Angle and frequency dependence of self-energy from spin fluctuation mediated d-wave pairing for high temperature superconductors

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Abstract

We investigated the characteristics of spin fluctuation mediated superconductivity employing the Eliashberg formalism. The effective interaction between electrons was modeled in terms of the spin susceptibility measured by inelastic neutron scattering experiments on single crystal La$_{2-x}$Sr$_x$CuO$_4$ superconductors. The diagonal self-energy and off-diagonal self-energy were calculated by solving the coupled Eliashberg equation self-consistently for the chosen spin susceptibility and tight-binding dispersion of electrons. The full momentum and frequency dependence of the self-energy is presented for optimally doped, overdoped, and underdoped LSCO cuprates in a superconductive state. These results may be compared with the experimentally deduced self-energy from ARPES experiments.

1. Introduction

One of the leading contenders for the d-wave pairing mechanism of cuprate superconductors is spin fluctuation. Superconductivity (SC) mediated by spin fluctuation has a long history [1–3]. In support of the spin fluctuation mechanism, Scalapino [1], noticing the commonalities among the heavy fermion, cuprate, and Fe superconductors, argued as follows. (a) Their chemical and structural makeup, their phase diagrams, and the observation of a neutron scattering spin resonance in the superconducting phase support the notion that they form a related class of superconducting materials. (b) A number of their observed properties are described by Hubbard-like models. (c) Numerical studies of the effective pairing interaction in the Hubbard-like models find unconventional pairing mediated by an $S = 1$ particle–hole channel. He proposed that spin fluctuation mediated pairing provides the common thread which is responsible for superconductivity in all of these materials.

Along the same lines, many works have been published. Noteworthy is the work by Dahm et al [4]. They measured the spin susceptibility from inelastic neutron scattering (INS) experiments on YBa$_2$Cu$_3$O$_{6.6}$ and used it as the effective interaction (the Eliashberg function) between electrons to calculate the diagonal self-energy from the Eliashberg equation. The calculated spectral function produced similar results to the measured angle resolved photoemission spectroscopy (ARPES) intensity from the same YBa$_2$Cu$_3$O$_{6.6}$ crystal. They claimed that a self-consistent description of ARPES and INS can be obtained within the Eliashberg formalism for the cuprates (by adjusting a single parameter, the fermion–spin coupling strength). Their work, however, did not take full consideration of the frequency and momentum dependence of the diagonal and...
off-diagonal self-energies. This point is crucial in that, for instance, the momentum dependence of the peak position of the self-energy, which is one of the ongoing discussions in the field, can only be addressed by calculations without assuming ad hoc momentum dependence. See the remarks in section 5.

Here, we revisit this spin fluctuation scenario by computing the angle, i.e., the momentum direction in the Brillouin zone (BZ), and frequency dependence of the diagonal, $\Sigma(k, \omega)$, and off-diagonal self-energy, $\phi(k, \omega)$. The cause of the angle and frequency dependence can be an important clue about the pairing mechanism [5, 6]. The diagonal self-energy is also called normal self-energy (‘normal’ here means the particle–hole channel) and should not be confused with the ‘normal’ as in the normal state meaning above $T_c$), and off-diagonal self-energy is also called anomalous or pairing self-energy. We employ the phenomenological fermion–spin coupling [2, 4],

$$H_{fs} = \alpha \sum_{k,q,a,b} c_{k+q,a}^\dagger c_{k,b} \sigma_{a,b},$$

where $\alpha$ is the coupling strength of the dimension of energy, and $c$ and $\sigma$ are the fermion and spin operators. Although the Eliashberg formalism is not firmly established for spin fluctuation mediated superconductivity, perhaps, our resort is that the ratio $\lambda \omega_c / E_F$ is $< 1$, $\lambda$ is the dimensionless coupling constant, $\omega_c$ the cutoff of the spin fluctuation frequency, and $E_F$ is the Fermi energy. Also, Millis argued in [7], in justifying the numerical Eliashberg approaches, that the d-wave superconductivity induced by antiferromagnetic (AF) spin fluctuations is due essentially to the high-energy part and not to the strong low-lying AF fluctuations producing the mass enhancement and scattering.

For the Eliashberg function, $\alpha^2 F(q, \omega)$, we take like Dahm et al the imaginary part of the spin susceptibility, $\chi_{sp}(q, \omega)$, measured from INS. High quality INS data require large size single crystals and the INS data over wide momentum and energy ranges are mainly from YBCO or LSCO compounds. A functional form of the spin susceptibility obtained by fitting the INS data is given in the literature for optimally doped (OP) La$_{2−x}$Sr$_x$CuO$_4$ ($x = 0.16$, $T_c = 38.5$ K) by Vignolle et al [8] and for overdoped (OV), ($x = 0.22$, $T_c = 26$ K) [9], and underdoped (UD) La$_{2−x}$Sr$_x$CuO$_4$ ($x = 0.08$, $T_c = 22$ K) [10] by Lipscombe et al [11]. The diagonal and off-diagonal self-energies and the quasi-particle (qp) energy shift, $\Sigma(k, \omega)$, are computed self-consistently for OP, OV, and UD La$_{2−x}$Sr$_x$CuO$_4$ using the INS measured spin susceptibility. See equations (12) and (4).

In section 2, we present the Eliashberg formalism used to calculate the self-energy from the given spin susceptibility spectrum, $\chi_{sp}(q, \omega)$. Some preliminary analysis for the energy scales of the self-energy is given in section 3 before presenting results of numerical calculations. In section 4, the numerical results are presented for OP, OV, and UD La$_{2−x}$Sr$_x$CuO$_4$ focusing on the angle dependence of the position and intensity of the peaks in the self-energy. There are two sources for the peaks in the self-energy in the SC state: the peaks in the density of states (DOS) and the spin susceptibility. We will discuss how the two between them show up in the self-energy. The summary and outlook follow in section 5.

### 2. Formalism

The d-wave Eliashberg equation is given by [12, 13]

$$\Sigma(k, \omega) = \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon' S \sum_{k'} A_{\delta}(k', \epsilon) \alpha^2 F^{(+)}(k', k, \epsilon'),$$

$$X(k, \omega) = \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon' S \sum_{k'} A_{\delta}(k', \epsilon) \alpha^2 F^{(+)}(k', k, \epsilon'),$$

$$\phi(k, \omega) = -\int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon' S \sum_{k'} A_{\delta}(k', \epsilon) \alpha^2 F^{(-)}(k', k, \epsilon'),$$

$$S = \frac{f(\epsilon) + n(-\epsilon')}{\epsilon + \epsilon' - \omega - i\delta},$$

where $f(\omega)$ and $n(\omega)$ are the Fermi and Bose distribution functions, respectively. $\Sigma$ is the symmetric part of the diagonal self-energy $\Sigma$, $X$ the shift of the qp dispersion, and $\phi$ is the off-diagonal self-energy. The diagonal and off-diagonal Eliashberg functions, $\alpha^2 F^{(+)}$ and $\alpha^2 F^{(-)}$, are given by

$$\alpha^2 F^{(+)}(k', k, \epsilon, \epsilon') = \alpha_{\delta}^2 (k, k') F\delta (k' - k, \epsilon', \epsilon') + \alpha_{ch}^2 (k, k') F_{ch} (k' - k, \epsilon', \epsilon'),$$

$$\alpha^2 F^{(-)}(k', k, \epsilon, \epsilon') = \alpha_{ch}^2 (k, k') F\delta (k' - k, \epsilon', \epsilon') - \alpha_{sp}^2 (k, k') F_{sp} (k' - k, \epsilon', \epsilon'),$$

where the subscripts ch and sp refer to the channels by which the bosonic modes transform. For instance, the charge fluctuations belong to the ch channel, and the spin and current fluctuations to the sp channel. The various spectral functions are given by

$$A_{\delta}(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{W(k, \omega)}{W^2 - Y^2 - \phi^2},$$

$$A_{ch}(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{Y(k, \omega)}{W^2 - Y^2 - \phi^2},$$

$$A_{sp}(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{\phi(k, \omega)}{W^2 - Y^2 - \phi^2},$$

where $\xi(k)$ is the bare dispersion,

$$W(k, \omega) = \omega - \Sigma(k, \omega) = \omega Z(k, \omega),$$

$$Y(k, \omega) = \xi(k) + X(k, \omega),$$

and $Z(k, \omega)$ is the renormalization function that appears, for example, in the gap function

$$\Delta(k, \omega) = \phi(k, \omega) / Z(k, \omega).$$

The $4 \times 4$ matrix self-energy may be written as [14]

$$\Sigma(k, \omega) = \Sigma_0 + X(k, \omega) \tau_3 + \phi(k, \omega) \tau_2 \sigma_2,$$

where $\Sigma_0$ is the bare self-energy.
where $\tau_i$ and $\sigma_i$ are the Pauli matrices in the particle–hole and spin space, respectively. The diagonal self-energy is given by

$$\Sigma(k, \omega) = \tilde{\Sigma}(k, \omega) + X(k, \omega),$$  

and the diagonal spectral function measured by ARPES is

$$A(k, \omega) = A_{\Sigma}(k, \omega) + A_X(k, \omega).$$  

The symmetry of the self-energy is as follows:

$$\tilde{\Sigma}(k, \omega) = -\tilde{\Sigma}^*(k, -\omega),$$  

$$X(k, \omega) = X^*(k, -\omega),$$  

$$\phi(k, \omega) = \phi^*(k, -\omega).$$

We choose the following tight-binding band as the bare dispersion for the doped La$_{2-x}$Sr$_x$CuO$_4$ [15].

$$\xi(k) = -2t(\cos k_x a + \cos k_y a) + 4t' \cos k_x a \cos k_y a$$

$$- 2t''(\cos 2k_x a + \cos 2k_y a) - \mu.$$  

The tight-binding parameters are $t = 0.25$ eV, $t' = 0.15 t$, $t'' = 0.5 t'$, and the chemical potential $\mu = -0.19$ eV for OP, and $t = 0.25$ eV, $t' = 0.13 t$, $t'' = 0.5 t'$, $\mu = -0.22$ eV for OV, and $t = 0.25$ eV, $t' = 0.17 t$, $t'' = 0.5 t'$, $\mu = -0.15$ eV for UD La$_{2-x}$Sr$_x$CuO$_4$. The UD and OP La$_{2-x}$Sr$_x$CuO$_4$ have a hole-like and the OV has an electron-like Fermi Surface (FS) as shown in figure 1. To denote the momentum direction in the BZ in two dimensions we use the tilt angle $\theta$ with respect to the nodal cut, that is, the diagonal cut along the $(0, 0) - (\pi, \pi)$ line, centered at $(\pi, \pi)$ for the hole-like FS and at $(0, 0)$ for the electron-like FS, as indicated in figure 1.  

The spin fluctuation mechanism in this formulation means that we take $F_{\Sigma}(q, \omega) = 0$ and $F_{\phi}(q, \omega)$ as the spin susceptibility $\chi_{sp}(q, \omega)$ measured by INS in equation (3). Then the imaginary parts of the self-energy may be rewritten from equation (2) as

$$\text{Im} \Sigma(k, \omega) = \pi \int_{-\infty}^{\infty} \text{d} \epsilon' \left[ f(\omega - \epsilon') + n(-\epsilon') \right]$$

$$\times \sum_{k'} A_{\Sigma}(k', \omega - \epsilon') a^2 \chi_{sp}(k - k', \epsilon'),$$

$$\text{Im} X(k, \omega) = \pi \int_{-\infty}^{\infty} \text{d} \epsilon' \left[ f(\omega - \epsilon') + n(-\epsilon') \right]$$

$$\times \sum_{k'} A_{X}(k', \omega - \epsilon') a^2 \chi_{sp}(k - k', \epsilon'),$$

$$\text{Im} \phi(k, \omega) = \pi \int_{-\infty}^{\infty} \text{d} \epsilon' \left[ f(\omega - \epsilon') + n(-\epsilon') \right]$$

$$\times \sum_{k'} A_{\phi}(k', \omega - \epsilon') a^2 \chi_{sp}(k - k', \epsilon').$$

The real parts were calculated from the imaginary parts using the Kramers–Kronig (KK) relation. Equations (12) and (4) were solved self-consistently via iterations.

The coupling strength $\alpha$ was chosen such that it reproduces the experimentally measured gap amplitude $\Delta_0$ of La$_{2-x}$Sr$_x$CuO$_4$ [16]. The coupling strength will be given in terms of the dimensionless coupling constant $\lambda$ below,

$$\lambda = \int_{-\infty}^{\infty} d\omega N(\omega) \frac{\alpha^2 \chi_{sp}(\omega)}{\omega},$$

where $N(\omega)$ is the density of states (DOS) and $\chi_{sp}(\omega)$ is the local spin susceptibility given by

$$\chi_{sp}(\omega) = \frac{\int dq \chi_{sp}(q, \omega)}{\int dq}.$$  

It is a measure of the density of spin excitation for a given energy. The gap function is determined by

$$\Delta(k) = \text{Re} \left[ \frac{\phi(k, \omega)}{Z(k, \omega)} \right]_{\omega = \Delta(k)},$$

and $\Delta_0$ was determined from the DOS peak position.

The measured spin susceptibility $\chi_{sp}(q, \omega)$ from INS was fitted by the form

$$\chi_{sp}(q, \omega) = \chi(\omega) \frac{\kappa^4(\omega)}{[\kappa^2(\omega) + R(q)]^2},$$

where the inplane wavevector is written in the reciprocal lattice as $q = ha^* + kb^* + le^*$, $\kappa(\omega) = 1/\xi$ is the inverse correlation length, the incommensurability $\delta(\omega)$ specifies the position of the four peaks, and $\lambda(\omega)$ controls the shape of the pattern. $\lambda = 4$ corresponds to four distinct peaks and $\lambda = 0$ corresponds to a pattern with circular symmetry. These fitting parameters were given in the references [8–11]. Notice, however, that in these references the authors used the wavevectors in the reciprocal lattice unit such that their $1/2$, for example, corresponds to $\pi$ of this paper.
The measured local susceptibility may be decomposed into three parts; a low frequency incommensurate (IC) peak centered around $Q_0 = (\pi \pm \delta, \pi)$ and the symmetry related points, a commensurate (CM) peak at $Q = (\pm \pi, \pm \pi)$, and a broad high frequency feature. The IC peak is around 18, 15, and 15 meV for OP, OV, and UD samples, respectively. The CM peak is around 50 meV for OP and 45 meV for UD samples, but is missing for OV La$_{2-x}$Sr$_x$CuO$_4$. On the other hand, the high frequency feature persisting up to measurable energy is common for all samples. The cutoff energy $\omega_c$ of the susceptibility spectrum was taken to be 0.3 eV. This is the upper limit of the spin wave spectrum \[17\] of around $2J$.

The absence of the CM peak in the spin susceptibility spectrum of overdoped La$_{2-x}$Sr$_x$CuO$_4$ is in accord with the infrared study on Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ by Hwang et al \[18\]. They separated a sharp feature from a broad background in the real part of the optical self-energy of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ using the extended Drude model. This sharp optical peak became suppressed with doping before a complete disappearance at a critical doping of 0.23 holes per copper atom. The qp are coupled with the spin fluctuations and the disappearance of the optical peak is caused by the absence of the corresponding CM peak of spin susceptibility. The superconductivity is still robust at the absence of the optical peak or the spin resonance peak. This conclusion is indeed borne out in the present work. In contrast, Carbotte et al emphasized the importance of the spin resonance feature in causing superconductivity \[19\].

The $k'$ summation in equation (12) was performed by using the 2D fast Fourier transform (FFT) between the momentum and real space using the convolution relation

$$\sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \sum_{\mathbf{k}'} F(\mathbf{k}' - \mathbf{k}) G(\mathbf{k}') = F(\mathbf{r})G(\mathbf{r})$$

on a $2^8 \times 2^8$ mesh of the first quadrant of BZ. No assumption about the $\mathbf{k}$ and $\omega$ dependence or a separable form of the diagonal and off-diagonal self-energy was made in the calculations. Self-consistency is reached in a couple of tens of iterations.

3. Preliminary analysis

Before presenting our results of the angle and frequency dependence of the self-energy, it will be useful to consider some simple cases. Let us first consider the Einstein model of frequency $\omega_b$ of the coupled boson.

$$\alpha^2 F(\mathbf{k}, \mathbf{k}', \epsilon') = \alpha^2(\mathbf{k}, \mathbf{k}') \left[ \delta(\epsilon' - \omega_b) - \delta(\epsilon' + \omega_b) \right].$$

Then the imaginary part of the diagonal self-energy from equation (12) is

$$\Sigma_2(\mathbf{k}, \omega) = \pi \left[ f(\omega - \omega_b) + n(-\omega_b) \right] D(\mathbf{k}, \omega - \omega_b) - \left[ f(\omega + \omega_b) + n(\omega_b) \right] D(\mathbf{k}, \omega + \omega_b),$$

where

$$D(\mathbf{k}, \omega) = \sum_{\mathbf{k}'} \alpha^2(\mathbf{k}, \mathbf{k}') A(\mathbf{k}', \omega).$$

In the low temperature limit of $T \to 0$, it is reduced to

$$-\Sigma_2(\mathbf{k}, \omega) = \pi \left[ \Theta(\omega - \omega_b) D(\mathbf{k}, \omega - \omega_b) + \Theta(-\omega - \omega_b) D(\mathbf{k}, \omega + \omega_b) \right],$$

where $\Theta$ is the step function. The peaks of $-\Sigma_2(\mathbf{k}, \omega)$ for the negative (positive) $\omega$ region are determined by those of $D(\mathbf{k}, \omega \pm \omega_b)$. Depending on the range of $\mathbf{k}'$ summation of equation (20) determined by $\alpha^2(\mathbf{k}, \mathbf{k}')$, either one peak (for $\kappa \to \infty$ or 0) or two peaks (for intermediate $\kappa$) may show up as discussed below.

Consider two limits of this expression: first, for momentum independent coupling of $\alpha^2(\mathbf{k}, \mathbf{k}') = \alpha^2$. Then, we have

$$-\Sigma_2(\mathbf{k}, \omega) = \begin{cases} \pi \alpha^2 N(\omega - \omega_b), & \text{for } \omega > \omega_b, \\ \pi \alpha^2 N(\omega + \omega_b), & \text{for } \omega < -\omega_b, \\ 0, & \text{otherwise} \end{cases}$$

where

$$N(\omega) = \sum_{\mathbf{k}'} A(\mathbf{k}', \omega)$$

is DOS. This clearly shows that the peaks of DOS at $\omega = \pm \Delta_0$ in the SC state are shifted to $\pm (\Delta_0 + \omega_b)$ in $-\Sigma_2(\omega)$ because of the coupling to the boson of frequency $\omega_b$ and that they are momentum independent. This case is relevant where the correlation length $\xi$ of a susceptibility peak is small (or, the inverse correlation length $\kappa \to \infty$) like the 50 meV CM peak of OP sample. See the angle independent peaks near $|\omega| \approx 65$ meV in $-\Sigma_2$ and $\varphi_2$ shown in figures 2(a) and 3(a).

Another limit is where the coupling is a delta function like $\alpha^2(\mathbf{k}, \mathbf{k}') = \alpha^2 \delta(\mathbf{k}' - \mathbf{k} - \mathbf{q})$, corresponding to $\kappa \to 0$. Then, instead of equation (22), we have

$$-\Sigma_2(\mathbf{k}, \omega) = \begin{cases} \pi \alpha^2 A(\mathbf{k} + \mathbf{q}, \omega - \omega_b), & \text{for } \omega > \omega_b, \\ \pi \alpha^2 A(\mathbf{k} + \mathbf{q}, \omega + \omega_b), & \text{for } \omega < -\omega_b, \\ 0, & \text{otherwise} \end{cases}$$

Because the spectral function $A(\mathbf{k}, \omega)$ has a peak around $\omega \approx \pm E(\mathbf{k})$ in the SC state, where

$$E(\mathbf{k}) = \sqrt{\xi^2(\mathbf{k}) + \Delta^2(\mathbf{k})},$$

and $\tilde{\xi}(\mathbf{k}) = (\xi(\mathbf{k}) + X)/Z$ is the renormalized dispersion; the peak of $-\Sigma_2(\mathbf{k}, \omega)$ occurs at $\omega \approx \pm (E(\mathbf{k} + \mathbf{q}) + \omega_b)$ which is clearly momentum and band structure dependent.

For intermediate values of $\kappa$, the self-energy of equation (24) is summed around $\mathbf{k} + \mathbf{q}$ over the width $\kappa$. Then, both energy scales of $(\Delta_0 + \omega_b)$ and $(E(\mathbf{k} + \mathbf{q}) + \omega_b)$ may appear in $-\Sigma_2(\mathbf{k}, \omega)$ from a single peak of $\chi(\mathbf{q}, \omega)$. A modification is that the energy $(\Delta_0 + \omega_b)$ of $\xi \to 0$ now becomes momentum dependent $(\Delta(\mathbf{k}) + \omega_b)$ because a non-zero $\xi$ implies a momentum selection in the $\mathbf{k}'$ summation. $\Delta(\mathbf{k})$ is an angle dependent energy of order $\Delta_0$. This seems to be the case for the IC peaks as will be discussed below.
Some complications arise from the band structure and momentum dependent coupling [12]. An interesting case is where the momentum sum covers the saddle point, which usually occurs at $(0, \pi)$. This introduces another energy scale in $-\Sigma_2(k, \omega)$ from the van Hove singularity (VHS). It occurs at $\omega \approx \text{sgn}(\xi_{\text{VHS}})(E_{\text{VHS}} + \omega_b)$, where $E_{\text{VHS}} = \sqrt{\xi_{\text{VHS}}^2(0, \pi) + \Delta_0^2}$ and $\text{sgn}(f) = \pm 1$ represents the sign of $f$, in addition to the two energy scales of the peaks discussed above. The shape of $\Sigma(k, \omega)$ is also modified by the impurity scatterings [20]. The VHS peak may be substantially suppressed by the coupling to boson spectrum and impurity scatterings. One should perform the self-consistent calculations to see their effects without misleading conclusion. The off-plane elastic impurities may induce interesting features of the self-energy in the SC state. In cases where the VHS peak is strongly suppressed and/or the $E_{\text{VHS}}$ and $\Delta_0$ are not well separated, the VHS feature may not clearly show up. The parameters of current LSCO calculations seem to belong to this case and we do not discuss the VHS features in the self-energy below. Also recall that the discussion so far is restricted to a sharp boson frequency of a single energy. A finite width in energy as well as in momentum space smoothens peak features in the self-energy.

4. Numerical results

We now turn to the self-consistent numerical calculations using the experimentally measured spin susceptibility as the Eliashberg function for the OP, OV, and UD $La_{2-x}Sr_xCuO_4$ as explained above. The angle $\theta$ in the BZ was chosen with respect to the nodal direction as shown in figure 1. We wish to discuss the position and intensity of peaks in the absolute value of the imaginary part, $-\Sigma_2(k, \omega)$, and the real part of the self-energy, $\Sigma_1(k, \omega)$, for $\omega < 0$. The $\omega > 0$ region with which we wish to compare our numerical results cannot be probed by ARPES. For the off-diagonal self-energy, $\phi_1(k, \omega)$ and $\phi_2(k, \omega)$ are, respectively, even and odd functions of $\omega$, and will be shown in the $\omega > 0$ region.

4.1. OP $La_{2-x}Sr_xCuO_4$

First, we consider the OP $La_{2-x}Sr_xCuO_4$ with the doping concentration $x = 0.16$ and the critical temperature $T_c = 38.5$ K. The spin susceptibility spectrum reported by Vignolle

![Figure 2.](image1.png)

Figure 2. The calculated imaginary and real parts of the diagonal self-energy at the Fermi momentum of OP LSCO along several cuts in the BZ in the SC state. The Vignolle spectrum was used for the $F_{\rho}$ in the Eliashberg equation. The nodal direction is $0^\circ$ and the anti-nodal direction is $45^\circ$.

![Figure 3.](image2.png)

Figure 3. The calculated imaginary and real parts of the off-diagonal self-energy of OP LSCO along several cuts perpendicular to the FS in the SC state. The angles are the same as figure 2.
et al. has three parts; the IC peak near 18 meV, the CM peak near 50 meV, and a broad high frequency feature extended to 0.3 eV. The coupling constant was chosen such that \( \lambda = 1.74 \) in the calculations to obtain the gap amplitude \( \Delta_0 = 17 \) meV in the \( T \rightarrow 0 \) limit [16].

Figures 2(a) and (b) are the imaginary and real parts of the diagonal self-energy along several cuts perpendicular to the FS in the BZ in the SC state. Figures 3(a) and (b) show the imaginary and real parts of the off-diagonal self-energy, respectively. The two peaks in both the real and imaginary parts of the diagonal and off-diagonal self-energies reflect the two peaks in the spin susceptibility with slight complication as explained below.

For the Vignolle spectrum from OP La\(_{2-x}\)Sr\(_x\)CuO\(_4\), the IC peak has an intermediate correlation length of \( \xi \approx 4.1a \), the CM peak has a small \( \xi \approx 0.8a \), and the broad high frequency feature has \( \xi \approx 0.7a \) [8]. From the discussion in section 3, we may expect two peaks at \( \omega_1 \approx -(\Delta'(k) + \omega_{IC}) \) and \( \omega'_1 \approx -(E(k + Q_3) + \omega_{IC}) \) from the IC peak, and one peak at \( \omega_2 \approx -(\Delta_0 + \omega_{CM}) \) from the CM peak. The \( \omega'_1 \) seems to overlap with \( \omega_2 \), and two peaks show up in \( -\Sigma_2(k, \omega) \). The \( \omega_1 \) is expected to be angle dependent and \( \omega_2 \) to be \( \approx -67 \) meV because \( \Delta_0 = 17 \) and \( \omega_{CM} \approx 50 \) meV. This is what we obtained in numerical calculations as shown in figure 2(a). Exactly the same argument holds for the off-diagonal self-energy, \( \phi_2(k, \omega) \), as shown in figure 3(a).

In order to understand the peak energy of the real parts of the self-energy, recall that the real and imaginary parts are related by the KK relation. This means that the peak energy of \( \Sigma_1(\omega) \) is shifted from that of \( -\Sigma_2(\omega) \) by the width of the peak, that is, the peak energy of \( \Sigma_1 \) is expected at \( \omega \approx -(\Delta'(k) + \omega_{IC} - \Gamma_{IC}) \) and \( \omega \approx -(\Delta_0 + \omega_{CM} - \Gamma_{CM}) \), where \( \Gamma \) is the width of the peak. This is indeed what we obtained from numerical calculations. See the plots of \( \Sigma_1(k, \omega) \) and \( \phi_1(k, \omega) \) as shown in figures 2(b) and 3(b), respectively.

Now, we turn to the intensity of the peaks of the self-energy. From equations (21) and (20) we see that \( -\Sigma_2(k, \omega) \) is given by the sum over \( k' \) of \( \alpha^2(k, k')A(k', \omega + \omega_b) \). This means that there is large contribution from the \( k' \) sum to \( -\Sigma_2(k, \omega) \) if both \( k' \approx k \approx Q_3 \) and \( \omega \approx -(E(k + Q_3) + \omega_{IC}) \) are satisfied. This is better satisfied near the anti-nodal region and \( -\Sigma_2(k, \omega) \) increases as the tilt angle increases for small \( |\omega| \). For large \( |\omega| \), however, either of the two conditions become ill satisfied and \( -\Sigma_2(k, \omega) \) is roughly angle independent. This is indeed what figure 2(a) shows. The IC peak in all four plots in figures 2 and 3 is not highest at 45° but \( \approx 40° \) because of the incommensurability \( \delta \). On the other hand, the CM peak near 65 meV is highest at 45° as expected because the broad CM peak connects the anti-nodal regions most effectively.

The angle dependence of the off-diagonal self-energy \( \phi(\theta, \omega) \) along several cuts is roughly d-wave, similar to that shown in figure 3. The imaginary part looks like the local spin susceptibility \( \chi_{sp}(\omega) \) with the suppressed high frequency part. The suppression of \( \phi_2(\theta, \omega) \) above \( \approx 0.1 \) eV shows that the high frequency part of the susceptibility does not contribute much to pairing because its broad momentum dependence is not very effective for d-wave pairing. The real part \( \phi_1(\theta, \omega) \) increases as \( \omega \) increases from 0 and exhibits two peaks induced by the two peaks in the spin susceptibility, and then decreases and makes a zero crossing near \( \omega_2 \). There, \( \phi_2(\theta, \omega) \) has a peak because of the KK relation.

4.2. OV La\(_{2-x}\)Sr\(_x\)CuO\(_4\)

The calculations were done for OV La\(_{2-x}\)Sr\(_x\)CuO\(_4\) as well. The difference from the OP case is that (a) the spin susceptibility spectrum does not have the CM component, and (b) the bare dispersion has smaller next nearest neighbor hopping amplitude of \( t'/t = 0.13 \) and has an electron-like FS. The IC peak at 15 meV of the spin susceptibility has the correlation length of \( \xi \approx 2.7a \) and the broad high-energy feature has \( \xi \approx 0.6a \) [10]. The coupling constant was chosen such that \( \lambda = 1.98 \) to obtain the gap amplitude \( \Delta_0 = 11 \) meV at \( T = 0 \) in calculations.

Figures 4(a) and (b) are the imaginary and real parts of the diagonal self-energy along several cuts perpendicular to the Fermi surface in the BZ. The results may be understood similarly to the OP case. The single IC peak in the spin susceptibility has an intermediate correlation length and induces two peaks in \( -\Sigma_2(k, \omega) \). Because the correlation length is rather small, the angle dependence of the peaks at \( \omega_1 \approx -25 \) and \( \omega_2 \approx -75 \) meV is weak. The peak at \( \omega_1 \) is the shift of the DOS peak because \( \Delta_0 + \omega_{IC} \approx 26 \) meV. The peak

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**Figure 4.** The calculated imaginary and real parts of the diagonal self-energy of OV LSCO along several cuts in the BZ in the SC state.
at $\omega_2$ is from the $-(E(k + Q) + \omega_{IC})$ as was discussed in the OP case. We note that the VHS peak cannot appear in the negative energy because OV LSCO has an electron-like Fermi surface.

Figures 5(a) and (b) show the imaginary and real parts of the off-diagonal self-energy along several cuts in the BZ. The angle dependence is roughly d-wave like. The imaginary part of the off-diagonal self-energy $\phi_2(\theta, \omega)$ has a peak near $\omega_1 \approx 25$ meV and looks like the local spin susceptibility with the suppressed high frequency part as the OP case. The real part $\phi_1(\theta, \omega)$ begins to increase as $\omega$ increases from 0, has a peak and then decreases and makes a zero crossing near $\omega_1$ where the $\phi_2(\theta, \omega)$ has the IC peak.

4.3. UD La$_{2-x}$Sr$_x$CuO$_4$

The calculations were carried out for UD La$_{2-x}$Sr$_x$CuO$_4$ as well. The spin susceptibility spectrum reported by Lipscombe et al [10, 11] for 8% doping La$_{2-x}$Sr$_x$CuO$_4$ was used in the calculations. The spectrum $\chi_{sp}(\omega)$ has three parts, as the OP case; the IC peak near 15 meV, the CM peak near 45 meV, and a broad high frequency feature extrapolated up to 0.38 eV. The IC and CM peaks have the correlation lengths of $\xi \approx 2.45a$ and $0.8a$, respectively [11]. The coupling constant was chosen such that $\lambda = 1.58$ to obtain the gap amplitude $\Delta_0 = 17$ meV at $T = 0$ in the calculations [16].

Figures 6(a) and (b) are the imaginary and real parts of the diagonal self-energy along several cuts perpendicular to the Fermi surface in the BZ. The results may be understood similarly to the OP and OV cases. Because the peaks of the susceptibility are broader in frequency than OP and OV materials, the peaks in the self-energy are not as sharp as the OP and OV cases.

Figures 7(a) and (b) show the imaginary and real parts of the off-diagonal self-energy along several cuts. The angle dependence is roughly d-wave like. The two peaks in the diagonal and off-diagonal self-energy are from the IC and CM peaks of the spin susceptibility. Their energy in the imaginary parts is expected at $\omega_1 \approx \Delta_0 + \omega_{IC} \approx 32$ and $\omega_2 \approx \Delta_0 + \omega_{CM} \approx 62$ meV. The peaks in the real parts are shifted by the width. This is what we obtained from the calculations as shown in figures 6 and 7.

5. Summary and concluding remarks

We have calculated the full momentum and frequency dependence of the self-energy by solving the Eliashberg equation using the measured spin susceptibility from inelastic neutron scattering experiments on optimally doped, overdoped, and underdoped La$_{2-x}$Sr$_x$CuO$_4$ cuprates in the SC state. The real and imaginary parts of the diagonal
The present results may be checked against the proposed spin-fluctuation theory for the cuprate superconductivity. The direct evidence of the spin fluctuation theory will be to detect the angle and frequency dependence of the diagonal and off-diagonal self-energy experimentally and compare it with the results presented here. This will be an extension of the McMillan–Rowell procedure of phonon superconductor [21] to d-wave pairing. The experiment of choice for this purpose will be ARPES because of its high momentum and frequency resolution capability.

Indeed, the self-energy has been deduced by performing the momentum distribution curve analysis of the ARPES intensity for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. For La$_{2-x}$Sr$_x$CuO$_4$ crystals high quality ARPES data are not available for comparison though. The requirement of high resolution ARPES intensity data is being met only recently for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ using Laser ARPES [22, 13, 23].

If we compare the present calculations on LSCO with the ARPES analysis from BSCO, bearing the difference in mind, we notice that the peak intensity of the real part of the self-energy from BSCO does not change so much as the present calculations. From the nodal ($\theta = 0$) to $30^\circ$, the peak height changes by less than a factor of 1.5. The angle dependence of the peak position is different too. From nodal to anti-nodal direction the peak position decreases in contrast to though. The requirement of high resolution ARPES intensity data is being met only recently for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ using Laser ARPES [22, 13, 23].

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