Effect of orbital currents on the restricted optical conductivity sum rule

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We derive the restricted optical-conductivity sum rule for a model with circulating orbital currents. It is shown that an unusual coupling of the vector potential to the interaction term of the model Hamiltonian results in a non-standard form of the sum rule. As a consequence, the temperature dependence of the restricted spectral weight could be compatible with existing experimental data for high-$T_c$ cuprates above the critical temperature $T_c$. We extend our results to the superconducting state, and comment on the differences and analogies between these two symmetry-breaking phenomena.

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I. INTRODUCTION

Recent results extracted from measurements [1, 2, 3, 4, 5] of the in-plane optical conductivity $\sigma(\omega)$ in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) place strong constraints on possible theories of high-$T_c$ superconductivity. Special attention has been devoted to the partial spectral weight extracted from the optical conductivity in the direction $\alpha = x, y$

$$W_\alpha(\omega_m, T) = \int_{-\omega_m}^{\omega_m} \text{Re} \sigma_{\alpha\alpha}(\omega, T)d\omega,$$

which is analyzed as a function of temperature $T$ and the cutoff frequency $\omega_m$, which varies between 1000 cm$^{-1}$ (0.12 eV) and 20000 cm$^{-1}$ (2.5 eV). According to this definition, the weight $W$ includes the condensate peak at $\omega = 0$ which develops in the superconducting (SC) state below $T_c$. When $\omega_m$ is of order of the plasma frequency, $\omega_p \sim 10^4$ cm$^{-1}$, only intraband optical transitions contribute to the measured spectral weight $\overline{W}$, and the so-called restricted or partial sum rule may be applied [1, 2, 3], which relates $W$ to the average value of the diamagnetic term $\tau_{\alpha\alpha}$ (see Eq. (6) below),

$$W_\alpha(\omega_p, T) \equiv W(T) = \frac{\pi e^2}{VN} \sum_{k,\sigma} \partial^2 \varepsilon_k \partial k^2_{\alpha} n_{k,\sigma} = -\frac{\pi e^2}{V} \frac{\langle K^2 \rangle}{d},$$

where $n_{k,\sigma}$ is the momentum occupation number, $V$ is the unit-cell volume, $N$ is the system size, $d = 2$ is the dimension of the system, $e$ is the electron charge, and we set $\hbar = c = 1$. The second line of Eq. (2) is obtained under the assumption that the interaction term of the Hamiltonian does not couple to the vector potential $A$, and the final equality in Eq. (2) is valid only for a nearest-neighbors tight-binding dispersion $\varepsilon_k = -2t(\cos k_x a + \cos k_y a)$ with the lattice constant $a$. In this case the spectral weight is a direct measure of the mean kinetic energy $K$ of the system, and depends on temperature and interaction strength. For a non-interacting system $n_{k,\sigma} = f(\xi_k)$, where $\xi_k = \varepsilon_k - \mu$, $\mu$ is the chemical potential, and $f(x)$ is the Fermi function, so that $W(T)$ increases as the temperature decreases. In the presence of a SC instability, the BCS theory predicts that the occupation number is modified below $T_c$ and the partial spectral weight is

$$\frac{W(T)}{\pi e^2 a^2} = -\frac{1}{2VN} \sum_k \varepsilon_k \left[ 1 - \frac{\xi_k}{E^SC_k} \tanh \frac{E^SC_k}{2T} \right],$$

where $\Delta_k = (\Delta_0/2)(\cos k_x a - \cos k_y a)$ is the $d$-wave SC gap and $E^SC_k = \sqrt{\varepsilon_k^2 + \Delta_k^2}$ is the quasiparticle dispersion in the SC state. The kinetic energy increases below $T_c$ because of particle-hole mixing, and as a consequence $W(T)$

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decreases. The restricted sum rule should be contrasted \[ \int_{-\infty}^{\infty} \text{Re} \sigma(\omega) d\omega = \frac{\pi n e^2}{m}, \] which relates the integral over all optical transitions ($\omega_m \to \infty$) to the total carrier density $n$ and bare mass $m$, and is independent of temperature and interactions. The difference between the full and restricted sum rules is made up by transitions between the orbitals described by the low-energy effective tight-binding model and orbitals with the energies above $\omega_p$, not included in this model. As noted in Ref. [11], there is as yet no complete understanding of the relevant orbitals or energy range over which the full sum rule is restored.

The experimental results and their implications \[1,2,3\] for the restricted sum rule are the following. (i) Above the critical temperature $T_c$, the partial spectral weight $W(T)$ does not decrease when $T$ decreases. Assuming that the mean-field Eq. \[8\] is already valid in the pseudogap state for $T > T_c$, so that $W(T)$ would decrease as $T$ decreases even above $T_c$, following Ref. \[2\] one may conclude that the observed increase of $W(T)$ is in contradiction with the opening of a pseudogap. (ii) Using the value $t = 0.25$ eV, which is typical for cuprates, the tight-binding estimate Eq. \[2\] for the relative thermal variation of $W(T)$ between $T_c$ and the room temperature $T_r$, with $T_r/t \approx 0.1$, gives $(W(T_r) - W(T_c))/W(T_c) \approx 2 \cdot 10^{-3}$. This variation appears to be at least one order of magnitude smaller than the experimentally observed change in $W(T)$ even for a large $\omega_m = 10^4$ cm$^{-1}$. There is even faster increase of $W(T)$ when smaller values of $\omega_m$ are used \[3\]. (iii) Below $T_c$ the situation is not clear yet. While early measurements in BSCCO samples show that there is an even faster increase of $W(T)$ \[11,12\], contrary to the prediction of the BCS theory, more recent results in BSCCO \[4\] show that there is a flattening of $W(T)$ in underdoped samples for $\omega_m = 8000$ cm$^{-1}$, while a BCS behavior below $T_c$ is seen in the overdoped BSCCO and in YBCO samples \[3,8\].

The possibility of a spectral-weight change below the superconducting critical temperature has been analyzed, for example, in Refs. \[13,14,15\] in terms of the lowering of the in-plane kinetic energy. In Ref. \[15\] the reduction of the kinetic energy at $T_c$ has been attributed to the transition from a phase-incoherent Cooper pair motion in the pseudogap regime above $T_c$ (see, e.g., review \[10\]) to a phase coherent motion at $T_c$, while in Ref. \[14\] a model with a frequency dependent scattering rate was used. More recently, the optical conductivity sum rule has been analyzed for a model with electron coupled to a single Einstein oscillator \[17\].

Here, in contrast to these papers, we focus primarily on the temperature dependence of $W(T)$ above $T_c$ and on the issue of the compatibility between the pseudogap opening and the absence of a lowering of the spectral weight. Our purpose is to show that if the pseudogap originates from a state with circulating orbital currents \[18,19,20,21,22,23,24\] the opening of the pseudogap can be accompanied by the increase of the partial spectral weight. For completeness we extend these results also to the SC state. We find that when a small SC gap opens in the presence of a large DDW gap $W(T)$ remains almost constant below $T_c$.

II. MODEL

We consider the model with bond currents circulating around elementary plaquettes of copper atoms which is described by the effective Hamiltonian

\[ H = \sum_{k, \sigma} \left[ \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + i D_k c_{k\sigma}^\dagger c_{k+Q \sigma} \right], \] (5)

where $c_{k\sigma}^\dagger$, $c_{k\sigma}$ are creation and annihilation operators for a particle with momentum $k$ and spin $\sigma$, $D_k = (D_0/2)(\cos k_x a - \cos k_y a)$ is the gap, known as the DDW gap \[26\], arising from the formation of the state with circulating currents, and $Q = (\pi/a, \pi/a)$ is the wave vector at which the density-wave ordering takes place. In the present paper we do not derive the Hamiltonian \[3\] by means of a Hartree-Fock analysis of a microscopic model, as it has been done elsewhere \[13,15,20,21,22,23,24\]. These studies showed that Hubbard-like Hamiltonians with additional finite-range repulsion and superexchange interaction can have a stable DDW saddle point. Thus we shall parametrize phenomenologically the DDW order parameter and we will analyze within the low-energy effective model \[3\] the effect of this symmetry breaking on the optical sum rule. It is worth noting that this approach has been often adopted in the literature to address several issues related to transport properties in the DDW state \[25,26,27,28,31,32,33\].

The derivation of the restricted sum rule depends crucially on the manner in which the vector potential $A$ enters the effective low-energy Hamiltonian \[17\]. For lattice models $A$ is usually inserted in a coordinate representation by means of the Peierls ansatz \[8,10\] $c_i \rightarrow c_i e^{-ie/\Lambda} dr$, which modifies the fermionic operator at every site $i$. The dependence of the resulting Hamiltonian on each component $A_n$ of the gauge field is $H(A_n) \approx H(0) -$
for a Hamiltonian expressed in coordinate representation. For a Hamiltonian in the momentum representation, it is hopping. This derivation of the optical-conductivity sum rule requires the knowledge of function $\Lambda_{\alpha\alpha}$ of the current density expressed in imaginary-time representation. The Kramers-Kronig relations for the response function \( e^{\alpha\alpha}_j \) is the Fourier transform of the particle density which satisfies the continuity equation

\[
\frac{\partial\rho(t, q)}{\partial t} + i\mathbf{q} \cdot \mathbf{j}^P(t, q) = 0.
\]

We note that substitution in Eq. (8) of \( \rho(t, q) = \sum_{k, \sigma} e^{\uparrow}_{k+q/2, \sigma} c_{k+q/2, \sigma} \) and of the free-electron expression \( j^P(t, q) = (1/m) \sum_{k, \sigma} k c_{k+q/2, \sigma} \) corresponding to \( \varepsilon_k = k^2/2m \), returns the full f-sum rule (12) (see [34]).

In most cases it is assumed that the interaction term of the Hamiltonian involves only density-density coupling, so that this is trivially gauge invariant and the Peierls ansatz modifies only the first, “kinetic”, term of the Hamiltonian [5]. For models with nearest-neighbors hopping, \( \tau_{\alpha\alpha} \) is then related directly to the kinetic energy, \( \langle \tau_{\alpha\alpha} \rangle = -(K)/d \) and one obtains the usual version of the sum rule given by Eq. (2). However, this assumption is invalid when for example “occupation modulated” hopping terms are considered [13]. In particular, if one assumes that the low-energy physics of the system can be described by the effective Hamiltonian [3], then any distinction in the total energy between a kinetic and a potential part is somehow ambiguous. Thus, by transforming the Hamiltonian [5] to the coordinate space, one finds that \( \tau_{\alpha\alpha} \) contains an extra term for \( D_0 \neq 0 \),

\[
\langle \tau_{\alpha\alpha} \rangle = -\frac{1}{2N} \sum_{k, \sigma} \varepsilon_k \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle + iD_k \langle c^\dagger_{k\sigma} c_{k+Q\sigma} \rangle.
\]

This result is consistent with the derivation [5] of the sum rule, when one uses the particle current operator compatible with the conservation law [21] and with the equations of motion for the operators \( c \) and \( c^\dagger \), [27, 29, 37, 33]

\[
\mathbf{j}^P(t, q) = \sum_{k, \sigma} \left[ v^F_k \epsilon_{k+q/2, \sigma} c_{k+q/2, \sigma} - i v^D_k \epsilon^\dagger_{k+q/2, \sigma} c_{k+q+Q/2, \sigma} \right],
\]

where \( v^F_k = \partial \varepsilon_k / \partial k \) and \( v^D_k = -\partial D_k / \partial k \). The first term of the previous expression relates as usual the particle current to the band velocity \( v^F_k \). The second term, which only appears for non-vanishing \( D_0 \), takes into account the contribution of the orbital currents to the electrical conductivity, arising when the DDW order is established. Substitution of Eq. (11) in (8) yields

\[
\frac{W(T)}{\pi e^2 a^2} = -\frac{1}{VN} \sum_{RBZ} E_k [f(\xi_++k) - f(\xi_-+k)],
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\[
\frac{W(T)}{\pi e^2 a^2} = -\frac{1}{VN} \sum_{RBZ} E_k [f(\xi_++k) - f(\xi_-+k)],
\]
The spectral weight in the DDW+SC state reads

\[ H = T \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^* c_{\mathbf{k}\sigma} c_{-\mathbf{k}\sigma} + h.c. \]

where \( E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + D_{\mathbf{k}}^2} \), and \( \xi_{\pm,\mathbf{k}} = -\mu \pm E_{\mathbf{k}} \) represent the two excitation branches associated with the formation of DDW order which breaks translation symmetry. The sum is taken over the reduced Brillouin zone (RBZ). Eq. (12) was derived using the fact that \( \partial_{\mathbf{k}} h_{\mathbf{k}} = 2ta^2 \cos k_x a \) (and \( \partial_{\mathbf{k},y} h_{\mathbf{k}} = \pm (D_0/2)a^2 \cos k_x a \)), and it reduces to Eq. (2) for \( D_0 = 0 \).

To extend this result to a state with both DDW and SC order present, we add to the Hamiltonian an additional d-wave mean-field pairing term \( H_p = \sum_{\mathbf{k},\sigma} \Delta_{\mathbf{k}} c_{\mathbf{k}\sigma} c_{-\mathbf{k}\sigma} + h.c. \), where \( \Delta_{\mathbf{k}} = (\Delta_0/2)(\cos k_x a - \cos k_y a) \). As a consequence, the spectral weight in the DDW+SC state reads

\[ W(T) = \frac{1}{2VN} \sum_{\text{RBZ}} E_{\pm,\mathbf{k}} \left[ \frac{\xi_+}{E_+} \tanh \frac{E_+}{2T} - \frac{\xi_-}{E_-} \tanh \frac{E_-}{2T} \right], \tag{13} \]

where \( E_{\pm,\mathbf{k}} = \sqrt{\varepsilon_{\pm,\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} \) is the quasiparticle dispersion in the presence of pairing, and the explicit dependence on \( \mathbf{k} \) has been omitted. Numerical calculation of the spectral weight defined by Eqs. (12) and (13) shows that below the temperature \( T_{DDW} \), at which the DDW state is formed, the spectral weight \( W(T) \) increases as the temperature decreases and the DDW gap opens. As stated above, this increase originates from the second term of Hamiltonian (5) which effectively enhances the low-frequency conductivity, as already observed in Ref. [33]. When the temperature is lowered further and the SC gap opens at a temperature \( T_c < T_{DDW} \), the spectral-weight increase is reduced with respect to the DDW state only.

A more quantitative comparison with experimental data requires the dependences of the gaps \( D_0 \) and \( \Delta_0 \) on temperature \( T \) and doping \( \delta \). This issue has been investigated within various microscopic models by several authors (see for example [23, 24]). Here, following the lines of Ref. [23, 27, 32], and consistently with our effective Hamiltonian (5), we adopt a mean-field dependence for the DDW gap. We assume that \( D_0 \) opens below a doping-dependent temperature \( T_{DDW}(\delta) = 40[1 - (\delta/\delta_0)^3] \) meV, where \( \delta \) is the doping with respect to half filling, and \( \delta_0 = 0.2 \) is the critical doping for the DDW formation. We adopt for the temperature dependence of \( D_0 \) the mean-field relation \( D_0(T,\delta) = cT_{DDW}(\delta)g(T/T_{DDW}(\delta)) \), where \( g(x) = (1 - x^4/3)\sqrt{1 - x^4} \), and \( c \) is a constant which is used as a fitting parameter. To describe the SC transition we solve self-consistently the BCS equations for \( \Delta_0 \) and \( \mu \) as functions of temperature. We use an analogous set of parameters as in Ref. [27] to estimate the thermal variation of \( W(T) \) in BSCCO. We focus on an underdoped \( (\delta = 0.13) \) and an optimally doped \( (\delta = 0.16) \) compound [1, 2]. The results are presented in Fig. 1, where the temperature dependence of \( W(T) \) for the tight-binding metal is shown for comparison. Below \( T_{DDW} \) the weight \( W(T) \) increases proportionally to \( D_0(T) \), so that the overall increase of \( W(T) \) with respect to \( W(T_{DDW}) \) is more pronounced in the underdoped case \( (\delta = 0.13) \), where \( D_0(0) \) is larger. In Ref. [1] it has been observed that \( W(T) \) shows a \( T^2 \) dependence above the critical temperature, as expected in the tight-binding model Eq. (2), but with a much larger slope. To make a comparison with the result of Eq. (12), in the inset of Fig. 1 we plot \( W(T) \) as a function of \( T^2 \). One can see that below \( T_{DDW} \) the \( T^2 \) temperature dependence of \( W(T) \) is still recovered over a wide range of temperature, and with a slope in good agreement with the experimental observation. Significant deviations are observed approaching \( T_c \) and below, where our mean-field approach does not reproduce the anomalous increasing of \( W(T) \) observed in BSCCO in early experiments [1]. Observe however that because at these dopings...
$\Delta_0 \ll D_0$, $W(T)$ is not explicitly decreasing below $T_c$, as expected in an ordinary metal-SC transition, but keeps almost constant resembling more recent experimental data \cite{1}. Finally, we find that the relative variations of $W(T)$ below $T_c = 0.1t$ is of order $W(0)/W(T_c) \simeq 3 \cdot 10^{-2}$, as observed experimentally \cite{1,2,3,4}, and is much larger than expected in the simple tight-binding model.

The previous analysis can be extended to the case where an additional next-nearest neighbor hopping term $t'$ is added to the bare band dispersion $\xi_k$ in Eq. \eqref{eq:5}. Even though both Eq. \eqref{eq:10} and Eq. \eqref{eq:12} are formally modified, the qualitative behavior of the reduced spectral weight is the same, with an increasing of $W(T)$ below the temperature for DDW formation. However, as suggested also in Ref. \cite{31}, it is likely that the analysis of the DDW state should be carried out with a value of $t'$ much smaller then suggested by ARPES experiments, leading to small quantitative corrections to the previous results. Also, as shown in \cite{12}, the effect of including next-neighbors hopping term $t'$ is small, so for qualitative considerations one may consider the model only with a hopping $t$.

### III. Discussion

A crucial step in the presented derivation of the sum rule is to use the current operator \eqref{eq:11} that was considered before in Refs. \cite{27,29,30,33}. A different current operator was used instead in Ref. \cite{32}, where it was suggested that the gauge field should couple via the Peierls ansatz to the quasiparticle fermionic operators that diagonalize the Hamiltonian \eqref{eq:5}. As far as the restricted sum rule is concerned, this corresponds to the replacement of the bare dispersion law $\xi_k$ in Eq. \eqref{eq:2} with the sum of the contributions from the new bands $\xi_{\pm}(k)$, and it would produce an extra term $(2/NV) \sum_{R \in (\pm D)} \sum_{\alpha \in \{\uparrow, \downarrow\}} [f(\xi_{\pm}(k) - \xi(k))] E^2$ that would be added to the spectral weight \eqref{eq:12}. Its contribution to $W(T)$ is negative and of order $t \sqrt{t}/D_0$, as one can check numerically and estimate analytically at low doping. The resulting $W(T)$ is then found to decrease below $T_{DDW}$, in contrast to the experimental observation and the result obtained with Eq. \eqref{eq:12}. Analogously, below $T_c$ the ansatz of coupling the gauge field to the quasiparticle DDW operators does not reproduced the expression for the superfluid density $\rho_s(T)$ proposed in Refs. \cite{27,28}, which is derived through the current operator \eqref{eq:11}.

The previous discussion shows that there is not yet an agreement in the literature about the proper treatment of the transport properties in the DDW state. However, it is worth noting that the form of thecurrent operator and of the diamagnetic term used to evaluate the electromagnetic response kernel $K_{\alpha\alpha}(q)$ in the DDW state are intimately related. If a Gauge invariant approximation is used, the response kernel satisfies $K_{\alpha\alpha}(\omega = 0, q \rightarrow 0) = 0$ above the SC critical temperature $T_c$ \cite{8,35}. This means for example that the diamagnetic contribution $\langle \tau_{\alpha\alpha} \rangle$ to the superfluid density $\rho_s(T)$ cancels the contribution $\Lambda_{\alpha\alpha}(i\Omega_n = 0, q \rightarrow 0)$ providing the vanishing of $\rho_s(T)$ for $T > T_c$. Within the low-energy model \eqref{eq:11} this cancellation holds only if the diamagnetic term \eqref{eq:10} is considered along with the current operator \eqref{eq:11}, derived from the requirement that the continuity equation \eqref{eq:9} be satisfied. The same result does not hold by using the mean-field correlation functions defined in Ref. \cite{32}.

A different approach, which was not investigated here, consists of deriving a proper gauge-invariant approximation for the response kernel $K_{\alpha\alpha}$ by starting from an underlying microscopic model that provides the basis for the Hamiltonian \eqref{eq:5} \cite{13,14,15,20,21,22,23,24} and including the vertex corrections to the mean-field correlation functions. In the case of SC symmetry breaking, one knows that vertex corrections are singular for $(\omega, q) \rightarrow 0$, satisfying the dispersion relations of the collective (phase) mode \cite{31,35}. In the DDW case, where the phase mode is locked by the commensurability, vertex corrections are always finite and at zero frequency are related by Ward identities to the $k$ derivative of the self-energy associated with the DDW state, i.e. to the term $v_k^D$ which appears in the definition \eqref{eq:11} of the current. As a consequence, as observed in Ref. \cite{32}, the d.c. conductivity, $\sigma(0)$ calculated with the current operator \eqref{eq:11} coincides with the exact results for a general, many-body formulation with nonzero vertex corrections.

This observation suggests that there exists an energy scale below which the approach followed here, where the sum rules \eqref{eq:12} for $T > T_c$ and \eqref{eq:10} for $T < T_c$ were derived directly from the effective Hamiltonian \eqref{eq:5}, describes properly the system behavior. However, since there is no straightforward extension of the previous arguments for $\sigma(\omega \neq 0)$, it is difficult to determine the value of $\omega_m$ at which the restoration of the more general sum rules \eqref{eq:2} and \eqref{eq:4} should be observed in the original microscopic model. In particular, if this cut-off energy resulted to be quite lower than the bare plasma edge, the comparison with the experimental data presented before should be reconsidered and referred to the data collected up to frequencies lower than $10^5$ cm$^{-1}$. As a consequence, the restricted sum rule derived here for the mean-field Hamiltonian \eqref{eq:5} has yet to be understood from a more general point of view, within a direct analysis of a microscopic Hubbard-type model with some short-range interaction that may result in the formation of DDW state. As mentioned above, this investigation is rather complicated and cannot be done within the framework considered here, so we reserve it for a future work.

To conclude, we have demonstrated within an effective model that circulating currents can act to modify the restricted optical sum rule in a such way that this acquires the same temperature dependence as that observed in experiments above $T_c$: the opening of the corresponding gap produces an increase in the spectral weight above $T_c$. 

Below the SC critical temperature the spectral weight keeps almost constant, as observed recently in Ref. [4], but in contrast with other measurements [1]. Since the experimental situation about the behavior of the spectral weight in the SC state is not settled, more data are certainly required to definitively establish the possible compatibility between our findings and the experiments. As far as our theoretical approach is concerned, we discussed that the exact range of validity of this result should still be clarified. Nonetheless, the analysis of the reduced low-energy model suggests the possibility that the same kind of deviations from the conventional form of the restricted sum rule could be expected in more sophisticated microscopic models (see e.g. [22]).

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