

# Optical integral and sum-rule violation in high- $T_c$ superconductors

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The purpose of this work is to investigate the role of the lattice in the optical Kubo sum rule in the cuprates. We compute conductivities, optical integrals  $W$ , and the change between  $W$  in superconducting and normal states ( $\Delta W = W_{SC} - W_{NS}$ ) for two-dimensional systems with lattice dispersion typical of the cuprates. We study four different models—a dirty BCS model, a single Einstein boson model, a marginal Fermi-liquid model, and a collective boson model with a feedback from superconductivity on a collective boson. The goal of the paper is twofold. First, we analyze the dependence of  $W$  on the upper cutoff ( $\omega_c$ ) placed on the optical integral because in experiments  $W$  is measured up to frequencies of order bandwidth. For a BCS model, the Kubo sum rule is almost fully reproduced at  $\omega_c$  equal to the bandwidth. But for other models only 70–80 % of Kubo sum rule is obtained up to this scale and even less so for  $\Delta W$ , implying that the Kubo sum rule has to be applied with caution. Second, we analyze the sign of  $\Delta W$ . In all models we studied  $\Delta W$  is positive at small  $\omega_c$ , then crosses zero and approaches a *negative* value at large  $\omega_c$ , i.e., the optical integral in a superconductor is smaller than in a normal state within the one band model. The point of zero crossing, however, increases with the interaction strength and in a collective boson model becomes comparable to the bandwidth at strong coupling. We argue that this model exhibits the behavior consistent with that in the cuprates.

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## I. INTRODUCTION

The analysis of sum rules for optical conductivity has a long history. Kubo, in an extensive paper<sup>1</sup> in 1957, used a general formalism of a statistical theory of irreversible processes to investigate the behavior of the conductivity in electronic systems. For a system of interacting electrons, he derived the expression for the integral of the real part of a (complex) electric conductivity  $\sigma(\Omega)$  and found that it is independent on the nature of the interactions and reduces to

$$\int_0^{\infty} \text{Re } \sigma(\Omega) d\Omega = \frac{\pi n e^2}{2 m}. \quad (1)$$

Here  $n$  is the density of the electrons in the system and  $m$  is the bare mass of the electron. This expression is exact provided that the integration extends truly up to infinity, and its derivation uses the obvious fact that at energies higher than the total bandwidth of a solid, electrons behave as free particles.

The independence of the right-hand side (rhs) of Eq. (1) on temperature and the state of a solid (e.g., a normal or a superconducting state—henceforth referred to as NS and SCS, respectively) implies that, while the functional form of  $\sigma(\Omega)$  changes with, e.g., temperature, the total spectral weight is conserved and only gets redistributed between different frequencies as temperature changes. This conservation of the total weight of  $\sigma(\Omega)$  is generally called a sum rule.

One particular case, studied in detail for conventional superconductors, is the redistribution of the spectral weight between normal and superconducting states. This is known as Ferrel-Glover-Tinkham (FGT) sum rule<sup>2,3</sup>

$$\int_{0+}^{\infty} \text{Re } \sigma_{NS}(\Omega) = \int_{0+}^{\infty} \text{Re } \sigma_{SC}(\Omega) + \frac{\pi n_s e^2}{2m}, \quad (2)$$

where  $n_s$  is the superfluid density and  $\pi n_s e^2 / (2m)$  is the spectral weight under the  $\delta$ -functional piece of the conductivity in the superconducting state.

In practice, the integration up to an infinite frequency is hardly possible, and more relevant issue for practical applications is whether a sum rule is satisfied, at least approximately, for a situation when there is a single electron band which crosses the Fermi level and is well separated from other bands. Kubo considered this case in the same paper of 1957 and derived the expression for the “band” or Kubo sum rule

$$\int_0^{\infty} \text{Re } \sigma(\Omega) d\Omega = W_K = \frac{\pi e^2}{2N} \sum_{\vec{k}} \nabla_{k_x}^2 \epsilon_{\vec{k}} n_{\vec{k}}, \quad (3)$$

where  $n_{\vec{k}}$  is the electronic distribution function and  $\epsilon_{\vec{k}}$  is the band dispersion. Prime in the upper limit of the integration has the practical implication that the upper limit is much larger than the bandwidth of a given band which crosses the Fermi level but smaller than the frequencies of interband transitions. Interactions with external objects, e.g., phonons or impurities, and interactions between fermions are indirectly present in the distribution function which is expressed via the full fermionic Green’s function as  $n_{\vec{k}} = T \Sigma_m G(\vec{k}, \omega_m)$ . For  $\epsilon_k = k^2 / 2m$ ,  $\nabla_{k_x}^2 \epsilon_{\vec{k}} = 1/m$ , and  $W_K = \pi n e^2 / (2m)$ , and Kubo sum rule reduces to Eq. (1). In general, however,  $\epsilon_{\vec{k}}$  is a lattice dispersion, and Eqs. (1) and (3) are different. Most important,  $W_K$  in Eq. (3) generally depends on  $T$  and on the state of the system because of  $n_{\vec{k}}$ . In this situation, the temperature evolution of the optical integral does not reduce to a simple redistribution of the spectral weight—the whole spectral weight inside the conduction band changes with  $T$ . This issue was first studied in detail by Hirsch<sup>4</sup> who introduced the now frequently used notation “violation of the conductivity sum rule.”

In reality, as already pointed out by Hirsch, there is no true violation as the change of the total spectral weight in a given band is compensated by an appropriate change in the spectral weight in other bands such that the total spectral

weight, integrated over all bands, is conserved, as in Eq. (1). Still, nonconservation of the spectral weight within a given band is an interesting phenomenon as the degree of nonconservation is an indicator of relevant energy scales in the problem. Indeed, when relevant energy scales are much smaller than the Fermi energy, i.e., changes in the conductivity are confined to a near vicinity of a Fermi surface (FS), one can expand  $\varepsilon_k$  near  $k_F$  as  $\varepsilon_k = v_F(k - k_F) + (k - k_F)^2 / (2m_B) + O(k - k_F)^3$  and obtain  $\nabla_{k_x}^2 \varepsilon_{\vec{k}} \approx 1/m_B$  [this approximation is equivalent to approximating the density of states (DOS) by a constant]. Then  $W_K$  becomes  $\pi n e^2 / (2m_B)$  which does not depend on temperature. The scale of the temperature dependence of  $W_K$  is then an indicator how far in energy the changes in conductivity extend when, e.g., a system evolves from a normal metal to a superconductor. Because relevant energy scales increase with the interaction strength, the temperature dependence of  $W_K$  is also an indirect indicator of whether a system is in a weak, intermediate, or strong coupling regime.

In a conventional BCS superconductor—with constant density of states approximation as only the physics close to the Fermi surface is relevant—the only relevant scales are the superconducting gap  $\Delta$  and the impurity scattering rate  $\Gamma$ . Both are generally much smaller than the Fermi energy so the optical integral should be almost  $T$ -independent, i.e., the spectral weight lost in a superconducting state at low frequencies because of gap opening is completely recovered by the zero-frequency  $\delta$  function. In a clean limit, the weight which goes into a  $\delta$  function is recovered within frequencies up to  $4\Delta$ . This is the essence of FGT sum rule.<sup>2,3</sup> In a dirty limit, this scale is larger,  $O(\Gamma)$ , but still  $W_K$  is  $T$ -independent and there was no violation of sum rule.

The issue of sum rule attracted substantial interest in the studies of high- $T_c$  cuprates<sup>5–24</sup> in which pairing is without doubts a strong coupling phenomenon. From a theoretical perspective, the interest in this issue was originally triggered by a similarity between  $W_K$  and the kinetic energy  $K = 2 \sum \varepsilon_{\vec{k}} n_{\vec{k}}$ .<sup>18,25,26</sup> For a model with a simple tight-binding cosine dispersion  $\varepsilon_k \propto (\cos k_x + \cos k_y)$ ,  $\frac{d^2 \varepsilon_{\vec{k}}}{dk_x^2} \sim -\varepsilon_{\vec{k}}$ , and  $W_K = -K$ . For a more complex dispersion there is no exact relation between  $W_K$  and  $K$  but several groups argued<sup>17,27,28</sup> that  $W_K$  can still be regarded as a good monitor for the changes in the kinetic energy. In a BCS superconductor, kinetic energy increases below  $T_c$  because  $n_k$  extends to higher frequencies (see Fig. 2). At strong coupling,  $K$  not necessary increases because of opposite trend associated with the fermionic self-energy: fermions are more mobile in the SCS due to less space for scattering at low energies than they are in the NS. Model calculations show that above some coupling strength, the kinetic energy decreases below  $T_c$ .<sup>31</sup> While, as we said, there is no one-to-one correspondence between  $K$  and  $W_K$ , it is still likely that, when  $K$  decreases,  $W_K$  increases.

The sign of  $\Delta W_K$  has been analyzed in detail for the Hubbard model with attractive  $U$ , within the framework of BCS to BEC crossover. The transformation from a potential-energy-driven (BCS) mechanism to kinetic-energy-driven Bose-Einstein condensation (BEC) mechanism has been found and parallels have been drawn to relate this to moving

from overdoped to underdoped regimes in the cuprates.<sup>32,33</sup> There were also several investigations on the doping dependence of the optical sum in the  $t$ - $J$  model, see Ref. 34.

A good amount of experimental effort has been put into addressing the issue of the optical sum rule in the  $c$ -axis<sup>7</sup> and in-plane conductivities<sup>8–16</sup> in overdoped, optimally doped, and underdoped cuprates. The experimental results demonstrated, above all, outstanding achievements of experimental abilities as these groups managed to detect the value of the optical integral with the accuracy of a fraction of a percent. The analysis of the change in the optical integral between normal and SCS is even more complex because one has to (i) extend NS data to  $T < T_c$  and (ii) measure superfluid density with the same accuracy as the optical integral itself. The analysis of the optical integral showed that in overdoped cuprates it definitely decreases below  $T_c$ , in consistency with the expectations at weak coupling.<sup>11</sup> For underdoped cuprates, all experimental groups agree that a relative change in the optical integral below  $T_c$  gets much smaller. There is no agreement yet about the sign of the change in the optical integral: Molegraaf *et al.*<sup>8</sup> and Santander-Syro *et al.*<sup>9</sup> argued that the optical integral increases below  $T_c$  while Boris *et al.*<sup>10</sup> argued that it decreases.

Theoretical analysis of these results<sup>19,20,23,28,29</sup> added one more degree of complexity to the issue. It is tempting to analyze the temperature dependence of  $W_K$  and relate it to the observed behavior of the optical integral and some earlier works<sup>23,28,29</sup> followed this route. We direct the reader to Ref. 35 for a comprehensive review.

In the experiments, however, optical conductivity is integrated only up to a certain frequency  $\omega_c$  and the quantity which is actually measured is

$$W(\omega_c) = \int_0^{\omega_c} \text{Re } \sigma(\Omega) d\Omega = W_K + f(\omega_c),$$

$$f(\omega_c) = - \int_{\omega_c}^{\infty} \text{Re } \sigma(\Omega) d\Omega. \quad (4)$$

The Kubo formula, Eq. (3) is obtained assuming that the second part is negligible. This is not guaranteed, however, as typical  $\omega_c \sim 1-2$  eV are comparable to the bandwidth.

The differential sum rule  $\Delta W$  is also a sum of two terms

$$\Delta W(\omega_c) = \Delta W_K + \Delta f(\omega_c), \quad (5)$$

where  $\Delta W_K$  is the variation in the rhs of Eq. (3) and  $\Delta f(\omega_c)$  is the variation in the cutoff term. Because conductivity changes with  $T$  at all frequencies,  $\Delta f(\omega_c)$  also varies with temperature. If  $\Delta W(\omega_c)$  depends heavily on  $\Delta f(\omega_c)$ , it becomes the issue whether the experimentally observed  $\Delta W(\omega_c)$  is actually the “intrinsic,” cutoff-independent  $\Delta W_K$ , or just an incomplete integrated sum due to nonzero  $\Delta f(\omega_c)$ . From this perspective, it becomes relevant to know how much of the Kubo sum is actually recovered up to the scale of the bandwidth. (There is also the issue of corrections to the Kubo formula because of the close proximity of other bands in an actual experiment. But we do not take that into account).

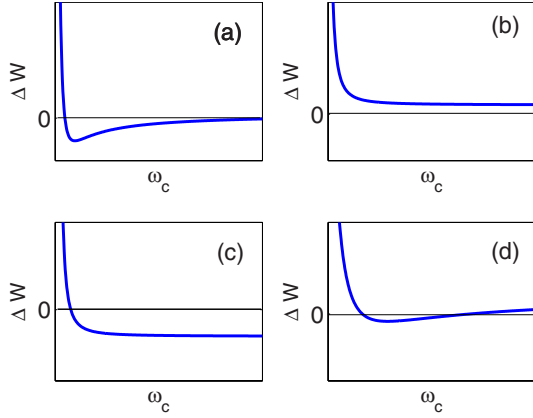


FIG. 1. (Color online) Schematic behavior of  $\Delta W$  vs  $\omega_c$ , Eq. (4). The limiting value of  $\Delta W$  at  $\omega_c = \infty$  is  $\Delta W_K$  given by Eq. (3). Depending on the value of  $\Delta W_K$ , there can be either one sign change of  $\Delta W$  (panels a and c), or no sign changes (panel b), or two sign changes (panel d).

For the NS, previous works<sup>19,20</sup> on particular models for the cuprates indicated that the origin of the temperature dependence of  $W(\omega_c)$  is likely the  $T$  dependence of the cutoff term  $f(\omega_c)$ . Specifically, Norman *et al.*<sup>20</sup> approximated a fermionic DOS by a constant (in which case, as we said,  $W_K$  does not depend on temperature) and analyzed the  $T$  dependence of  $W(\omega_c)$  which is now entirely due to the  $T$  dependence of the cut-off term. They found a good agreement with the experiments. This still does not solve the problem fully as amount of the  $T$  dependence of  $W_K$  in the same model but with a lattice dispersion has not been analyzed. For a superconductor, which of the two terms [ $\Delta W_K$  or  $\Delta f(\omega_c)$ ] contributes more, remains an open issue.

The conventional evolution of  $\Delta W(\omega_c)$  with the cutoff is explained as follows: at small cut-off frequencies,  $\Delta W(\omega_c)$  between SCS and NS is positive simply because  $\sigma(\Omega)$  in SCS has a  $\delta$ -functional term. In the models with a constant DOS (i.e., without the lattice)  $\Delta W_K = 0$ , and previous calculations<sup>19</sup> show that  $\Delta W(\omega_c)$  changes sign at some  $\omega_c$ , becomes negative at larger  $\omega_c$  and approaches zero from a negative side. The frequency when  $\Delta W(\omega_c)$  changes sign is of order  $\Delta$  at weak coupling but increases as the coupling increases and at large coupling becomes comparable to a bandwidth ( $\sim 1$  eV).

In the lattice models,  $\Delta W_K$  is nonzero, and the sign of  $\Delta W$  in the formal limit  $\omega_c = \infty$  is decided by  $\Delta W_K$ , i.e., it is positive for positive  $\Delta W_K$ , or negative for negative  $\Delta W_K$ . Still, in a physical system one has to restrict oneself to  $\omega_c$  comparable to the bandwidth to stay within the single-band picture. In this intermediate regime ( $\omega_c \sim$  bandwidth)  $\Delta W_K$  can still be potentially overshadowed by the cut-off term, i.e., the sign of  $\Delta W(\omega_c)$  at these  $\omega_c$  is not necessary the same as that of  $\Delta W_K$ . In particular,  $\Delta W$  can remain positive over a wide frequency range even when  $\Delta W_K$  is negative.  $\Delta W$  can even show more exotic behavior with more than one sign change (for a small positive  $\Delta W_K$ ). We show various cases schematically in Fig. 1.

In our work, we perform direct numerical calculations of optical integrals at  $T=0$  for a lattice dispersion extracted

from angle resolved photoemission (ARPES) studies of the cuprates. The goal of our work is twofold. First, we perform calculations of the optical integral in the NS and analyze how rapidly  $W(\omega_c)$  approaches  $W_K$ , in other words we check how much of the Kubo sum is recovered up to the scale of the bandwidth. Second, we analyze the difference between optical integral in the SCS at  $T=0$  and in the NS extrapolated to  $T=0$  and compare the cut-off effect  $\Delta f(\omega_c)$  to  $\Delta W_K$  term. We also analyze the sign of  $\Delta W(\omega_c)$  at large frequencies and discuss under what conditions theoretical  $W(\infty)$  increases in the SCS.

We perform calculations for four models. First is a conventional BCS with impurities (BCSI) model. Second is an Einstein boson (EB) model of fermions interacting with a single Einstein boson whose propagator does not change between NS and SCS. These two cases will illustrate a conventional idea of the spectral weight in SCS being less than in NS. Then we consider two more sophisticated models: a phenomenological “marginal Fermi liquid with impurities” (MFLI) model of Norman and Pépin,<sup>29</sup> and a microscopic collective-boson (CB) model<sup>36</sup> in which in the NS fermions interact with a gapless continuum of bosonic excitations, but in a  $d$ -wave SCS a gapless continuum splits into a resonance and a gaped continuum. This model describes, in particular, interaction of fermions with their own collective spin fluctuations<sup>37</sup> via

$$\Sigma(k, \Omega) = 3g^2 \int \frac{d\omega}{2\pi} \frac{d^2q}{(2\pi)^2} \chi(q, \omega) G(k+q, \omega + \Omega), \quad (6)$$

where  $g$  is the spin-fermion coupling, and  $\chi(q, \omega)$  is the spin susceptibility whose dynamics changes between NS and SCS.

From our analysis we found that the introduction of a finite fermionic bandwidth by means of a lattice has generally a notable effect on both  $W$  and  $\Delta W$ . We found that for all models except for BCSI model, only 70–80 % of the optical spectral weight is obtained by integrating up to the bandwidth. In these three models, there also exists a wide range of  $\omega_c$  in which the behavior of  $\Delta W(\omega_c)$  is due to variation in  $\Delta f(\omega_c)$  which is dominant comparable to the  $\Delta W_K$  term. This dominance of the cut-off term is consistent with the analysis in Refs. 19, 20, and 38.

We also found that for all models except for the original version of the MFLI model the optical weight at the highest frequencies is greater in the NS than in the SCS (i.e.,  $\Delta W < 0$ ). This observation is consistent with the findings of Abanov and Chubukov,<sup>58</sup> Benfatto *et al.*,<sup>28</sup> and Karakozov and Maksimov.<sup>39</sup> In the original version of the MFLI model<sup>29</sup> the spectral weight in SCS was found to be greater than in the NS ( $\Delta W > 0$ ). We show, however, that the behavior of  $\Delta W(\omega_c)$  in this model crucially depends on how the fermionic self-energy modeled to fit ARPES data in a NS is modified when a system becomes a superconductor.

The negative  $\Delta W_K$  implies that  $\Delta W$  is negative, when the integration is extended to sufficiently large frequencies (if, indeed, there exists a sufficiently wide range between a given band and other bands). This behavior would be consistent with Ref. 10.

We also found, however, that  $\omega_c$  at which  $\Delta W$  becomes negative rapidly increases with the coupling strength and at strong coupling becomes comparable to the bandwidth, i.e., at strong enough coupling  $\Delta W$  may remain positive up to 1 eV. This would be consistent with Refs. 8 and 9. In the CB model, which, we believe, is most appropriate for the application to the cuprates,  $\Delta W_K = \Delta W(\infty)$  is quite small, and at strong coupling a positive  $\Delta W(\omega_c)$  up to  $\omega_c \sim 1$  eV is nearly compensated by the optical integral between  $\omega_c$  and “infinity,” which, in practice, is an energy of interband transitions, which is roughly 2 eV. This is again consistent with Refs. 8 and 9.

Our result about  $\Delta W$  being negative is consistent with previous works.<sup>23,40</sup> Ref. 23 had found that  $\Delta W$  can change sign and become positive near a van Hove singularity. Our consideration is for doping far away from van Hove singularity (see Sec. II).

We begin with formulating our calculational basis in the next section. Then we take up the four cases and consider in each case the extent to which the Kubo sum is satisfied up to the order of bandwidth and the functional form and the sign of  $\Delta W(\omega_c)$ . The last section presents our conclusions.

## II. OPTICAL INTEGRAL IN NORMAL AND SUPERCONDUCTING STATES

The generic formalism of the computation of the optical conductivity and the optical integral has been discussed several times in the literature<sup>19–21,24,31,41</sup> and we just list the formulas that we used in our computations. The conductivity  $\sigma(\Omega)$  and the optical integral  $W(\omega_c)$  at  $T=0$ , which we consider here, are given by<sup>41</sup>

$$\sigma'(\Omega) = \text{Im} \left[ -\frac{\Pi(\Omega)}{\Omega + i\delta} \right] = -\frac{\Pi''(\Omega)}{\Omega} + \pi\delta(\Omega)\Pi'(0), \quad (7a)$$

$$W(\omega_c) = \int_0^{\omega_c} \sigma'(\Omega) d\Omega = -\int_{0+}^{\omega_c} \frac{\Pi''(\Omega)}{\Omega} d\Omega + \frac{\pi}{2}\Pi'(0), \quad (7b)$$

where “ $X'$ ” and “ $X''$ ” stand for real and imaginary parts of  $X$ .

Note that these equations are correct when the integration over intermediate momenta is performed before the integration over intermediate frequencies. In our numerical computational scheme we perform the integration over frequency first and then sum over the momenta in the first Brillouin zone. In this situation, the expression for  $\Pi'(0)$  in Eq. (8c) contains the extra term equal to  $\Sigma \nabla^2 \varepsilon_{\vec{k}} n_{\vec{k}}$ . This term reduces to the usual  $ne^2/m$ , (or 1 in our units) for the continuum case (see Ref. 41).

The polarization operator  $\Pi(\Omega)$  is (see Ref. 42)

$$\Pi(i\Omega) = T \sum_{\omega} \sum_{\vec{k}} (\nabla_{\vec{k}} \varepsilon_{\vec{k}})^2 [G(i\omega, \vec{k})G(i\omega + i\Omega, \vec{k}) + F(i\omega, \vec{k})F(i\omega + i\Omega, \vec{k})], \quad (8a)$$

TABLE I. Dispersion fit using tight-binding basis functions (Ref. 44).

$c_i$ (in eV)	$\eta_i(\vec{k})$
0.1305	1
-0.5951	$\frac{1}{2}(\cos k_x + \cos k_y)$
0.1636	$\cos k_x \cos k_y$
-0.0519	$\frac{1}{2}(\cos 2k_x + \cos 2k_y)$
-0.1117	$\frac{1}{2}(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y)$
0.0510	$\cos 2k_x \cos 2k_y$

$$\Pi''(\Omega) = -\frac{1}{\pi} \sum_{\vec{k}} (\nabla_{\vec{k}} \varepsilon_{\vec{k}})^2 \int_{-\Omega}^0 d\omega [G''(\omega, \vec{k})G''(\omega + \Omega, \vec{k}) + F''(\omega, \vec{k})F''(\omega + \Omega, \vec{k})], \quad (8b)$$

$$\Pi'(0) = \frac{1}{\pi^2} \sum_{\vec{k}} (\nabla_{\vec{k}} \varepsilon_{\vec{k}})^2 \int' \int' dx dy [G''(x, \vec{k})G''(y, \vec{k}) + F''(x, \vec{k})F''(y, \vec{k})] \frac{n_F(y) - n_F(x)}{y - x}, \quad (8c)$$

where  $\int'$  denotes the principal value of the integral,  $\Sigma_{\vec{k}}$  is understood to be  $\frac{1}{N} \sum_{\vec{k}}$ , ( $N$  is the number of lattice sites),  $n_F(x)$  is the Fermi function which is a step function at zero temperature,  $G$  and  $F$  are the normal and anomalous Green's functions given by<sup>43</sup> for a NS

$$G(\omega, \vec{k}) = \frac{1}{\omega - \Sigma(k, \omega) - \varepsilon_{\vec{k}} + i\delta} \quad (9a)$$

for a SCS

$$G(\omega, \vec{k}) = \frac{Z_{k,\omega} \omega + \varepsilon_{\vec{k}}}{Z_{k,\omega}^2 (\omega^2 - \Delta_{k,\omega}^2) - \varepsilon_{\vec{k}}^2 + i\delta \text{sgn}(\omega)}, \quad (9b)$$

$$F(\omega, \vec{k}) = \frac{Z_{k,\omega} \Delta_{k,\omega}}{Z_{k,\omega}^2 (\omega^2 - \Delta_{k,\omega}^2) - \varepsilon_{\vec{k}}^2 + i\delta \text{sgn}(\omega)}, \quad (9c)$$

where  $Z_{k,\omega} = 1 - \frac{\Sigma(k,\omega)}{\omega}$ , and  $\Delta_{k,\omega}$  is the SC gap. We emphasize that  $\Sigma(\omega)$  defined this way is the “normal” self-energy. Throughout the text, the term “self-energy” would refer to this normal self-energy. Following earlier works,<sup>36,38</sup> we assume that the fermionic self-energy  $\Sigma(k, \omega)$  predominantly depends on frequency and approximate  $\Sigma(k, \omega) \approx \Sigma(\omega)$  and also neglect the frequency dependence of the gap, i.e., approximate  $\Delta_{k,\omega}$  by a  $d$ -wave  $\Delta_k$ .

The lattice dispersion  $\varepsilon_{\vec{k}} = \sum c_i \eta_i(\vec{k})$  is taken from Ref. 44, where tight-binding basis functions  $\eta_i(\vec{k})$  were used to fit the experimental dispersion. These  $\eta_i(\vec{k})$  are summarized in Table I. In the calculations, we rescaled all  $c_i$  to obtain the bandwidth of 1 eV. The chemical potential is chosen to satisfy Luttinger theorem. For dopings relevant to the cuprates, this gives a Fermi surface consisting of four “quadrants” at the corners of the Brillouin zone. Also, with this choice we

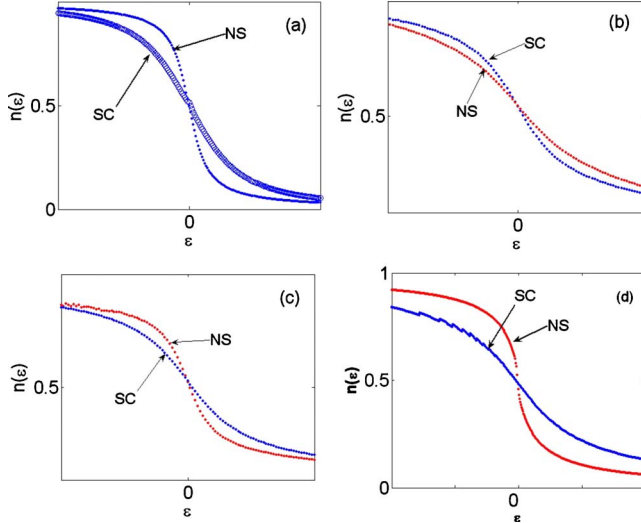


FIG. 2. (Color online) Distribution functions in four cases (a) BCSI model, where one can see that for  $\epsilon > 0$ ,  $SC > NS$  implying KE increases in the SCS. (b) The original MFLI model of Ref. 29, where for  $\epsilon > 0$ ,  $SC < NS$ , implying KE decreases in the SCS. (c) Our version of MFLI model (see text) and (d) the CB model. In both cases,  $SC > NS$ , implying KE increases in the SCS. Observe that in the impurity-free CB model there is no jump in  $n(\epsilon)$  indicating lack of fermionic coherence. This is consistent with ARPES (Ref. 30). In MFLI case, the smearing of  $n(\epsilon)$  is due to impurity scattering.

are far from van Hove singularities. To calculate  $W_K$ , one has to evaluate the Kubo term in Eq. (3) wherein the distribution function  $n_{\vec{k}}$ , is calculated from

$$n(\epsilon_{\vec{k}}) = -2 \int_{-\infty}^0 \frac{d\omega}{2\pi} G''(\omega, \vec{k}). \quad (10)$$

The 2 is due to the trace over spin indices. We show the distribution functions in the NS and SCS under different circumstances in Fig. 2.

The  $\vec{k}$  summation is done over first Brillouin zone for a two-dimensional lattice with a  $62 \times 62$  grid. The frequency integrals are done analytically wherever possible, otherwise performed using Simpson's rule for all regular parts. Contributions from the poles are computed separately using Cauchy's theorem. For comparison, in all four cases we also calculated FGT sum rule by replacing  $\int d^2k = d\Omega_k d\epsilon_k \nu_{\epsilon_k, \Omega_k}$  and keeping  $\nu$  constant. We remind that the FGT is the result when one assumes that the integral in  $W(\omega_c)$  predominantly comes from a narrow region around the Fermi surface.

We will first use Eq. (3) and compute  $W_K$  in NS and SCS. This will tell us about the magnitude of  $\Delta W(\omega_c = \infty)$ . We next compute the conductivity  $\sigma(\omega)$  using the equations listed above, find  $W(\omega_c)$  and  $\Delta W(\omega_c)$  and compare  $\Delta f(\omega_c)$  and  $\Delta W_K$ .

For simplicity and also for comparisons with earlier studies, for BCSI, EB, and MFLI models we assumed that the gap is just a constant along the FS. For CB model, we used a  $d$ -wave gap and included into consideration the fact that, if

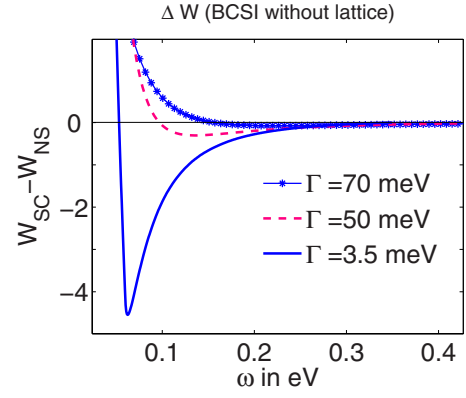


FIG. 3. (Color online) The BCSI case with a dispersion linearized around the Fermi surface. Evolution of the difference of optical integrals in the SCS and the NS with the upper cutoff  $\omega_c$ . Observe that the zero-crossing point increases with impurity scattering rate  $\Gamma$  and also the “dip” spreads out with increasing  $\Gamma$ .  $\Delta = 30$  meV.

a CB is a spin fluctuation, its propagator develops a resonance when the pairing gap is  $d$  wave.

#### A. BCS case

In BCS theory the quantity  $Z(\omega)$  is given by

$$Z_{\text{BCSI}}(\omega) = 1 + \frac{\Gamma}{\sqrt{\Delta^2 - (\omega + i\delta)^2}} \quad (11)$$

and

$$\Sigma_{\text{BCSI}}(\omega) = \omega[Z(\omega) - 1] = i\Gamma \frac{\omega}{\sqrt{(\omega + i\delta)^2 - \Delta^2}}. \quad (12)$$

This is consistent with having in the NS,  $\Sigma = i\Gamma$  in accordance with Eq. (6). In the SCS,  $\Sigma(\omega)$  is purely imaginary for  $\omega > \Delta$  and purely real for  $\omega < \Delta$ . The self-energy has a square-root singularity at  $\omega = \Delta$ .

It is worth noting that Eq. (12) is derived from the integration over infinite band. If one uses Eq. (6) for finite band, Eq. (12) acquires an additional frequency dependence at large frequencies of the order of bandwidth [the low-frequency structure still remains the same as in Eq. (12)]. In principle, in a fully self-consistent analysis, one should indeed evaluate the self-energy using a finite bandwidth. In practice, however, the self-energy at frequencies of order bandwidth is generally much smaller than  $\omega$  and contribute very little to optical conductivity which predominantly comes from frequencies where the self-energy is comparable or even larger than  $\omega$ . Keeping this in mind, below we will continue with the form of self-energy derived from infinite band. We use the same argument for all four models for the self-energy.

For completeness, we first present some well-known results about the conductivity and optical integral for a constant DOS and then extend the discussion to the case where the same calculations are done in the presence of a particular lattice dispersion. For a constant DOS,  $\Delta W(\omega_c) = W_{\text{SC}}(\omega_c) - W_{\text{NS}}(\omega_c)$  is zero at  $\omega_c = \infty$  and Kubo sum rule reduces to FGT sum rule. In Fig. 3 we plot for this case

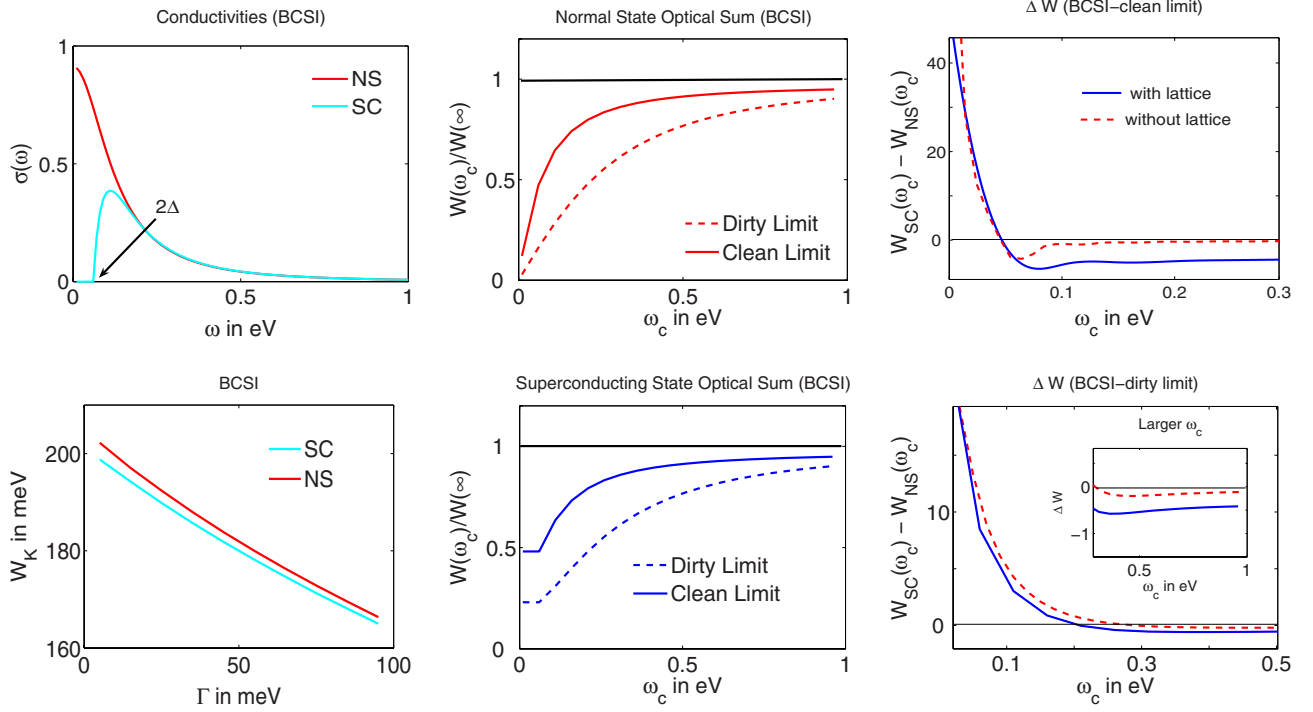


FIG. 4. (Color online) Left Panel: top—conductivity plot for the BCS case in the presence of a lattice. The parameters are  $\Delta=30$  meV and  $\Gamma=3.5$  meV. Bottom—the behavior of Kubo sums ( $W_K$ ). Note that the spectral weight in the NS is always greater in the SCS and decreases with  $\Gamma$ . Center panel: the evolution of optical integral in NS (top) and SCS (bottom). Plots are made for clean limit (solid lines,  $\Gamma=3.5$  meV) and dirty limit (dashed lines,  $\Gamma=150$  meV) for  $\Delta=30$  meV. Observe that  $\sim 90$ – $95\%$  of the spectral weight is recovered up to 1 eV. Right panel: evolution of  $\Delta W$  in the presence of a lattice (solid line) compared with the case of no lattice (a constant DOS, dashed line) for clean and dirty limits.

$\Delta W(\omega_c)$  as a function of the cutoff  $\omega_c$  for different  $\Gamma$ 's. The plot shows the two well-known features: zero-crossing point is below  $2\Delta$  in the clean limit  $\Gamma \ll \Delta$  and is roughly  $2\Gamma$  in the dirty limit<sup>19,45</sup>. The magnitude of the “dip” decreases quite rapidly with increasing  $\Gamma$ . Still, there is always a point of zero crossing and  $\Delta W(\omega_c)$  at large  $\omega_c$  approaches zero from below.

We now perform the same calculations in the presence of lattice dispersion. The results are summarized in Fig. 4.

Figure 4 shows conductivities  $\sigma(\omega)$  in the NS and the SCS and Kubo sums  $W_K$  plotted against impurity scattering  $\Gamma$ . We see that the optical integral in the NS is always greater than in the SCS. The negative sign of  $\Delta W_K$  is a consequence of the fact that  $n_k$  is larger in the NS for  $\epsilon_k > 0$  and smaller for  $\epsilon_k < 0$ , and  $\nabla^2 \epsilon_{\vec{k}}$  closely follows  $-\epsilon_{\vec{k}}$  for our choice of dispersion<sup>44</sup>). Hence  $n_k$  is larger in the NS for  $\nabla^2 \epsilon_{\vec{k}} > 0$  and smaller for  $\nabla^2 \epsilon_{\vec{k}} < 0$  and the Kubo sum rule, which is the integral of the product of  $n_k$  and  $\nabla^2 \epsilon_{\vec{k}}$  [Eq. (3)], is larger in the normal state.

We also see from Fig. 4 that  $\Delta W_K$  decreases with  $\Gamma$  reflecting the fact that with too much impurity scattering there is little difference in  $n_k$  between NS and SCS. The center panel in the figure shows the optical sum in NS and SCS in clean and dirty limits (the parameters are stated in the figure). This plot shows that the Kubo sums are almost completely recovered by integrating up to the bandwidth of 1 eV: the recovery is 95% in the clean limit and  $\sim 90\%$  in the dirty limit. In the right panel we plot  $\Delta W(\omega_c)$  as a function of  $\omega_c$  in clean and dirty limits.  $\Delta W(\infty)$  is now nonzero, in agree-

ment with the plot for  $\Delta W_K$  and we also see that there is little variation in  $\Delta W(\omega_c)$  above 0.1–0.3 eV what implies that for larger  $\omega_c$ ,  $\Delta W(\omega_c) \approx \Delta W_K \gg \Delta f(\omega_c)$  or in simpler terms no cut-off dependence.

To make this more quantitative, we compare in Fig. 4 right panel  $\Delta W(\omega_c)$  obtained for a constant DOS, when  $\Delta W(\omega_c) = \Delta f(\omega_c)$ , and for the actual lattice dispersion, when  $\Delta W(\omega_c) = \Delta W_K + \Delta f(\omega_c)$ . In the clean limit there is obviously little cutoff dependence beyond 0.1 eV, i.e.,  $\Delta f(\omega_c)$  is truly small, and the difference between the two cases is just  $\Delta W_K$ . In the dirty limit, the situation is similar but there is obviously more variation with  $\omega_c$  and  $\Delta f(\omega_c)$  becomes truly small only above 0.3 eV. Note also that the position of the dip in  $\Delta W(\omega_c)$  in the clean limit is at a larger  $\omega_c$  in the presence of the lattice than in a continuum.

## B. Einstein boson model

We next consider the case of electrons interacting with a single boson mode which by itself is not affected by superconductivity. The primary candidate for such mode is an optical phonon. The imaginary part of the NS self-energy has been discussed numerous times in the literature. We make one simplifying assumption—approximate the DOS by a constant in calculating fermionic self-energy. We will, however, keep the full lattice dispersion in the calculations of the optical integral. The advantage of this approximation is that the self-energy can be computed analytically. The full self-energy obtained with the lattice dispersion is more involved

and can only be obtained numerically but its structure is quite similar to the one obtained with a constant DOS.

The self-energy for a constant DOS is given by

$$\Sigma(i\omega) = -\frac{i}{2\pi}\lambda \int d\epsilon_k d(i\Omega)\chi(i\Omega)G(\epsilon_k, i\omega + i\Omega), \quad (13)$$

where

$$\chi(i\Omega) = \frac{\omega_0^2}{\omega_0^2 - (i\Omega)^2} \quad (14)$$

and  $\lambda$  is a dimensionless electron-boson coupling. Integrating and transforming to real frequencies, we obtain

$$\begin{aligned} \Sigma''(\omega) &= -\frac{\pi}{2}\lambda\omega_0\Theta(|\omega| - \omega_0), \\ \Sigma'(\omega) &= -\frac{1}{2}\lambda\omega_0 \log\left|\frac{\omega + \omega_0}{\omega - \omega_0}\right|. \end{aligned} \quad (15)$$

In the SCS, we obtain for  $\omega < 0$

$$\begin{aligned} \Sigma''(\omega) &= -\frac{\pi}{2}\lambda\omega_0 \operatorname{Re}\left(\frac{\omega + \omega_0}{\sqrt{(\omega + \omega_0)^2 - \Delta^2}}\right), \\ \Sigma'(\omega) &= -\frac{1}{2}\lambda\omega_0 \operatorname{Re} \int d\omega' \frac{1}{\omega_0^2 - \omega'^2 - i\delta} \frac{\omega + \omega'}{\sqrt{(\omega + \omega')^2 - \Delta^2}}. \end{aligned} \quad (16)$$

Observe that  $\Sigma''(\omega)$  is nonzero only for  $\omega < -\omega_0 - \Delta$ . Also, although it does not straightforwardly follow from Eq. (16) but real and imaginary parts of the self-energy do satisfy  $\Sigma'(\omega) = -\Sigma'(-\omega)$  and  $\Sigma''(\omega) = \Sigma''(-\omega)$ .

Figure 5 shows conductivities  $\sigma(\omega)$  and Kubo sums  $W_K$  as a function of the dimensionless coupling  $\lambda$ . We see that, like in the previous case, the Kubo sum in the NS is larger than that in the SCS. The difference  $\Delta W_K$  is between 5 and 8 meV.

The figure also shows the evolution of the optical integrals. Here we see the difference with the BCS model—only about 75% of the optical integral is recovered, both in the NS and SCS, when we integrate up to the bandwidth of 1 eV. The rest will be recovered from higher frequencies.

In Fig. 6 we plot  $\Delta W(\omega_c)$  as a function of  $\omega_c$ . We see the same behavior as in the BCS model in a clean limit— $\Delta W(\omega_c)$  is positive at small frequencies, crosses zero at some  $\omega_c$ , passes through a deep minimum at a larger frequency, and eventually saturates at a negative value at the largest  $\omega_c$ . However, in distinction to BCS model,  $\Delta W(\omega_c)$  keeps varying with  $\omega_c$  up a much larger scale and saturates only at around 0.8 eV. In between the dip at 0.1 and 0.8 eV, the behavior of the optical integral is predominantly determined by the variation of the cut-off term  $\Delta f(\omega_c)$  up to larger  $\omega_c$ . When compared to the BCS case we see that the cut-off term is significant for relatively larger  $\omega_c$  and when it eventually saturates deviation is then explained by  $\Delta W_K$ .

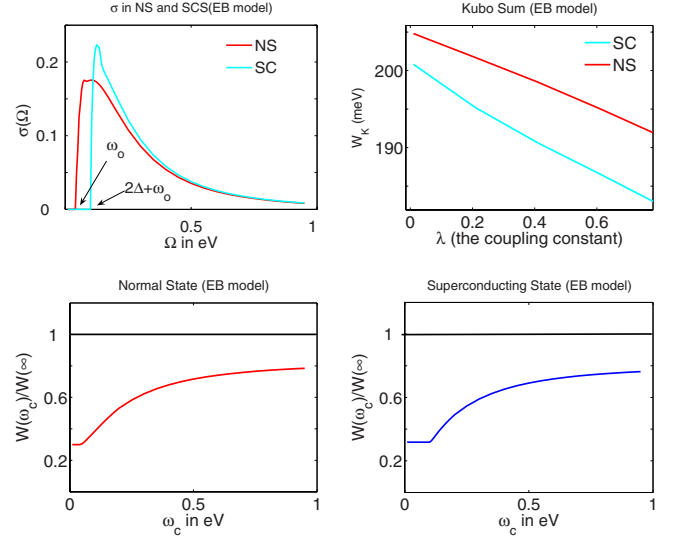


FIG. 5. (Color online) Top Panel: left—conductivities in the NS and the SCS for the EB model. The conductivity in the NS vanishes below  $\omega_0$  because of no phase space for scattering. Right—Kubo sums as a function of coupling. Observe that  $W_K$  in the SCS is below that in the NS. Bottom Panel: evolution of the optical integrals in the EB model. Note that  $W(0)$  has a nonzero value at  $T=0$  in the NS because the self-energy at small frequencies is purely real and linear in  $\omega$  hence the polarization bubble  $\Pi(0) \neq 0$ , as in an ideal Fermi gas. We set  $\omega_0=40$  meV,  $\Delta=30$  meV, and  $\lambda=.5$

### C. Marginal Fermi-liquid model

For their analysis of the optical integral, Norman and Pépin<sup>29</sup> introduced a phenomenological model for the self-energy which fits normal-state scattering-rate measurements by ARPES.<sup>46</sup> It constructs the NS  $\Sigma''(\omega)$  out of two contributions—impurity scattering and electron-electron scattering which they approximated phenomenologically by the marginal Fermi-liquid form of  $\alpha\omega$  at small frequencies<sup>6</sup> (MFLI model). The total  $\Sigma''$  is

$$\Sigma''(\omega) = \Gamma + \alpha|\omega|f\left(\frac{\omega}{\omega_{sat}}\right), \quad (17)$$

where  $\omega_{sat}$  is about  $\sim \frac{1}{2}$  of the bandwidth, and  $f(x) \approx 1$  for  $x < 1$  and decreases for  $x > 1$ . In Ref. 29  $f(x)$  was assumed to

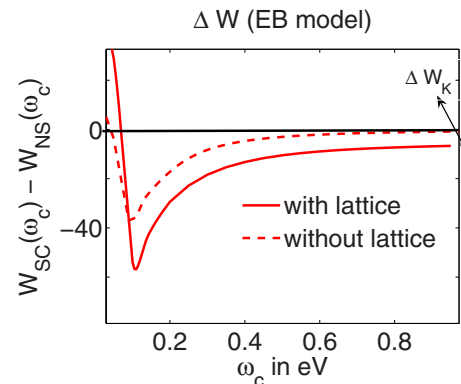


FIG. 6. (Color online)  $\Delta W$  vs the cutoff for the EB model. It remains negative for larger cutoffs. Parameters are the same as before. The dot indicates the value of  $\Delta W(\infty) = \Delta W_K$ .

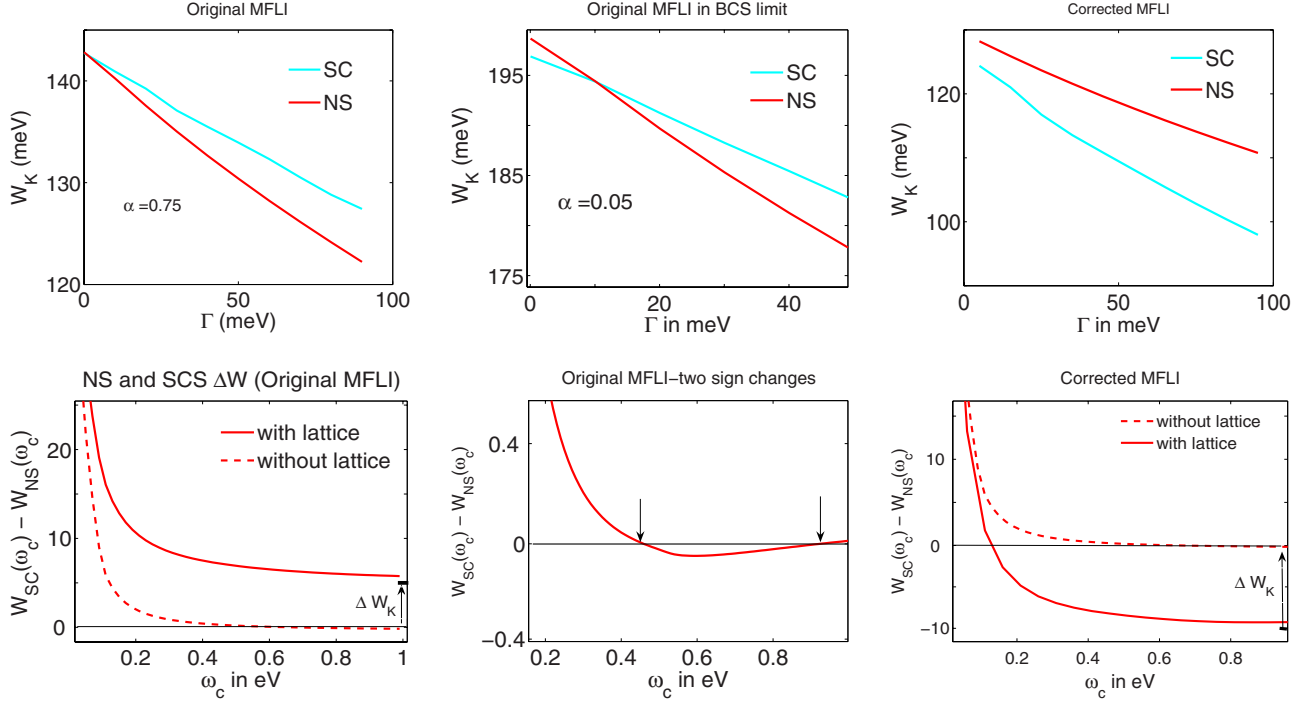


FIG. 7. (Color online) Left panel: top  $W_K$  in the original MFLI model of Ref. 29. We use  $\Gamma=70$  meV,  $\alpha=0.75$ ,  $\Delta=32$  meV, and  $\omega_1=71$  meV. Bottom—evolution of  $\Delta W(\omega_c)$  with the upper cutoff  $\omega_c$ . Observe that  $\Delta W(\omega_c) > 0$  and that it has not yet reached  $\Delta W_K$  up to the bandwidth. The dashed line is the FGT result. Center panel: top—behavior of  $W_K$  with  $\Gamma$  for the original MFLI model in BCS limit ( $\alpha=0.05$ ,  $\omega_1=\Delta=32$  meV). Observe the inconsistency with  $W_K$  in the BCS model in Fig. 4. Bottom—showing the possibility of two sign changes (indicated by the arrows) in original MFLI ( $\alpha=1.5$ ,  $\Gamma=5$  meV). Right panel: the same as left panel but in the corrected MFLI model (see main text). Observe that here  $\Delta W(\omega_c) < 0$ .

scale as  $1/x$  at large  $x$  such that  $\Sigma''$  is flat at large  $\omega$ . The real part of  $\Sigma(\omega)$  is obtained from Kramers-Krönig relations. For the superconducting state, they obtained  $\Sigma''$  by cutting off the NS expression on the lower end at some frequency  $\omega_1$  (the analog of  $\omega_0 + \Delta$  that we had for EB model)

$$\Sigma''(\omega) = \left[ \Gamma + \alpha |\omega| f\left(\frac{\omega}{\omega_{sat}}\right) \right] \Theta(|\omega| - \omega_1), \quad (18)$$

where  $\Theta(x)$  is the step function. In reality,  $\Sigma''$  which fits ARPES in the NS has some angular dependence along the Fermi surface<sup>47</sup> but this was ignored for simplicity. This model had gained a lot of attention as it predicted the optical sum in the SCS to be larger than in the NS, i.e.,  $\Delta W > 0$  at large frequencies. This would be consistent with the experimental findings in Refs. 8 and 9 if, indeed, one identifies  $\Delta W$  measured up to 1eV with  $\Delta W_K$ .

We will show below that the sign of  $\Delta W$  in the MFLI model actually depends on how the normal state results are extended to the superconducting state and, moreover, will argue that  $\Delta W_K$  is actually negative if the extension is done such that at  $\alpha=0$  the results are consistent with BCS model. However, before that, we show in Fig. 7 the conductivities and the optical integrals for the original MFLI model.

In Fig. 7 we plot the conductivities in the NS and the SCS and Kubo sums  $W_K$  vs  $\Gamma$  at  $\alpha=0.75$  showing that the spectral weight in the SCS is indeed larger than in the NS. We find that only  $\sim 75-80\%$  of the Kubo sum is recovered up to the scale of the bandwidth implying that there is indeed a sig-

nificant spectral weight well beyond the bandwidth. We also show the behavior of  $\Delta W(\omega_c)$ . We see that it does not change sign and remain positive at all  $\omega_c$ , very much unlike the BCS case. Comparing the behavior of  $W(\omega_c)$  with and without a lattice (solid and dashed lines in the figure) we see that the “finite-bandwidth effect” just shifts the curve in the positive direction. We also see that the solid line flattens above roughly half of the bandwidth, i.e., at these frequencies  $\Delta W(\omega_c) \approx \Delta W_K$ . Still, we found that  $\Delta W$  continues going down even above the bandwidth and truly saturates only at about 2 eV (not shown in the figure) supporting the idea that there is “more” left to recover from higher frequencies.

The rationale for  $\Delta W_K > 0$  in the original MFLI model has been provided in Ref. 29. They argued that this is closely linked to the absence of quasiparticle peaks in the NS and their restoration in the SCS state because the phase space for quasiparticle scattering at low energies is smaller in a superconductor than in a normal state. This clearly affects  $n_k$  because it is expressed via the full Green’s function and competes with the conventional effect of the gap opening. The distribution function from this model, which we show in Fig. 2(b) brings this point out by showing that in a MFLI model, at  $\epsilon < 0$ ,  $n_k$  in a superconductor is larger than  $n_k$  in the normal state, in clear difference with the BCS case.

We analyzed the original MFLI model for various parameters and found that the behavior presented in Fig. 7 left panel, where  $\Delta W(\omega_c) > 0$  for all frequencies, is typical but not a generic one. There exists a range of parameters  $\alpha$  and  $\Gamma$  where  $\Delta W_K$  is still positive but  $\Delta W(\omega_c)$  changes the sign



twice and is negative at intermediate frequencies. We show an example of such behavior also in right panel in Fig. 7. Still, for most of the parameters, the behavior of  $\Delta W(\omega_c)$  is the same as in the left panel of Fig. 7.

On more careful looking we found the problem with the original MFLI model. We recall that in this model the self-energy in the SCS state was obtained by just cutting the NS self energy at  $\omega_1$  [see Eq. (18)]. We argue that this phenomenological formalism is not fully consistent, at least for small  $\alpha$ . Indeed, for  $\alpha=0$ , the MFLI model reduces to BCSI model for which the behavior of the self-energy is given by Eq. (12). This self-energy evolves with  $\omega$  and  $\Sigma''$  has a square-root singularity at  $\omega=\Delta+\omega_o$  (with  $\omega_o=0$ ). Meanwhile  $\Sigma''$  in the original MFLI model in Eq. (18) simply jumps to zero at  $\omega=\omega_1=\Delta$  and this happens for all values of  $\alpha$  including  $\alpha=0$  where the MFLI and BCSI model should merge. This inconsistency is reflected in Fig. 7 center panel, where we plot the near-BCS limit of MFLI model by taking a very small  $\alpha=0.05$ . We see that the optical integral  $W_K$  in the SCS still remains larger than in the NS over a wide range of  $\Gamma$ , in clear difference with the exactly known behavior in the BCSI model, where  $W_K$  is larger in the NS for all  $\Gamma$  (see Fig. 4). In other words, the original MFLI model does not have the BCSI theory as its limiting case.

We modified the MFLI model in a minimal way by changing the damping term in a SCS to  $\frac{\Gamma}{\sqrt{-\omega^2+\Delta^2}}$  to be consistent with BCSI model. We still use Eq. (18) for the MFL term simply because this term was introduced in the NS on phenomenological grounds and there is no way to guess how it gets modified in the SCS state without first deriving the normal state self-energy microscopically (this is what we will do in the next section). The results of the calculations for the modified MFLI model are presented in Fig. 7 right panel. We clearly see that the behavior is now different and  $\Delta W_K < 0$  for all  $\Gamma$ . This is the same behavior as we previously found in BCSI and EB models. So we argue that the ‘‘unconventional’’ behavior exhibited by the original MFLI model is most likely the manifestation of a particular phenomenological approach towards modeling the NS and SCS self-energies. Nevertheless it did make a valid point that the quasiparticles behave more close to free fermions in a SCS than in a NS, and this effect tends to reverse the signs of  $\Delta W_K$  and of the kinetic energy.<sup>48</sup> It just happens that in the corrected MFLI model the optical integral is still larger in the NS.

#### D. Collective boson model

We now turn to a more microscopic model—the CB model. The model describes fermions interacting by exchanging soft, overdamped collective bosons in a particular, near-critical, spin, or charge channel.<sup>36,49,50</sup> This interaction is responsible for the normal state self-energy and also gives rise to a superconductivity. A peculiar feature of the CB model is that the propagator of a collective boson changes below  $T_c$  because this boson is not an independent degree of freedom (as in EB model) but is made out of low-energy fermions which are affected by superconductivity.<sup>37</sup>

The most relevant point for our discussion is that this model contains the physics which we identified above as a

source of a potential sign change of  $\Delta W_K$ . Namely, at strong coupling the fermionic self-energy in the NS is large because there exists strong scattering between low-energy fermions mediated by low-energy collective bosons. In the SCS, the density of low-energy fermions drops and a continuum collective excitations becomes gaped. Both effects reduce fermionic damping and lead to the increase in  $W_K$  in a SCS. If this increase exceeds a conventional loss of  $W_K$  due to a gap opening, the total  $\Delta W_K$  may become positive.

The CB model has been applied numerous times to the cuprates, most often under the assumption that near-critical collective excitations are spin fluctuations with momenta near  $Q=(\pi, \pi)$ . This version of a CB boson is commonly known as a spin-fermion model. This model yields  $d_{x^2-y^2}$  superconductivity and explains in a quantitative way a number of measured electronic features of the cuprates, in particular, the near absence of the quasiparticle peak in the NS of optimally doped and underdoped cuprates<sup>30</sup> and the peak-dip-hump structure in the ARPES profile in the SCS.<sup>36,37,51,52</sup> In our analysis we assume that a CB is a spin fluctuation.

The results for the conductivity within a spin-fermion model depend in quantitative (but not qualitative) way on the assumption for the momentum dispersion of a collective boson. This momentum dependence comes from high-energy fermions and is an input for the low-energy theory. Below we follow Refs. 36 and 38 and assume that the momentum dependence of a collective boson is flat near  $(\pi, \pi)$ . The self-energy within such model has been worked out consistently in Refs. 36 and 38. In the normal state

$$\begin{aligned}\Sigma''(\omega) &= -\frac{1}{2}\lambda\omega_{sf}\log\left(1+\frac{\omega^2}{\omega_{sf}^2}\right), \\ \Sigma'(\omega) &= -\lambda\omega_{sf}\arctan\frac{\omega}{\omega_{sf}},\end{aligned}\quad (19)$$

where  $\lambda$  is the spin-fermion coupling constant and  $\omega_{sf}$  is a typical spin relaxation frequency of overdamped spin collective excitations with a propagator

$$\chi(q \sim Q, \Omega) = \frac{\chi_Q}{1 - i\frac{\Omega}{\omega_{sf}}}, \quad (20)$$

where  $\chi_Q$  is the uniform static susceptibility. If we use Ornstein-Zernike form of  $\chi(q)$  and use either Eliashberg<sup>50</sup> or FLEX computational schemes,<sup>53</sup> we get rather similar behavior of  $\Sigma$  as a function of frequency and rather similar behavior of optical integrals.

The collective nature of spin fluctuations is reflected in the fact that the coupling  $\lambda$  and the bosonic frequency  $\omega_{sf}$  are related:  $\lambda$  scales as  $\xi^2$ , where  $\xi$  is the bosonic mass (the distance to a bosonic instability), and  $\omega_{sf} \propto \xi^{-2}$  (see Ref. 54). For a flat  $\chi(q \sim Q)$  the product  $\lambda\omega_{sf}$  does not depend on  $\xi$  and is the overall dimensional scale for boson-mediated interactions.

In the SCS fermionic excitations acquire a gap. This gap affects fermionic self-energy in two ways: directly, via the change in the dispersion of an intermediate boson in the exchange process involving a CB, and indirectly, via the

change in the propagator of a CB. We remind ourselves that the dynamics of a CB comes from a particle-hole bubble which is indeed affected by  $\Delta$ .

The effect of a  $d$ -wave pairing gap on a CB has been discussed in a number of papers, most recently in Ref. 36. In a SCS a gapless continuum described by Eq. (20) transforms into a gaped continuum, with a gap about  $2\Delta$  and a resonance at  $\omega = \omega_0 < 2\Delta$ , where for a  $d$ -wave gap we define  $\Delta$  as a maximum of a  $d$ -wave gap.

The spin susceptibility near  $(\pi, \pi)$  in a superconductor can generally be written up as

$$\chi(q \sim Q, \Omega) = \frac{\chi_Q}{1 - i \frac{\Pi(\Omega)}{\omega_{sf}}}, \quad (21)$$

where  $\Pi$  is evaluated by adding up the bubbles made out of two normal and two anomalous Green's functions. Below  $2\Delta$ ,  $\Pi(\Omega)$  is real ( $\sim \Omega^2/\Delta$  for small  $\Omega$ ), and the resonance emerges at  $\Omega = \omega_0$  at which  $\Pi(\omega_0) = \omega_{sf}$ . At frequencies larger than  $2\Delta$ ,  $\Pi(\Omega)$  has an imaginary part, and this gives rise to a gaped continuum in  $\chi(\Omega)$ .

The imaginary part of the spin susceptibility around the resonance frequency  $\omega_0$  is<sup>36</sup>

$$\chi''(q, \Omega) = \frac{\pi Z_o \omega_0}{2} \delta(\Omega - \omega_0), \quad (22)$$

where  $Z_o \sim 2\omega_{sf} \chi_0 / \frac{\partial \Pi}{\partial \omega} |_{\Omega=\omega_0}$ . The imaginary part of the spin susceptibility describing a gaped continuum exists for  $\Omega \geq 2\Delta$  and is

$$\Sigma_B''(\omega) = -\lambda \int_{2\Delta}^{|\omega|} dx \operatorname{Re} \frac{\omega + x}{\sqrt{(\omega + x)^2 - \Delta^2}} \left[ \frac{\frac{x}{\omega_{sf}} K_2 \left( 1 - \frac{4\Delta^2}{x^2} \right)}{\left[ 1 - \frac{4\Delta^2}{x\omega_{sf}} D \left( \frac{4\Delta^2}{x^2} \right) \right]^2 + \left[ \frac{x}{\omega_{sf}} K_2 \left( 1 - \frac{4\Delta^2}{x^2} \right) \right]^2} \right] \quad (25)$$

comes from the interaction with the gaped continuum. The real part of  $\Sigma$  is obtained by Kramers-Krönig transform of the imaginary part.

We performed the same calculations of conductivities and optical integrals as in the previous three cases. The results are summarized in Figs. 8–10. Figure 8 shows conductivities in the NS and the SCS for two couplings  $\lambda=1$  and  $\lambda=10$  (keeping  $\lambda\omega_{sf}$  constant). Other parameters  $Z_o$  and  $\omega_o$  are calculated according to the discussion after Eq. (21). For  $\omega_{sf}=26$  meV,  $\lambda=1$ , we find  $\omega_o=40$  meV,  $Z_o=0.77$ . And for  $\omega_{sf}=2.6$  meV,  $\lambda=10$ , we find  $\omega_o=13.5$  meV,  $Z_o=1.22$ . Note that the conductivity in the SCS starts at  $2\Delta + \omega_o$  (i.e., the resonance energy shows up in the optical gap), where as in the BCSI case it would have always begun from  $2\Delta$ . In Fig. 9 (left) we plot the Kubo sums  $W_K$  vs coupling  $\lambda$ . We see that for all  $\lambda$ ,  $W_K$  in the NS stays larger than in the SCS. Figure 9 (center and right) shows the cut-off dependence of the optical integrals  $W(\omega_c)$  for  $\lambda=1$  separately in the NS and

$$\chi''(Q, \Omega) = \operatorname{Im} \left[ \frac{\chi_0}{1 - \frac{1}{\omega_{sf}} \left( \frac{4\Delta^2}{\Omega} D \left( \frac{4\Delta^2}{\Omega^2} \right) + i\Omega K_2 \left( 1 - \frac{4\Delta^2}{\Omega^2} \right) \right)} \right] \approx \operatorname{Im} \left[ \frac{\chi_0}{1 - \frac{1}{\omega_{sf}} \left( \frac{\pi\Delta^2}{\Omega} + i\frac{\pi}{2}\Omega \right)} \right] \quad \text{for } \Omega \gg 2\Delta. \quad (23)$$

In Eq. (23)  $D(x) = \frac{K_1(x) - K_2(x)}{x}$ , and  $K_1(x)$  and  $K_2(x)$  are Elliptic integrals of first and second kind. The real part of  $\chi$  is obtained by Kramers-Krönig transform of the imaginary part.

Substituting Eq. (6) for  $\chi(q, \Omega)$  into the formula for the self-energy one obtains  $\Sigma''(\omega)$  in a SCS state as a sum of two terms<sup>36</sup>

$$\Sigma''(\omega) = \Sigma_A''(\omega) + \Sigma_B''(\omega), \quad (24)$$

where

$$\Sigma_A''(\omega) = \frac{\pi Z_o}{2} \lambda \omega_o \operatorname{Re} \left( \frac{\omega + \omega_o}{\sqrt{(\omega + \omega_o)^2 - \Delta^2}} \right)$$

comes from the interaction with the resonance and

the SCS. We again see that only about 75% of the Kubo sum is recovered up to the bandwidth of 1 eV indicating that there is a significant amount left to recover beyond this energy scale. Figure 8 also shows  $\Delta W$  for the two different couplings. We see that, for both  $\lambda$ 's, there is only one zero crossing for the  $\Delta W$  curve, and  $\Delta W$  is negative at larger frequencies. The only difference between the two plots is that for larger coupling the dip in  $\Delta W$  gets “shallower.” In this case we see that the solid line in Fig. 8 for  $\Delta W(\omega_c)$  is rather far away from the dashed line at  $\omega_c > 1$  meV, which indicates that, although  $\Delta W(\omega_c)$  in this region has some dependence on  $\omega_c$ , still the largest part of  $\Delta W(\omega_c)$  is  $\Delta W_K$ , while the contribution from  $\Delta f(\omega_c)$  is smaller.

The negative sign of  $\Delta W(\omega_c)$  above a relatively small  $\omega_c \sim 0.1-0.2$  eV implies that the compensating effect from the fermionic self-energy on  $\Delta W$  is not strong enough to overshadow the decrease in the optical integral in the SCS due to gap opening. In other words, the CB model displays

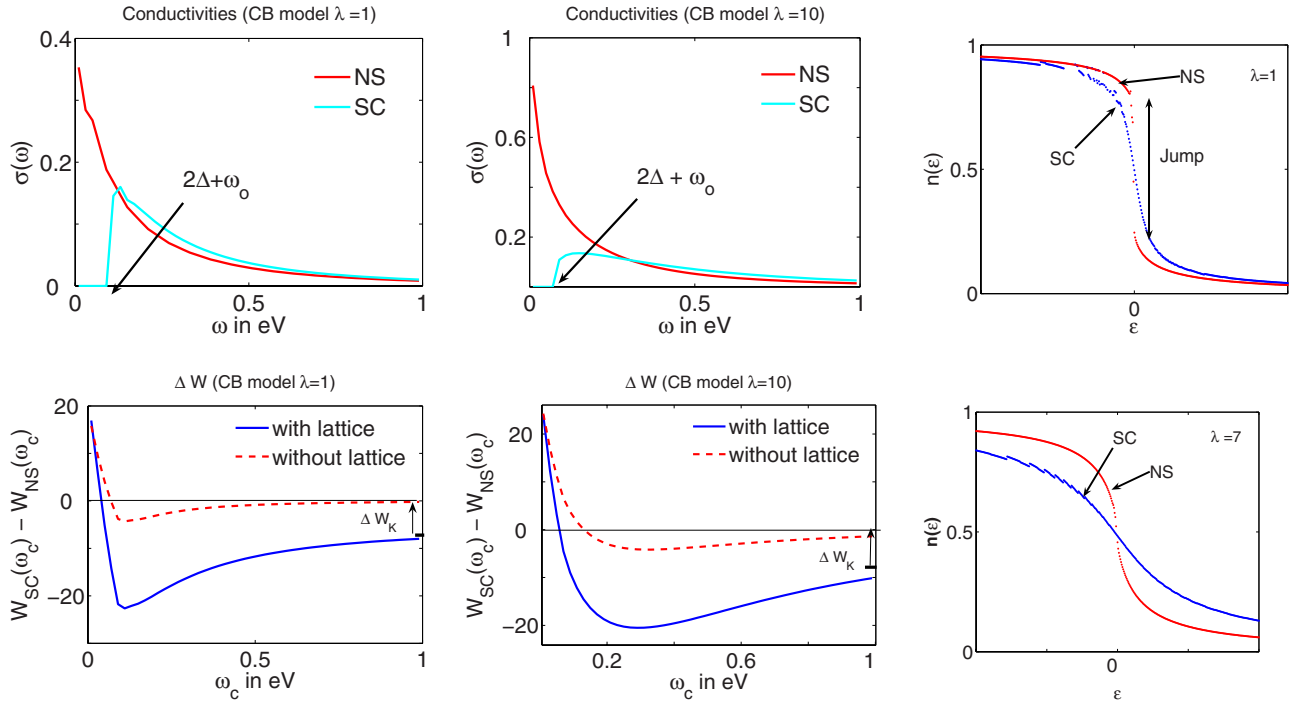


FIG. 8. (Color online) Conductivities and  $\Delta W$  for a fixed  $\lambda\omega_{sf}$  for the CB model. Left panel— $\omega_{sf}=26$  meV,  $\lambda=1$ ,  $\omega_0=40$  meV, and  $Z_0=0.77$ . Center panel— $\omega_{sf}=2.6$  meV,  $\lambda=10$ ,  $\omega_0=13.5$  meV, and  $Z_0=1.22$ . We set  $\Delta=30$  meV. Right panel—distribution functions  $n(\epsilon)$  for CB model for  $\lambda=1$  and  $\lambda=7$ , and a constant  $\omega_{sf}=26$  meV. We set  $\Delta=30$  meV. For smaller  $\lambda$  (top), quasiparticles near the FS are well defined as indicated by the well-pronounced jump in  $n(\epsilon)$ . For  $\lambda=7$ ,  $n(\epsilon)$  is rather smooth implying that a coherence is almost lost. Some irregularities in the SCS distribution function are due to finite sampling in the frequency domain. The irregularities disappear when finer mesh for frequencies is chosen.

the same behavior as BCSI, EB, and modified MFLI models. It is interesting that this holds despite the fact that for large  $\lambda$  CB model displays the physics one apparently needs to reverse the sign of  $\Delta W_K$ —the absence of the quasiparticle peak in the NS and its emergence in the SCS accompanied by the dip and the hump at larger energies. The absence of coherent quasiparticle in the NS at large  $\lambda$  is also apparent from Fig. 8 (right panel) where we show the normal-state distribution functions for two different  $\lambda$ . For large  $\lambda$  the jump (which indicates the presence of quasiparticles) virtually disappears.

On a more careful look, we found that indifference of  $\Delta W(\omega_c)$  to the increase in  $\lambda$  is merely the consequence of the

fact that above we kept  $\lambda\omega_{sf}$  constant. Indeed, at small frequencies, fermionic self-energy in the NS is  $\Sigma'=\lambda\omega$ ,  $\Sigma''=\lambda^2\omega^2/(\lambda\omega_{sf})$ , and both  $\Sigma'$  and  $\Sigma''$  increase with  $\lambda$  if we keep  $\lambda\omega_{sf}$  constant. But at frequencies larger than  $\omega_{sf}$ , which we actually probe by  $\Delta W(\omega_c)$ , the self-energy essentially depends only on  $\lambda\omega_{sf}$ , and increasing  $\lambda$  but keeping  $\lambda\omega_{sf}$  constant does not bring us closer to the physics associated with the recovery of electron coherence in the SCS. To detect this physics, we need to see how things evolve when we increase  $\lambda\omega_{sf}$  above the scale of  $\Delta$ , i.e., consider a truly strong coupling when not only  $\lambda \gg 1$  but also the normal state  $\Sigma_{NS}(\omega \geq \Delta) \gg \Delta$ .

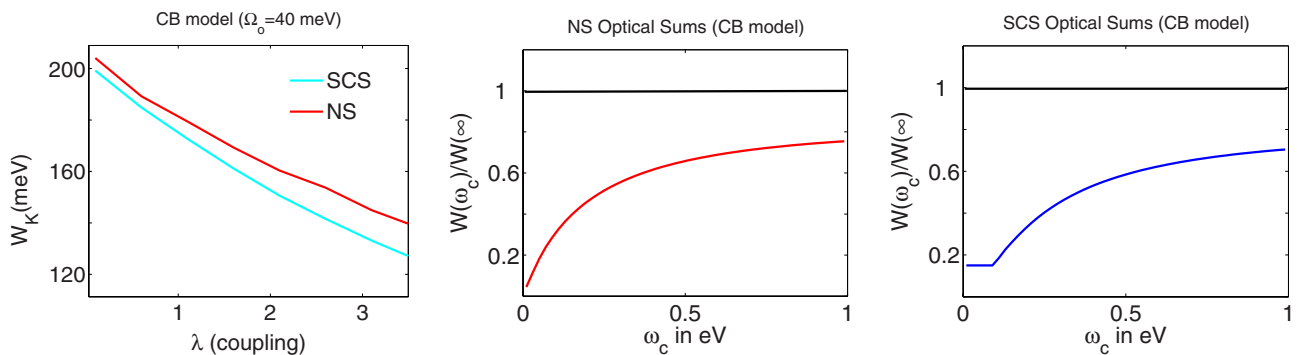


FIG. 9. (Color online) Left—the behavior of Kubo sums in the CB model. Note that the spectral weight in the NS is always larger than in the SCS. Center and right—the evolution of the optical integrals in the NS and the SCS in the CB model. Note that about  $\sim 75\%$  of the spectral weight is recovered up to 1 eV. We set  $\omega_{sf}=26$  meV,  $\lambda=1$ , and  $\Delta=30$  meV.

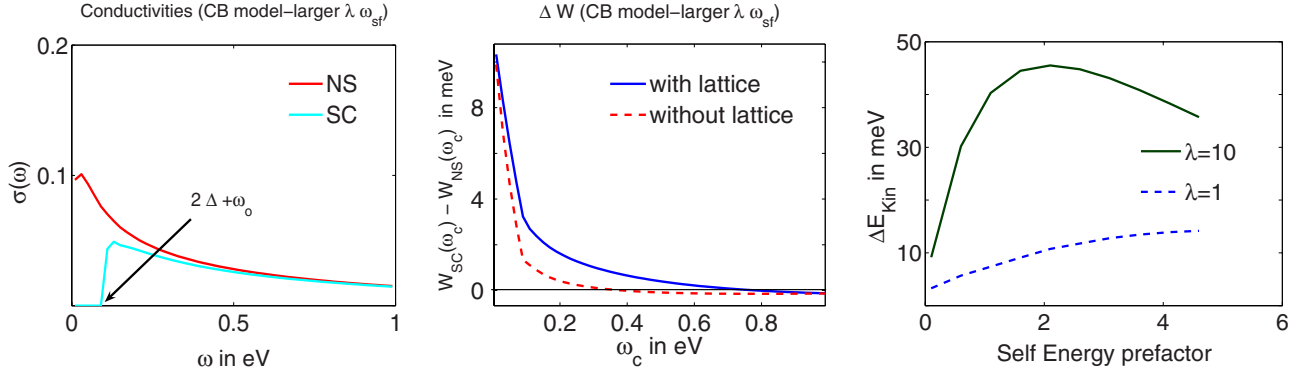


FIG. 10. (Color online) Left—conductivity at a larger value of  $\omega_{sf}\lambda$  ( $\omega_{sf}=26$  meV,  $\lambda=7$ ) consistent with the one used in Ref. 38). Center— $\Delta W$  with and without lattice. Observe that the frequency of zero crossing of  $\Delta W$  enhances compared to the case of a smaller  $\lambda\omega_{sf}$  and becomes comparable to the bandwidth. At energies smaller than the bandwidth,  $\Delta W > 0$ , as in the Norman-Pépin model. Right—kinetic-energy difference between the SCS and the NS,  $\Delta E_{Kin}$ . We set  $\lambda$  to be either  $\lambda=1$  or  $\lambda=10$  and varied  $\omega_{sf}$  thus changing the overall prefactor in the self-energy. At weak coupling ( $\lambda=1$ ) the behavior is BCS-like— $\Delta E_{Kin}$  is positive and increases with the overall factor in the self-energy. At strong coupling ( $\lambda=7$ ),  $\Delta E_{Kin}$  shows a reverse trend at larger  $\omega_{sf}$ .

To address this issue, we took a larger  $\lambda$  for the same  $\omega_{sf}$  and re-did the calculation of the conductivities and optical integrals. The results for  $\sigma(\omega)$  and  $\Delta W(\omega_c)$  are presented in Fig. 10. We found the same behavior as before, i.e.,  $\Delta W_K$  is negative. But we also found that the larger is the overall scale for the self-energy, the larger is a frequency of zero crossing of  $\Delta W(\omega_c)$ . In particular, for the same  $\lambda$  and  $\omega_{sf}$  that were used in Ref. 38 to fit the NS conductivity data, the zero crossing is at  $\sim 0.8$  eV which is quite close to the bandwidth. This implies that at a truly strong coupling the frequency at which  $\Delta W(\omega_c)$  changes sign can well be larger than the bandwidth of 1 eV in which case  $\Delta W$  integrated up to the bandwidth does indeed remain positive. Such behavior would be consistent with Refs. 8 and 9.

We note in this regard that the strength of coupling constant is generally related to doping and increases as doping decreases, i.e., larger  $\lambda$  correspond to smaller dopings. For detailed account of the dependence of the optical integral on the doping in the NS see Ref. 55.

We also see from Fig. 10 that  $\Delta W_K$  becomes small at a truly strong coupling, and over a wide range of frequencies the behavior of  $\Delta W(\omega_c)$  is predominantly governed by  $\Delta f(\omega_c)$ , i.e. by the cut-off term.<sup>56</sup> The implication is that, to first approximation,  $\Delta W_K$  can be neglected and positive  $\Delta W(\omega_c)$  integrated to a frequency where it is still positive is almost compensated by the integral over larger frequencies. This again would be consistent with the experimental data in Refs. 8 and 9.

For a more detailed comparison between theory and experiment, we plot in Fig. 11 our  $\Delta W(\omega_c)$  vs the data for optimally doped  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$  ( $\text{Bi}2223$ ) (Ref. 57). We see that the functional form of our  $\Delta W(\omega_c)$  agrees well with the experiment over a wide frequency range, however, to match the data we had to shift our  $\Delta W(\omega_c)$  by a constant. There are several possible explanations for the shift. One possibility is that this constant is the contribution to  $\Delta W$  from other bands.

It is also instructive to understand the interplay between the behavior of  $\Delta W(\omega_c)$  and the behavior of the difference of the kinetic energy between the SCS and the NS,  $\Delta E_{Kin}$ . We

computed the kinetic energy as a function of  $\lambda\omega_{sf}$  and present the results in Fig. 10 (right) for  $\lambda=1$  and 10. For a relatively weak  $\lambda=1$  the behavior is clearly BCS-like  $\Delta E_{Kin} > 0$  and increases with increasing  $\lambda\omega_{sf}$ . However, at large  $\lambda=10$ , we see that the kinetic energy begins decreasing at large  $\lambda\omega_{sf}$ . The behavior of  $\Delta E_{Kin}$  at a truly strong coupling is consistent with earlier calculation of the kinetic energy for Ornstein-Zernike form of the spin susceptibility.<sup>48</sup>

We clearly see that the increase of the zero-crossing frequency of  $\Delta W(\omega_c)$  at a truly strong coupling is correlated with the non-BCS behavior of  $\Delta E_{Kin}$ . At the same time, the behavior of  $\Delta W(\omega_c)$  is obviously not driven by the kinetic energy as eventually  $\Delta W(\omega_c)$  changes sign and become negative. Rather, the increase in the frequency range where  $\Delta W(\omega_c)$  remains positive and non-BCS behavior of  $\Delta E_{Kin}$  are two indications of the same effect that fermions are incoherent in the NS but acquire coherence in the SCS.

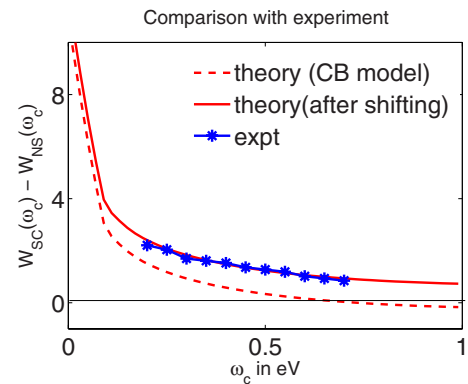


FIG. 11. (Color online) A comparison between the calculated optical spectral weight change between SC and NS and the measured  $\Delta W(\omega_c)$  in optimally doped  $\text{Bi}2223$  (Ref. 57). The theoretical calculation is for the CB model with parameters  $\omega_{sf}=26$  meV and  $\lambda=7$ . The functional form of theoretical  $\Delta W(\omega_c)$  agrees well with the data but theoretical curve has to be shifted up by a constant to match the experimental curve.

TABLE II. Table summarizing our results regarding the sign of  $\Delta W(\omega_c)$  for various models.  $B$  means bandwidth. The recovery refers to what percentage of  $W_K$  is  $W(\omega_c=B)$ .

Model	$\Delta W(\sim\Delta)$	$\Delta W(0.7B)$	$W(\infty)=\Delta W_K$	Recovery
BCSI	+	-	-	90–95 %
EB	+	-	-	75–80 %
MFLI (corrected)	+	-	-	75–80 %
CB (small coupling)	+	-	-	70–75 %
CB (large coupling)	+	+	-	

### III. CONCLUSION

In this work we analyzed the behavior of optical integrals  $W(\omega_c) \propto \int_0^{\omega_c} \sigma(\omega) d\omega$  and Kubo sum rules in the normal and superconducting states of interacting fermionic systems on a lattice. Our key goal was to understand what sets the sign of  $\Delta W_K = \Delta W(\infty)$  between the normal and superconducting states and what is the behavior of  $W(\omega_c)$  and  $\Delta W(\omega_c)$  at finite  $\omega_c$ . In a weak coupling BCS superconductor,  $\Delta W(\omega_c)$  is positive at  $\omega_c < 2\Delta$  due to a contribution from superfluid density, but becomes negative at larger  $\omega_c$ —the exact location turns out to be sensitive to the interaction considered—and approaches a negative value of  $\Delta W_K$  eventually. Our study was motivated by fascinating optical experiments on the cuprates.<sup>7–10</sup> In overdoped cuprates, there is clear indication<sup>11</sup> that  $\Delta W(\omega_c)$  becomes negative above a few  $\Delta$ , consistent with BCS behavior. In underdoped cuprates, two groups argued<sup>8,9</sup> that  $\Delta W$  integrated up to the bandwidth remains positive while the other group argued<sup>10</sup> that it is negative.

The reasoning why  $\Delta W_K$  may potentially change sign at strong coupling involves the correlation between  $-W_K$  and the kinetic energy. In the BCS limit, kinetic energy obviously increases in a SCS because of gap opening, hence  $-W_K$  increases and  $\Delta W_K$  is negative. At strong coupling, there is a counter effect—fermions become more mobile in a SCS due to a smaller self-energy.

We considered four models: a BCS model with impurities, a model of fermions interacting with an Einstein boson, a phenomenological MFL model with impurities, and a model of fermions interacting with collective spin fluctuations. In all cases, we found that  $\Delta W_K$  is negative but how it evolves with  $\omega_c$  and how much of the sum rule is recovered by integrating up to the bandwidth depends on the model. We summarize our results in the Table II.

Recovery farther from 100% simply tells us that the  $\Delta W(\omega_c)$  is sensitive to the experimental cutoff  $\omega_c$ . The result

most relevant to the experiments on the cuprates is obtained for the spin fluctuation CB model. We found that at strong coupling, the zero crossing of  $\Delta W(\omega_c)$  occurs at a frequency which increases with the coupling strength and become comparable to (or even larger than depending on the scale of interaction) the bandwidth at a truly strong coupling. Still, at even larger frequencies,  $\Delta W(\omega_c)$  is eventually negative.

The conclusion of our analysis is that the difference in the Kubo sums between SCS and NS,  $\Delta W_K$  is negative, but  $\Delta W(\omega_c)$ , which approaches  $\Delta W_K$  only at very large  $\omega_c$ , is positive at small frequencies, and the range where it remains positive increases with underdoping. The frequency at which  $\Delta W(\omega_c)$  changes sign becomes comparable to the bandwidth at strong coupling and the sign of  $\Delta W(\omega_c)$  becomes sensitive to fine interplay between the parameters. It is then possible that some experiments on underdoped cuprates probe the spectral weight integrated over the range where  $\Delta W(\omega_c)$  is still positive, while other experiments probe  $\Delta W(\omega_c)$  integrated up to a frequency, where it is already negative. Another possibility, consistent with Fig. 11, is that there is additional constant contribution to  $\Delta W$  from other bands. This constant offset between theoretical and experimental  $\Delta W$  can also, potentially, be due to error bars in the experimental determination of the condensate contribution to the optical integral.

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