rho}^{0}(q, \omega, T)$ and $\sigma_{\rho}(q, \omega, T)$ in frequency range of $\hbar \omega \le 2\Delta \le qv_F \le k_{\beta}T \le k_{\beta}T_c$, using another model calculation of $\prod(q, \omega, T)$. Where, q, Δ , v_F , k_{β} and T are the components of the wave vector in the *a-b* plane, the binding energy of Cooper-pair, Fermi velocity, Boltzman's constant and temperature, respectively. We applied our calculation to $La_{2x}Sr_xCuO_4$ by modelling it in terms of following values of parameters: $m^*=3.5m_e$, $n_2=1.277\times10^{14}$ cm⁻², d=13.25 A⁰ and $v_F= 0.9414\times10^7$ cm s⁻¹. We computed $\sigma'_1(\omega, T)$ and $\sigma''_1(\omega, T)$ (real and imaginary part of $\sigma(\omega, T)$, respectively) as a function of ω for both the cases of with and without including impurity scattering. It is found that on inclusion of impurity scattering the peak height of $\sigma'_1(\omega, T)$ drastically reduces by an order of 10^3 and becomes much broader as compared to that in $\sigma'_1(\omega, T)$ without impurity scattering. The behavior of $\sigma'_1(\omega, T)$ is almost insignificant for frequencies which are not close to pasma frequency. The position of peak in $\sigma'_1(\omega, T)$ represents plasma frequency of our model $La_{2x}Sr_xCuO_4$ just below T_e . Computation of $\omega: \{\sigma'_1(\omega, T)/\sigma''_1(\omega, T)\}$ versus ω for $T/T_c=0.997$ yields an approximate estimate of γ_s which exhibits almost linear ω -dependence for $\omega \le 0.8$ meV. Linear ω -dependence of γ_s is characteristics of quasi-two dimensional charge carries which exist in CS. Our computed $R_s(\omega)$ (real part of impedance) shows a sudden change at frequencies near to plasma frequency representing the collective excitation state of system, which exists in our model system just below T_c . It also almost linearly increases with ω for $\omega > 0.8$ meV.

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