Ward identity and optical conductivity sum rule in the *d*-density wave state

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We consider the role of the Ward identity in dealing with the transport properties of an interacting system forming a *d*-wave modulated charge-density wave or staggered flux phase. In particular, we address this issue from the point of view of the restricted optical-conductivity sum rule. Our aim is to provide a controlled approximation for the current-current correlation function which allows us also to determine analytically the corresponding sum rule. By analyzing the role of the vertex functions in both the microscopic interacting model and in the effective mean-field Hamiltonian, we propose a nonstandard low-energy sum-rule for this system. We also discuss the possible applicability of these results for the description of cuprate superconductors in the pseudogap regime.

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I. INTRODUCTION

In the last years a quite important re-examination of the optical conductivity of high-T_c superconductors (HTSC) has been performed, due to the improved experimental resolution. Despite the variety of features observed in the different families of cuprates, when the integral up to large frequencies of the optical spectra is concerned a common behavior can be found.[1–6] This result is particularly interesting, because it would allow us to distinguish between different theoretical scenarios for HTSC, in particular for the pseudogap phase observed in underdoped compounds. The optical spectral weight is defined as the integral of the optical conductivity in a given direction $i=x,y,z$,

$$W_i(\omega_M,T)=\int_{-\omega_M}^{\omega_M}\mathrm{Re}\,\sigma_{ii}(\omega,T)d\omega, \tag{1.1}$$

and can be analyzed as a function of both the temperature T and the cutoff frequency ω_M. According to this definition, the weight W_i includes also the condensate peak at $\omega=0$ which develops in the superconducting (SC) state below T_c. Depending on the cutoff ω_M the sum rule (1.1) acquires different meanings. When all the optical transitions are taken into account, Eq. (1.1) expresses simply the so-called full f-sum rule,[7–9] relating the optical spectral weight to the total carrier density n,

$$\int_{-\infty}^{\infty}\mathrm{Re}\,\sigma(\omega)d\omega=\frac{\pi ne^2}{m}, \tag{1.2}$$

where m is the bare electronic mass. However, it is usually assumed that when ω_M is of the order of the plasma frequency only intraband optical transitions relative to the lowest conduction band $\varepsilon_{\mathbf{k}}$ contribute to $W(T)$, so that one obtains the *restricted* or *partial sum rule*,[10–12] which relates W_i to the average value of the diamagnetic term τ_{ii} [see Eq. (2.10) below],

$$W_i(\omega_P,T)\equiv W(T)=\frac{\pi e^2}{V}\langle\tau_{ii}\rangle=\frac{\pi e^2}{VN}\sum_{\mathbf{k},\sigma}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_i^2}n_{\mathbf{k},\sigma}, \tag{1.3}$$

where $n_{\mathbf{k},\sigma}$ is the momentum occupation number, V is the unit-cell volume, N is the number of unit cells, e is the electron charge, and we set $\hbar=c=1$. In the two-dimensional (2D) case $V=a^2$, and in the quasi-2D case $V=a^2s$, where a is the lattice spacing and s is the distance between the layers. In the following we will consider mainly in-plane processes and isotropic systems, where $W_x=W_y=W$.

The main difference between the restricted and full sum rule is that while $W(\omega_M\to\infty,T)$ is a constant, $W(T)$ given by Eq. (1.3) is in general a function of temperature, which provides information about the interactions between the electrons in the system. In particular, in a 2D lattice model with a nearest-neighbors tight-binding dispersion $\varepsilon_{\mathbf{k}}=-2t(\cos k_xa+\cos k_ya)$ the spectral weight Eq. (1.3) is proportional to the mean kinetic energy of the system, $W(T)=-(\pi e^2/V)(\langle K\rangle/2)$. In the absence of interactions $n_{\mathbf{k}\sigma}=f(\xi_{\mathbf{k}})$, where $\xi_{\mathbf{k}}=\varepsilon_{\mathbf{k}}-\mu$, μ is the chemical potential, and $f(x)$ is the Fermi function. In this case the main temperature dependence of the spectral weight (1.3) comes from the temperature smearing of the Fermi function, and can be easily evaluated using the Sommerfeld expansion:

$$\begin{aligned}\frac{W(T)}{(\pi e^2a^2/V)}&=-\frac{1}{N}\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}f(\xi_{\mathbf{k}})\\&=-\int d\varepsilon N(\varepsilon)f(\varepsilon-\mu)\\&=\frac{W(0)}{(\pi e^2a^2/V)}-\frac{\pi^2}{6}c(\mu)T^2,\end{aligned} \tag{1.4}$$

where $N(\varepsilon)$ is the density of states for the tight-binding dispersion and $c(\varepsilon)=\varepsilon N'(\varepsilon)+N(\varepsilon)$. By making a quadratic approximation for the two-dimensional tight-binding band dispersion one would find $c(\mu)=1/4\pi t$, which is also a good

estimate of the exact value obtained using the true band dispersion and by doping the system away from half-filling (see also Appendix A). However, for an interacting system $n_{\mathbf{k}\sigma}$ can acquire in general a different temperature dependence, which influences also $W(T)$. An example is provided by the case of a SC instability. Indeed, according to the BCS theory, in the SC state the occupation number becomes

$$n_{\mathbf{k}\sigma} = [1 - \xi_{\mathbf{k}}/E_{\mathbf{k}}^{\mathrm{SC}} \tanh(E_{\mathbf{k}}^{\mathrm{SC}}/2T)], \tag{1.5}$$

where $\Delta_{\mathbf{k}}$ is the SC gap and $E_{\mathbf{k}}^{\mathrm{SC}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ is the quasiparticle dispersion in the SC state, so that the spectral weight (1.3) decreases below T_c. When $W(T)$ corresponds to the kinetic energy this result is understood as the increase of $\langle K \rangle$ below T_c due to the particle-hole mixing in the SC state.

These general expectations about the behavior of the restricted optical sum rule were not confirmed, within several respects, in the experiments on HTSC. Early measurements of the *c*-axis spectral weight up to frequencies of the order of the plasma edge, $\omega_P \propto 10^4$ cm^{-1}, showed that in $YB_2Cu_3O_{6+\delta}$ (YBCO) compounds $W_z(T)$ exhibits a quite anomalous temperature dependence, with a decrease below the pseudogap temperature, followed by an increase below T_c.[13] Such a behavior was indeed attributed to the effect of pseudogap opening, combined with the tunneling character of the transport along the *c*-axis direction.

Recently more attention has been instead devoted to the issue of the spectral-weight behavior for the in-plane optical conductivity, which is a better probe of the degrees of freedom mostly responsible for the properties of HTSC. The measurements were performed in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO),[1,2,4] YBCO,[3,5] and $La_{2-x}Sr_xCu_2O_4$ (LSCO) (Ref. 6) compounds at various cutoff frequencies ω_M between 1000 cm^{-1} (0.12 eV) and 20 000 cm^{-1} (2.5 eV). A first issue is the behavior of $W(T)$ below T_c. While early measurements in BSCCO samples show that there is an even faster *increase* of $W(T)$ below T_c,[1,2] contrary to the prediction of the BCS theory, more recent results in BSCCO (Ref. 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.[3,5] Also from the theoretical point of view many proposals arose relative to the problem of the lowering of in-plane kinetic energy in the SC state.[14–17]

Interestingly the behavior of $W(T)$ above the SC transition also shows unexpected features, which deserve more investigation. Indeed, as observed in Ref. 2, the in-plane optical sum rule does not show any decrease below the temperature at which the pseudogap forms, contrary to what found for the *c*-axis response. In addition, when the plasma edge is considered as a cutoff, $W(T)$ shows a "standard" T^2 temperature dependence, even though these are clearly strongly interacting non-Fermi-liquid systems. However, this result is misleading, because despite the *qualitative* analogy with the free tight-binding result (1.4), the measured $W(T)$ is in a strong *quantitative* disagreement with the estimate (1.4). Indeed, as we show in Appendix A, the coefficient $c(\mu)$ of Eq. (1.4) is about one order of magnitude larger than expected by using a t value estimated by other probes (as photoemission measurements of the Fermi surface), showing that the sum rule is far from being conventional already in the normal (non-SC) state.[6] Moreover, even faster increase of $W(\omega_M, T)$ is observed at smaller values of ω_M.[4,6]

For these reasons, the issue that we address in the present paper is the behavior of the optical-conductivity spectra and sum rule above T_c, but within a model system for the pseudogap state. Between the several proposals existing in the literature about the origin of the pseudogap,[18] we focus in the present paper on the case where a competing order parameter is formed before the SC state is established. In particular, we refer to the so-called flux phase or *d*-density wave state (DDW).[19–27] We would like to stress that while a flux phase does not present modulated charge, the same phenomenological spectrum can be considered as emerging due to the tendency of the system to form charge order near a quantum critical point.[28] This scenario was studied in Ref. 26, and we will refer in the present paper also to this point of view, which could be useful in relating the results presented here not only to cuprates, where they can be only partly applied, but also to other materials displaying a true *k*-space modulated CDW (as, for example, dichalcogenide materials[29,30]).

In a previous publication,[31] we discussed briefly how a mean-field description of the DDW state can be compatible with an increase of the spectral weight below the temperature at which the order parameter forms. However, this result was not considered from a more general point of view, which consists in relating the sum rule to the problem of providing a gauge-invariant approximation for the response functions in a given microscopic model. As we shall see, the basic requirement of respecting the charge conservation imposes simultaneously several constraints on the definition of the current operator, the diamagnetic term and the corresponding electromagnetic correlation functions. The sum rule then follows naturally when all these requirements are satisfied within a given approximation for the microscopic interacting model, and different approximations can lead to different sum rules. As we shall see, while the anomalous sum rule derived in Ref. 31 can be proposed to reproduce the experimental data for cuprates, the agreement with the theoretically obtained optical conductivity is more subtle, and more detailed features specific of different materials should be considered. A more difficult task is to properly define the change of behavior of the sum rule at different cutoff ω_M; this problem is quite general, and while it is clear that for $\omega_M \to \infty$ the full sum rule (1.2) must be recovered, there is as yet no clear understanding of a proper experimental and theoretical definition of the correct cutoff for the restricted sum rule in Eq. (1.3). In our case, we shall discuss how the various restricted sum rules should be realized at different energy scales, even though an exact result cannot be obtained in this respect.

The structure of the paper is the following. We begin by presenting in Sec. II the general formalism which is needed to analyze the optical-conductivity sum rule in an interacting system. In Sec. III we explicitly study the case of a DDW state, and we show that we can derive a good approximation for the low-energy optical conductivity which is however no more related to a known sum rule. In Sec. IV we solve this problem by analyzing directly the reduced, low-energy DDW model Hamiltonian, and we calculate explicitly the sum rule

and the optical conductivity within the proposed mean-field approach to the DDW transition. We then discuss in Sec. V the results obtained and summarize the procedure described in the paper. In Appendix A we report the evaluation of the sum-rule behavior for the noninteracting tight-binding model, to quantify the discrepancy with the experimental data, and some details about the role of disorder are presented in Appendix B.

II. SUM RULE IN A MODEL WITH GAUGE INVARIANT INTERACTION

Let us start by considering a general Hamiltonian describing interacting electrons in a two-dimensional lattice,

$$H = -t\sum_{\langle ij\rangle} c^{\dagger}_{i\sigma}c_{j\sigma} - \mu\sum_{i} c^{\dagger}_{i\sigma}c_{i\sigma} + \sum_{ij,\sigma\sigma'} c^{\dagger}_{i\sigma}c_{i\sigma}V(\mathbf{r}_i-\mathbf{r}_j)c^{\dagger}_{j\sigma'}c_{j\sigma'}, \tag{2.1}$$

where the field operator $c^{\dagger}_{i\sigma}$ creates an electron of spin σ at $\mathbf{r}_i$, t is the hopping parameter, $\langle ij\rangle$ is the sum over nearest-neighbor sites, $V(\mathbf{r}_i-\mathbf{r}_j)$ is the translationally invariant electron-electron interaction. When rewritten in reciprocal space, the band dispersion corresponds to $\varepsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a)$. Throughout the paper units $\hbar = k_B = c = 1$ are chosen.

In the DDW state a particle-hole coupling is considered at the characteristic wave vector $\mathbf{Q}=(\pi/a,\pi/a)$. The notation is then simplified by halving the Brillouin zone and introducing two-component electron operators (the DDW equivalent of Nambu spinors[32])

$$\chi_{\mathbf{k}\sigma} = \begin{pmatrix} c_{\mathbf{k}\sigma} \\ c_{\mathbf{k}+\mathbf{Q},\sigma}\end{pmatrix}, \quad \chi^{\dagger}_{\mathbf{k}\sigma} = \begin{pmatrix} c^{\dagger}_{\mathbf{k}\sigma} & c^{\dagger}_{\mathbf{k}+\mathbf{Q},\sigma}\end{pmatrix}, \tag{2.2}$$

where $c^{\dagger}_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}\sigma}$ are the Fourier transforms of $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$. The Hamiltonian (2.1) written in terms of χ becomes

$$H = \sum_{\mathbf{k},\sigma}^{\mathrm{RBZ}} \chi^{\dagger}_{\mathbf{k}\sigma}\left[\frac{1}{2}(\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{k}+\mathbf{Q}}) - \mu + \frac{1}{2}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{Q}})\sigma_3\right]\chi_{\mathbf{k}\sigma} + \frac{1}{N}\sum_{\mathbf{q}}^{\mathrm{BZ}} V(\mathbf{q})\sum_{\mathbf{k},\sigma}^{\mathrm{RBZ}} \chi^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}\chi_{\mathbf{k}\sigma}\sum_{\mathbf{p},\sigma'}^{\mathrm{RBZ}} \chi^{\dagger}_{\mathbf{p}-\mathbf{q},\sigma'}\chi_{\mathbf{p}\sigma'}, \tag{2.3}$$

where $V(\mathbf{q})$ is the Fourier transform of the potential, σ_3 is the Pauli matrix and the sums are over the reduced (RBZ) and full Brillouin zone (BZ).

After employing the nesting property $\varepsilon_{\mathbf{k}+\mathbf{Q}} = -\varepsilon_{\mathbf{k}}$ the kinetic term of the Hamiltonian (2.3) takes a simple form

$$H_0 = \sum_{\mathbf{k},\sigma}^{\mathrm{RBZ}} \chi^{\dagger}_{\mathbf{k}\sigma}[\varepsilon_{\mathbf{k}}\sigma_3 - \mu]\chi_{\mathbf{k}\sigma}. \tag{2.4}$$

Accordingly, the free electron Green's function reads

$$G_0^{-1}(\mathbf{k}, i\omega_n) = (i\omega_n + \mu)\sigma_0 - \varepsilon_{\mathbf{k}}\sigma_3, \tag{2.5}$$

where $\omega_n = (2n+1)\pi T$ is the fermionic (odd) Matsubara frequency. The full Green's function of the system $G(p)$, $p=(\mathbf{p}, i\omega)$ is given by the Dyson equation

$$G^{-1}(p) = G_0^{-1}(p) - \Sigma(p), \tag{2.6}$$

where the self-energy $\Sigma(p)$ is evaluated at Hartree-Fock level as

$$\Sigma(p) = \sum_{k} G(k)V(\mathbf{p}-\mathbf{k}), \tag{2.7}$$

where Σ_k is a short-hand notation for $T/N\Sigma_{i\omega_n}\Sigma^{\mathrm{RBZ}}_{\mathbf{k}}$. Observe that for a time-independent interaction, as the one considered in Eq. (2.1), the self-energy (2.7) does not depend explicitly on the frequency, but we will keep for convenience this more general notation in the following. In the case of superconductivity, the Hartree-Fock approximation for the self-energy, equivalent to the Eq. (2.7) rewritten in the particle-particle channel, gives the usual BCS result for the Green's function.[33] In the case of DDW order it corresponds instead to the mean-field Green's function usually considered in the literature.[31,34–41]

A. The electrical conductivity and the conductivity sum rule

The optical conductivity can be calculated from the electromagnetic response kernel

$$K_{\mu\nu}(\mathbf{q}, i\Omega_m) = -\tau_{\mu\mu}\delta_{\mu\nu}(1-\delta_{\nu 0}) + \Pi_{\mu\nu}(\mathbf{q}, i\Omega_m), \tag{2.8}$$

where $\Pi_{\mu\nu}(\mathbf{q}, i\Omega_m)$ is the correlation function

$$\Pi_{\mu\nu}(\mathbf{q}, i\Omega_m) = \frac{1}{N}\int_0^{\beta} d\tau e^{i\Omega_m\tau}\langle T_{\tau} j_{\mu}(\mathbf{q},\tau) j_{\nu}(-\mathbf{q},0)\rangle. \tag{2.9}$$

Here τ_{ii} is the diamagnetic (or stress) tensor, τ is imaginary time, $\beta = 1/T$, and $\Omega_m = 2\pi mT$ is the bosonic Matsubara frequency. The index $\mu=(i,0)$ with $i=1,2$ indicates spatial and time components, respectively, so that the particle current operator $j_{\mu}(\mathbf{q},\tau) = (j_i(\mathbf{q},\tau), j_0(\mathbf{q},\tau))$ consists of the particle current density, $j_i(\mathbf{q},\tau)$ and the particle density, $j_0(\mathbf{q},\tau)$. As usual, the particle current and the diamagnetic tensor are defined as the first and second order derivatives of the Hamiltonian $H(\mathbf{A})$ in the presence of the vector potential $\mathbf{A}$ with respect to $\mathbf{A}$ itself,[12]

$$H(A_i) \approx H(0) - \sum_j \left[eA_i(\mathbf{r_j})j_i(\mathbf{r_j}) - \frac{e^2}{2}A_i^2(\mathbf{r_j})\tau_{ii}(\mathbf{r_j})\right], \tag{2.10}$$

so that the total current density is expressed as $J_i(\mathbf{r}) = -\delta H/\delta A_i(\mathbf{r}) = ej_i(\mathbf{r}) - e^2\tau_{ii}(\mathbf{r})A_i(\mathbf{r})$, and by evaluating $\langle J_i(q)\rangle$ within the linear response theory,[12,33,42] one obtains $J_{\mu}(q) = e^2K_{\mu\nu}(q)A_{\nu}(q)$ with the electromagnetic kernel (2.8). Then using that $\mathbf{A}(\omega) = \mathbf{E}(\omega)/i(\omega+i0)$, where $\mathbf{E}$ is the electric field, one finally arrives at the Kubo formula

$$\sigma(\omega) = -ie^2\frac{K_{ii}(\mathbf{q}=0,\omega)}{V(\omega+i0)} = ie^2\frac{\langle\tau_{ii}\rangle - \Pi_{ii}(\mathbf{q}=0,\omega)}{V(\omega+i0)}, \tag{2.11}$$

where the standard analytic continuation $i\Omega_m \to \omega + i0$ was made. To avoid confusion, along the paper we will indicate

the imaginary bosonic frequencies with $i\Omega_m$, the imaginary fermionic frequencies with $i\omega_n$ and the real frequencies with ω. Since an isotropic system is considered we can omit the index i as done in the left-hand side (LHS) of Eq. (2.11) and in what follows.

Taking the real part of (2.11), one obtains $\mathrm{Re}\,\sigma(\omega) = (\pi e^2/V)\delta(\omega)[\langle\tau\rangle - \mathrm{Re}\,\Pi(\mathbf{0},\omega)] + (e^2/V)\mathrm{Im}\,\Pi(\mathbf{0},\omega)/\omega$. In the presence of disorder the coefficient of the $\delta(\omega)$ vanishes, so that $\mathrm{Re}\,\Pi(\mathbf{q}=0,\omega\to 0) = \langle\tau\rangle$ and only the regular part of $\sigma(\omega)$ survives. As a consequence, one usually defines the optical conductivity only through the imaginary part of $\Pi(\mathbf{q}=0,\omega)$:

$$\mathrm{Re}\,\sigma(\omega) = \frac{e^2}{V}\frac{\mathrm{Im}\,\Pi(\mathbf{q}=\mathbf{0},\omega)}{\omega}, \tag{2.12}$$

so that using the Kramers-Kronig (KK) relations for $\Pi(\mathbf{q}=0,\omega)$ one can derive the well-known sum rule,

$$\begin{aligned} W(T) &= \int_{-\infty}^{\infty} \mathrm{Re}\,\sigma(\omega)d\omega \\ &= \frac{e^2}{V}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,\Pi(\mathbf{q}=\mathbf{0},\omega)}{\omega}d\omega \\ &= \frac{\pi e^2}{V}\,\mathrm{Re}\,\Pi(\mathbf{q}=\mathbf{0},\omega=0) = \frac{\pi e^2}{V}\langle\tau\rangle. \end{aligned} \tag{2.13}$$

The form of $H(\mathbf{A})$ itself depends on the microscopic model and thus on the way the vector potential $\mathbf{A}$ enters the Hamiltonian of the system. When a continuum model is considered instead of Eq. (2.1), the kinetic term is expressed as $\int(-\nabla^2)/2m$ and $\mathbf{A}$ is inserted using the minimal coupling prescription $-i\nabla \to -i\nabla - e\mathbf{A}$. For lattice systems the equivalent of the minimal coupling prescription is the so-called *Peierls ansatz*,[7,8,12] which corresponds to insert the gauge field $\mathbf{A}$ in Eq. (2.1) by means of the substitution $c_i \to c_i e^{-ie\int \mathbf{A}\cdot d\mathbf{r}}$. In this case, it is clear that when the interaction term of the Hamiltonian is a density-density interaction, as in Eq. (2.1), only the kinetic hopping term is modified, while the interaction term is gauge invariant (GI). As a result, the current/density operator and the diamagnetic tensor can be expressed (for small $\mathbf{q}$) as

$$\begin{aligned} j_\mu(\mathbf{q},t) &= \frac{1}{N}\sum_{\mathbf{k},\sigma} v_\mu(\mathbf{k}) c^\dagger_{\mathbf{k}-\mathbf{q}/2\sigma} c_{\mathbf{k}+\mathbf{q}/2\sigma} \\ &= \frac{1}{N}\sum_{\mathbf{k},\sigma}^{\mathrm{RBZ}} \chi^+_{\mathbf{k}-\mathbf{q}/2}\gamma_\mu(\mathbf{k}-\mathbf{q}/2,\mathbf{k}+\mathbf{q}/2)\chi_{\mathbf{k}+\mathbf{q}/2}, \quad \mathbf{q}\to 0, \end{aligned} \tag{2.14}$$

$$\tau_{ii} = \frac{1}{N}\sum_{\mathbf{k},\sigma}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_i^2} n_{\mathbf{k},\sigma}, \tag{2.15}$$

where

$$v_\mu(\mathbf{k}) = (v^F_{\mathbf{k}},1), \quad \gamma_\mu(\mathbf{k}-\mathbf{q}/2,\mathbf{k}+\mathbf{q}/2) = (v^F_{\mathbf{k}}\sigma_3,\sigma_0), \quad \mathbf{q}\to 0, \tag{2.16}$$

and $(v^F_{\mathbf{k}})_i = \partial\varepsilon_{\mathbf{k}}/\partial k_i$ is the Fermi velocity.[43] Note that if a quadratic band dispersion $\varepsilon_{\mathbf{k}} = \mathbf{k}^2/2m$ is assumed, the tensor τ_{ii} reduces to n/m, where n is the total carrier density, so that Eq. (2.13) reduces to the f-sum rule (1.2), which is temperature independent. Instead, for a tight-binding nearest-neighbors lattice dispersion, according to the definition (2.15), τ_{ii} is proportional to the kinetic energy, and the sum rule (1.4) is recovered. Observe that formally the sum rule (2.13) always requires the integration up to an infinite cut off energy. Nevertheless, an intrinsic finite cutoff energy is provided by the energy scale below which a given model can be considered as a good approximation for the real system. As a consequence, while the full f-sum rule is always satisfied at enough large energy scales, the restricted optical sum rule relative to a given tight-binding interacting model is expected to hold only below some intrinsic energy scale, whose definition is not universal. We would like to stress that the definitions (2.14) and (2.15) follow from the Hamiltonian (2.1) once that a gauge-invariant form is chosen for the interaction term. However, this assumption is invalid when, for example, "occupation modulated" hopping terms are present,[14] or when an "effective" interacting model is considered, in a sense that we will specify below (see Sec. IV).

B. Gauge invariance and the sum rule

The derivation of the sum rule presented above is rather formal, and does not allow one to understand that the sum rule is just a different way of stating the gauge invariance of the theory. To gain a deeper insight into the relation between these two aspects, it is useful to consider here the sum-rule derivation presented in Ref. 42. The starting point is the observation that in a GI theory there is a gauge freedom to choose whether the applied electric field $\mathbf{E} = -\partial_t\mathbf{A} - \nabla\varphi$ is included in the Hamiltonian (2.1) either via the vector potential $\mathbf{A}(\varphi=0)$ or by considering a scalar potential $\varphi(\mathbf{A}=0)$. Obviously, the conductivity derived from two equivalent Hamiltonians $H(\mathbf{A})$ and $H(\varphi)$ must be the same, but this is only guaranteed by the charge conservation

$$e\partial j_0(\mathbf{q},t) + ie\mathbf{q}\cdot\mathbf{j}(\mathbf{q},t) = 0. \tag{2.17}$$

The proof considered in Ref. 42 that $\sigma(\omega)$ derived from $H(\mathbf{A})$ and $H(\varphi)$ are the same is based on the identity

$$\int_{-\infty}^{\infty} d\omega\,\mathrm{Re}\,\sigma(\omega) = \frac{\pi e^2}{VN}\lim_{q_i\to 0}\frac{1}{q_i}\langle[j_0(\mathbf{q},t), j_i(-\mathbf{q},t)]\rangle, \tag{2.18}$$

which is obtained by using the charge conservation (2.17). For example, substituting in Eq. (2.18) $j_0(\mathbf{q},t) = \sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}-\mathbf{q}/2,\sigma} c_{\mathbf{k}+\mathbf{q}/2,\sigma}$ and the free-electron expression $\mathbf{j}(\mathbf{q},t) = (1/m)\sum_{\mathbf{k},\sigma}\mathbf{k} c^\dagger_{\mathbf{k}-\mathbf{q}/2,\sigma} c_{\mathbf{k}+\mathbf{q}/2,\sigma}$, corresponding to $\varepsilon_{\mathbf{k}} = \mathbf{k}^2/2m$, returns the full f-sum rule (1.2).

Another way to state the relation between the sum rule and the GI uses instead the generalized electromagnetic kernel (2.8). As discussed in Ref. 33 with reference to the SC

case, the requirements of charge conservation $[q_\mu J_\mu(q)=0]$ and invariance of the theory under the gauge transformation $A_\mu(q)\to A_\mu(q)+iq_\mu\Lambda(q)$ are fulfilled when the condition

$$q_\mu K_{\mu\nu}(q)=K_{\mu\nu}(q)q_\nu=0, \quad q=(\mathbf{q},\omega) \tag{2.19}$$

is satisfied. In particular, the following relation must hold:

$$\Pi_{ii}(\mathbf{q}\to 0,\omega=0)=\langle\tau_{ii}\rangle. \tag{2.20}$$

This equality states that the diamagnetic term is canceled out by the *static* limit $(\omega=0,\mathbf{q}\to 0)$ of the (real) part of the current-current bubble, while deriving the Eq. (2.13) we used the relation between the *dynamic* $(\mathbf{q}=0,\omega\to 0)$ limit of the bubble and the stress tensor. However, in deriving Eq. (2.13) we assumed the presence of disorder, whose role is crucial in restoring the equality between the static and dynamic limits of the current-current correlator $\Pi(q)$. Indeed, while in a clean system the dynamic limit of the bubble vanishes, in the presence of disorder it coincides with the static limit, which in turn is equal to the diamagnetic term: $\mathrm{Re}\,\Pi(\omega\to 0,\mathbf{q}=0)=\mathrm{Re}\,\Pi(\omega=0,\mathbf{q}\to 0)=<\tau>$, and then Eq. (2.13) follows.

C. Ward identity and vertex function

The advantage of the derivations (2.18) and (2.20) of the sum rule is that they show explicitly that it must be regarded as a consequence of the charge conservation. Moreover, it allows one to see that once a given approximation is used in evaluating the current-current correlation function, it also fixes the sum rule that will follow from such an approximation. However, a quite difficult task is to implement an approximation for both the Green's function and the current-current correlator which preserves the condition (2.19), necessary for maintaining the GI of the theory. In particular, when the Hartree-Fock self-energy (2.7) is used and the bubbles $\Pi_{\mu\nu}$ are evaluated in the lowest-order approximation,

$$\begin{aligned}\Pi^{(\gamma)}_{\mu\nu}(\mathbf{q},i\Omega_m)=-2\sum_k \mathrm{Tr}[&G(\mathbf{k}-\mathbf{q}/2,i\omega_n+i\Omega_m)\\ &\times\gamma_\mu(\mathbf{k}-\mathbf{q}/2,\mathbf{k}+\mathbf{q}/2)G(\mathbf{k}+\mathbf{q}/2,i\omega_n)\\ &\times\gamma_\nu(\mathbf{k}+\mathbf{q}/2,\mathbf{k}-\mathbf{q}/2)],\end{aligned} \tag{2.21}$$

the GI is *not* in general preserved, as it is known for SC and as we shall see explicitly in Sec. IV in the case of DDW (the factor 2 in the previous equation is due to the spin summation). A general field theoretical approach that solves the difficulties with charge conservation and gauge invariance, originally present in the mean-field (bare vertex) formulation of the BCS theory, was developed by Nambu[32] and discussed in detail in Chap. 8 of Ref. 33, so that here we only introduce the main definitions and stress the points necessary for the consideration of the DDW state.

As shown in Ref. 33, the current-current correlator, defined above in Eq. (2.9), can be expressed in terms of the full Green's functions (2.6), the bare vertex γ_μ and the full vertex function Γ_ν as follows:

$$\Pi_{\mu\nu}(\mathbf{q},i\Omega_m)=-2\sum_k \mathrm{Tr}[G(k_-)\gamma_\nu(\mathbf{k}_-,\mathbf{k}_+)G(k_+)\Gamma_\mu(k_+,k_-)], \tag{2.22}$$

where $k_+=(\mathbf{k}_+,i\omega_n+i\Omega_m,)$, $k_-=(\mathbf{k}_-,i\omega_n,)$ with $\mathbf{k}_\pm=\mathbf{k}\pm\mathbf{q}/2$. The important property of the current-current correlation function (2.22) is that the condition (2.19) is preserved whenever the vertex function satisfies the *generalized Ward identity* (GWI):

$$q_\mu\Gamma_\mu(p_+,p_-)=G^{-1}(p_-)-G^{-1}(p_+). \tag{2.23}$$

The GWI is nothing but the charge conservation law (2.17) rewritten using the Green's and vertex functions. If the Green's function given by Dyson equation (2.6) is evaluated within the Hartree-Fock approximation (2.7), then the vertex function satisfying the GWI is also the solution of the following integral equation:

$$\Gamma_\mu(p_+,p_-)=\gamma_\mu(\mathbf{p}_+,\mathbf{p}_-)+\sum_k G(k_+)\Gamma_\mu(k_+,k_-)G(k_-)V(\mathbf{p}-\mathbf{k}). \tag{2.24}$$

The analytical solution of Eq. (2.24) cannot be easily determined, except that in the static limit, when Γ_i is given by

$$\begin{aligned}\Gamma_i(p,p)&=\gamma_i(\mathbf{p},\mathbf{p})+\frac{\partial\Sigma(p)}{\partial\mathbf{p}_i}\\ &=-\frac{\partial G^{-1}(p)}{\partial\mathbf{p}_i}\\ &=G^{-1}(p)\frac{\partial G(p)}{\partial\mathbf{p}_i}G^{-1}(p).\end{aligned} \tag{2.25}$$

Indeed, if one sets $q=0$ in Eq. (2.24) (which corresponds, as usual, to the static limit $\omega=0$, $\mathbf{q}\to 0$ when analytical continuation $i\Omega_m\to\omega+i0$ is made), by means of the previous relation one obtains

$$\begin{aligned}\Gamma_i(p,p)&=\gamma_i(p,p)+\sum_k G(k)\Gamma_i(k,k)G(k)V(\mathbf{p}-\mathbf{k})\\ &=\gamma_i(p,p)+\sum_k\frac{\partial G(k)}{\partial\mathbf{k}_i}V(\mathbf{p}-\mathbf{k})\\ &=\gamma_i(p,p)-\sum_k G(k)\frac{\partial V(\mathbf{p}-\mathbf{k})}{\partial\mathbf{k}_i}\\ &=\gamma_i(p,p)+\frac{\partial}{\partial\mathbf{p}_i}\sum_k G(k)V(\mathbf{p}-\mathbf{k})\\ &=\gamma_i(p,p)+\frac{\partial\Sigma(p)}{\partial\mathbf{p}_i}.\end{aligned} \tag{2.26}$$

Here we used the fact that the potential V is nonseparable, viz. it depends on the difference $\mathbf{p}-\mathbf{k}$, as it is expected for a GI density-density interaction. Observe also that this result can be obtained directly from the GWI (2.23) by taking the limit $\omega=0$, $\mathbf{q}\to 0$. For example, one can easily check that WI (2.25) is satisfied for the free electron Green's function (2.5) taken together with the bare vertex (2.16). It is worth noting that in the case of SC the behavior of the vertex function at

zero frequency and momentum is completely different, and indeed $\Gamma_i(p,p)$ is divergent as the inverse of the phase-mode dispersion.[32,33] Indeed, the equivalent of Eq. (2.23) contains for the SC case a combination of Green's functions and Pauli matrices that cannot be reduced to the derivative of G^{-1} as in Eq. (2.25). Here, however, the equivalent of the gapless phase mode is not present, because there is no Goldstone mode when a discrete symmetry is broken, and $\Gamma_i(p,p)$ turns out to be finite.

D. Symmetrized expression for $T=0$ dc conductivity

In practice, since the exact expressions for G and Γ_i are unknown, the consistency of an approximated calculation of the conductivity can be guaranteed if the *approximated* expressions for G and Γ_i satisfy the GWI (2.23). Observe that what we obtained in (2.26) is the limit $\omega=0$, $\mathbf{q}\to 0$ of Γ, but in the calculation of the optical conductivity it is the opposite limit which is needed. However, at least in the presence of impurities, or at $T=0$, the static and dynamic limits commute. Unfortunately, a generalization of the result (2.26) to finite frequency cannot be obtained from the equation (2.24) for a generic potential, by means of, e.g., a perturbative method. Since our final task is to find an approximation for the optical conductivity which allows us also to estimate the corresponding sum rule, let us analyze the utility of the result (2.26). First, we note that the knowledge of the vertex function at zero frequency allows one to find an exact result for the dc conductivity at $T=0$. To show this it is convenient to think of 2×2 matrices A and B as being represented by two column vectors of 2×2 matrix elements and rewrite Tr of the matrix product as the scalar product,

$$\mathrm{Tr}[AB] \equiv \sum_{\alpha\beta} (\vec{A})_{\alpha\beta}(\vec{B})_{\beta\alpha} = \vec{A}\cdot\vec{B}. \tag{2.27}$$

Accordingly, by introducing the vector

$$(\mathcal{G}(k_+,k_-)\vec{\Gamma}(k_+,k_-))_{\alpha\beta} \equiv \sum_{\gamma\delta} G_{\alpha\gamma}(k_+)G_{\delta\beta}(k_-)\Gamma_{\gamma\delta}(k_+,k_-), \tag{2.28}$$

we can rewrite correlation function (2.22) as follows:

$$\Pi_{ij}(q) = -2\int \frac{d^3k}{(2\pi)^3}\mathcal{G}(k_+,k_-)\vec{\Gamma}_i(k_+,k_-)\cdot\vec{\gamma}_j(\mathbf{k}_-,\mathbf{k}_+), \tag{2.29}$$

where since we are considering the $T=0$ case we have an integration over the real frequency instead of the Matsubara sum and the argument of the polarization operator is $q=(\mathbf{q},\omega)$.

The dc conductivity is determined by the imaginary part of the derivative of the correlation function, which in turn is given by

$$\left.\frac{\partial\Pi_{ij}(\mathbf{q}=0,\omega)}{\partial\omega}\right|_{\omega=0} = -2\int \frac{d^3k}{(2\pi)^3}[\mathcal{G}'_\omega(k_+,k_-)\vec{\Gamma}_i(k_+,k_-)\cdot\vec{\gamma}_j(\mathbf{k}_-,\mathbf{k}_+) + \mathcal{G}(k_+,k_-)\vec{\Gamma}'_{\omega i}(k_+,k_-)\cdot\vec{\gamma}_j(\mathbf{k}_-,\mathbf{k}_+)]\Big|_{\omega=0,\mathbf{q}=0}, \tag{2.30}$$

where $\mathcal{G}'_\omega$, Γ'_ω indicate the derivative with respect to ω. The expression (2.30) can be further simplified by using the equation for vertex (2.24) taken at $T=0$ and its derivative with respect to ω,

$$\vec{\gamma}_i(\mathbf{k},\mathbf{k}) = \vec{\Gamma}_i(k_+,k_-) - \int \frac{d^3p}{(2\pi)^3}\mathcal{G}(p_+,p_-)\vec{\Gamma}_i(p_+,p_-)V(\mathbf{k}-\mathbf{p}),$$

$$\mathbf{q}=0, \tag{2.31a}$$

$$\vec{\Gamma}'_{\omega i}(k_+,k_-) = \int \frac{d^3p}{(2\pi)^3}[\mathcal{G}'_\omega(p_+,p_-)\vec{\Gamma}_i(p_+,p_-) + \mathcal{G}(p_+,p_-)\vec{\Gamma}'_{\omega i}(p_+,p_-)]V(\mathbf{k}-\mathbf{p}). \tag{2.31b}$$

Substituting $\vec{\gamma}_i$ from Eq. (2.31a) in Eq. (2.29) and using (2.31b) we obtain

$$\left.\frac{\partial\Pi_{ij}(\mathbf{q}=0,\omega)}{\partial\omega}\right|_{\omega=0} = -2\int \frac{d^3k}{(2\pi)^3}\mathcal{G}'_\omega(k_+,k_-;\mathbf{q}=0)\vec{\Gamma}_i(k,k)\cdot\vec{\Gamma}_j(k,k)\Big|_{\omega=0}. \tag{2.32}$$

Our derivation is similar to the derivation of the symmetrized expressions for the derivatives of the polarization operator considered in Ref. 44, where also the derivative of Bethe-Salpeter kernel enters the analog of Eq. (2.31b). The useful property of the representation (2.32) for Π'_ω is that it contains two full vertex functions Γ_i. The corresponding expression for the dc conductivity σ_{dc} coincides with the result derived by Langer [Eq. (4.8) of Ref. 45] in the early 1960s using a completely different approach, consisting in introducing a *symmetric bubble*

$$\Pi^{\mathrm{sym}}_{ij}(i\Omega_m) = -2\frac{T}{N}\sum_{\mathbf{k},i\omega_n}^{\mathrm{RBZ}} \mathrm{Tr}[G(\mathbf{k},i\omega_n+i\Omega_m)\Gamma_i(k,k)G(\mathbf{k},i\omega_n)\Gamma_j(k,k)], \tag{2.33}$$

obtained by using *two* corrected vertices, evaluated at zero external frequency, and whose derivative at zero frequency and temperature coincides with the result (2.32). Then in the limit $T\to 0$ the leading term of Langer's expression for the dc conductivity is obtained from (2.33) via

$$\sigma_{\rm dc} = \lim_{\omega\to 0} \mathrm{Re}\ \sigma(\omega) = \frac{e^2}{V}\ \mathrm{Im}\ \partial_\omega[\Pi_{ii}^{\rm sym}(i\Omega_m \to \omega)]\big|_{\omega=0}. \tag{2.34}$$

In Eq. (2.26) the vertex function with coinciding fermion momenta and energies, $k_+ = k_- = k$ is related to the self-energy $\Sigma(k)$ by the WI (2.25).[39,45] Thus one can immediately see that whenever $\Sigma(k)$ depends on the momentum $\mathbf{k}$, the dc conductivity (2.34) would be different from the value obtained using the bare bubble (2.21).

From the previous considerations one can argue that, in the absence of a solution for the vertex function Γ at finite frequency, a better approximation for the conductivity in the DDW state is provided by the bubble (2.33), which gives at least an *exact* result for the dc conductivity at $T=0$ (see also Ref. 39). In other words, by evaluating the symmetric bubbles (2.33) at finite frequency one can still capture the behavior of $\sigma(\omega)$ at small ω. At the same time, we do also expect that this assumption will lead to a new result for the sum rule (2.13), because the symmetric bubble (2.33) is no more connected to the diamagnetic term (2.15) by any relation. However, as we shall see in the next section, the sum rule for the bubbles (2.33) can be obtained analytically by using the analogies between the results discussed up to now and the properties of the reduced Gaussian model, where the vertex equation admits the solution Eq. (2.26) at all frequencies.

III. VIOLATION OF THE GI WITH THE BARE VERTEX IN THE DDW STATE

A. The mean-field DDW Hamiltonian

The previous discussion was generically referred to any system displaying a particle-hole instability at the wave vector $\mathbf{Q}$. However, in the Hartree-Fock approach one usually selects a particular form for the mean-field Green function G and then solves the self-consistency equation corresponding to implement the Dyson equation (2.7). In the DDW case, one approximates the general interacting Hamiltonian (2.1) with the model,

$$H_I = -\frac{V_0}{2N}\sum_{\substack{k,k'\\ \sigma,\sigma'}} w_d(\mathbf{k}) w_d(\mathbf{k}') c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{Q}\sigma} c^\dagger_{\mathbf{k}'+\mathbf{Q}\sigma'} c_{\mathbf{k}'\sigma'}, \tag{3.1}$$

where $w_d(\mathbf{k}) = (\cos k_x a - \cos k_y a)/2$. By defining $iD_0 = -(V_0/N)\Sigma_{\mathbf{k}\sigma} w_d(\mathbf{k}) \langle c^\dagger_{\mathbf{k}+\mathbf{Q}\sigma} c_{\mathbf{k}\sigma}\rangle$ we obtain the following mean-field DDW Hamiltonian,

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma} [(\epsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + iD_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{Q}\sigma}] \\ &= \sum_{\mathbf{k},\sigma}^{\rm RBZ} \chi^\dagger_{\mathbf{k}\sigma} [\varepsilon_{\mathbf{k}}\sigma_3 - D_{\mathbf{k}}\sigma_2 - \mu] \chi_{\mathbf{k}\sigma}, \end{aligned} \tag{3.2}$$

where $D_{\mathbf{k}} = D_0 w_d(\mathbf{k})$ is the gap, known as the DDW gap,[27] arising from the formation of the state with circulating currents below a characteristic temperature $T_{\rm DDW}$.[46] This Hamiltonian corresponds to an explicit solution of Eqs. (2.6) and (2.7) with

$$\Sigma(\mathbf{k}) = -D_{\mathbf{k}}\sigma_2, \tag{3.3}$$

so that the full Green's function (2.6) reads

$$G^{-1}(\mathbf{k}, i\omega_n) = (i\omega_n + \mu)\sigma_0 - \varepsilon_{\mathbf{k}}\sigma_3 + D_{\mathbf{k}}\sigma_2. \tag{3.4}$$

The corresponding self-consistency equations for the order parameter D_0 and for the chemical potential μ read

$$\frac{2V_0}{N}\sum_{\mathbf{k}}^{\rm RBZ} \frac{w_d^2(\mathbf{k})}{E_{\mathbf{k}}} [f(\xi_{-,\mathbf{k}}) - f(\xi_{+,\mathbf{k}})] = 1, \tag{3.5}$$

$$\frac{2}{N}\sum_{\mathbf{k}}^{\rm RBZ} [f(\xi_{-,\mathbf{k}}) + f(\xi_{+,\mathbf{k}})] = n, \tag{3.6}$$

where $E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + D_{\mathbf{k}}^2}$, and $\xi_{\pm,\mathbf{k}} = -\mu \pm E_{\mathbf{k}}$ are the two excitation branches associated with the formation of DDW order, which breaks translation symmetry. Observe that to obtain the Eq. (3.6) we used the fact that the occupation number $n_{\mathbf{k}\sigma}$ in the DDW is given, according to the Green's function (3.4), by $n_{\mathbf{k}\sigma} = (1/2E_{\mathbf{k}})[E_{\mathbf{k}}(f(\xi_+) + f(\xi_-)) + \varepsilon_{\mathbf{k}}(f(\xi_+) - f(\xi_-))]$. This allows us also to evaluate the diamagnetic term (2.15) and the corresponding sum rule as

$$\frac{W(D,T)}{(\pi e^2 a^2/V)} = \langle\tau\rangle = -\frac{1}{N}\sum_{\mathbf{k}}^{\rm RBZ} \frac{\varepsilon^2}{E}[f(\xi_+) - f(\xi_-)], \tag{3.7}$$

where we used the fact that $(\partial^2\varepsilon_{\mathbf{k}}/\partial k_i^2) = +2ta^2\cos(k_i a)$ and we omitted the explicit dependence of ε, E, $\xi_\pm$ on $\mathbf{k}$. At this level we have performed an approximation on both the self-energy and the Green's function of the original, interacting system. To obtain now a GI approximation for the optical conductivity, i.e. an approximation which gives Eq. (3.7) as the integral of $\sigma(\omega)$, we should also evaluate the vertex function (2.24). Indeed, as we show with an explicit calculation in the next section, the bubble (2.21) with a bare vertex γ violates this requirement. In general, if the optical conductivity cannot be calculated by means of the exact vertex function (2.24), but a different approximation is used, one cannot expect any more to find Eq. (3.7) as the corresponding sum rule, but this must be calculated explicitly, as we do in Sec. IV.

Before showing the details of this calculation we would like to comment on the relation between the microscopic interaction (2.1) and the approximated one given in Eq. (3.1). If one restrict in the interacting part of Eq. (2.1) the sum over nearest-neighbors sites one can easily show that $H_{\rm int}$ can be rewritten as

$$H_{\rm int} = -V_0 \sum_{\substack{\alpha,k,k',q\\ \sigma\sigma'}} w_\alpha(\mathbf{k}) w_\alpha(\mathbf{k}') c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma'} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma}, \tag{3.8}$$

where the factor $(1/4)\Sigma_\delta e^{i(\mathbf{k}-\mathbf{k}')}$ coming from the sum over nearest-neighboring sites δ has been decomposed in the two-dimensional basis of wave functions $w_\alpha(\mathbf{k})$, which includes the sum of contributions from several channels displaying

different symmetries with respect to the discrete rotation group for the square lattice. One can see that even selecting only the *d*-wave channel and the contribution at $\mathbf{q}=\mathbf{Q}$, Eq. (3.8) does not contain only the coupling in the particle-hole channel of Eq. (3.1), because the spin structure in Eq. (3.8) and Eq. (3.1) are different. This problem does not exist if the original microscopic model is given by a *current-current* interaction, as the formation of a DDW state would naturally require,

$$H_{\rm int}=\frac{V_0}{2}\sum_{\substack{\langle i,j\rangle\\ \sigma\sigma'}} c^\dagger_{i\sigma}c_{i\sigma'}c^\dagger_{j\sigma'}c_{j\sigma}=-\frac{V_0}{2}\sum_{\substack{\langle i,j\rangle\\ \sigma\sigma'}} c^\dagger_{i\sigma}c_{j\sigma}c^\dagger_{j\sigma'}c_{i\sigma'}. \tag{3.9}$$

Observe that (i) Eq. (3.9) is still gauge invariant, since the Peierls transformation does not depend on the spin index; (ii) the self-energy for the interaction (3.9) is still given by Eq. (2.7), with $V(\mathbf{q})=2V_0$. In the following we will never face the problem of solving explicitly Eq. (3.5) for a given microscopic interaction. However, it is worth noting that Eq. (3.1) can be directly derived by selecting a specific channel of a microscopic GI model. Other examples can be also found in Refs. 20–25.

B. The current-current correlation function evaluated with the bare vertex γ

To evaluate the bubbles (2.21) it is useful to introduce the spectral representation for the Green's function (3.4),

$$G(\mathbf{k},i\omega_n)=\int_{-\infty}^{\infty}dz\frac{A(\mathbf{k},z)}{i\omega_n-z} \tag{3.10}$$

with the spectral function

$$A(\mathbf{k},z)=\frac{E_{\mathbf{k}}+\varepsilon_{\mathbf{k}}\sigma_3-D_{\mathbf{k}}\sigma_2}{2E_{\mathbf{k}}}\delta(z-\mu-E_{\mathbf{k}})+\frac{E_{\mathbf{k}}-\varepsilon_{\mathbf{k}}\sigma_3+D_{\mathbf{k}}\sigma_2}{2E_{\mathbf{k}}}\delta(z-\mu+E_{\mathbf{k}}). \tag{3.11}$$

The correlation functions (2.21) can then be written as

$$\Pi^{(\gamma)}_{\mu\nu}(\mathbf{q},i\Omega_m)=-\frac{2}{N}\sum_{\mathbf{k}}^{\rm RBZ}\int dz_1dz_2\,{\rm Tr}[A(\mathbf{k}_+,z_1)\gamma_\mu(\mathbf{k}_+,\mathbf{k}_-)\times A(\mathbf{k}_-,z_2)\gamma_\nu(\mathbf{k}_-,\mathbf{k}_+)]\frac{f(z_1)-f(z_2)}{z_1-z_2-i\Omega_m} \tag{3.12}$$

which gives, according to (3.11), the following current-current correlation function:

$$\Pi^{(\gamma)}_{ii}(\mathbf{q},i\Omega_m)=-\frac{1}{N}\sum_{\mathbf{k}}^{\rm RBZ}(v^F_{\mathbf{k}_i})^2\left(\frac{f(-\mu+E_+)-f(-\mu+E_-)}{E_+-E_--i\Omega_m}+\frac{f(-\mu-E_+)-f(-\mu-E_-)}{E_+-E_-+i\Omega_m}\right)\left(1+\frac{\varepsilon_+\varepsilon_--D_+D_-}{E_+E_-}\right)$$
$$+(v^F_{\mathbf{k}_i})^2\left(\frac{f(-\mu+E_+)-f(-\mu-E_-)}{E_++E_--i\Omega_m}-\frac{f(-\mu-E_+)-f(-\mu+E_-)}{E_++E_-+i\Omega_m}\right)\left(1-\frac{\varepsilon_+\varepsilon_--D_+D_-}{E_+E_-}\right), \tag{3.13}$$

where $D_\pm=D_{\mathbf{k}\pm\mathbf{q}/2}$, $\varepsilon_\pm=\varepsilon_{\mathbf{k}\pm\mathbf{q}/2}$, $E_\pm=E_{\mathbf{k}\pm\mathbf{q}/2}$.

The issue then arises of the relation between the approximation (3.12) for the correlation function and the sum rule (3.7). Let us consider again the GI relation (2.20). When the static limit of the current-current bubble is considered [corresponding in Matsubara formalism to set $q=0$ in the expression (3.13)], we find that $\Pi^{(\gamma)}(0,0)$ is real and given by

$$\Pi^{(\gamma)}_{ii}(\mathbf{0},0)=-\frac{2}{N}\sum_{\mathbf{k}}^{\rm RBZ}\frac{(v^F_i)^2D^2}{E^3}[f(\xi_+)-f(\xi_-)]+\frac{(v^F_i)^2\varepsilon^2}{E^2}[f'(\xi_+)+f'(\xi_-)]. \tag{3.14}$$

The usual procedure used to demonstrate that $\Pi(\mathbf{0},0)$ cancels out $\langle\tau\rangle$ given by Eq. (3.7) consists in integrating by parts the term in $\Pi(\mathbf{0},0)$ which contains the derivative of the Fermi distribution $f'(\xi_\pm)$.[12] In order to do that one would need a term like $df(\xi_\pm)/d\mathbf{k}_i=\pm f'(\xi_\pm)(\varepsilon v^F_{\mathbf{k}_i}-Dv^D_{\mathbf{k}_i})/E$, which in addition to the Fermi velocity, $v^F_{\mathbf{k}}$, contains also the DDW gap velocity, $v^D_{\mathbf{k}_i}=-\partial D_{\mathbf{k}}/\partial\mathbf{k}_i$. However, as one can easily see, the second term of Eq. (3.14) does not contain any contribution proportional to v^D_i, so that the gauge-invariant relation $\Pi(\mathbf{q}\to 0,\omega=0)=\langle\tau\rangle$ cannot be satisfied with the bubble $\Pi^{(\gamma)}$.

According to the discussion of the preceding section, the GI can only be restored when the vertex corrections are included in the correlation functions. Observe that the static-limit result (2.26) reads in the case of DDW state:

$$\Gamma_i(k,k)=\gamma_i(\mathbf{k},\mathbf{k})+v^D_{\mathbf{k}_i}\sigma_2=v^F_{\mathbf{k}_i}\sigma_3+v^D_{\mathbf{k}_i}\sigma_2\equiv V_i(\mathbf{k}), \tag{3.15}$$

where $V_i(\mathbf{k})$ is the generalized velocity representing the $q=0$ limit of the vertex function. It is important to stress that in deriving Eq. (2.26) for $\Gamma_i(k,k)$ it was crucial to keep the translation invariant form $V(\mathbf{p}-\mathbf{k})$ of the potential until the end. This point has been often overlooked in the literature, at least while discussing the corresponding problem for the superconducting case.[33] If one used in Eq. (2.24) defining the vertex function the approximated form $V(\mathbf{k}-\mathbf{p})\approx V_0w_d(\mathbf{k})w_d(\mathbf{p})$, which is appropriate for selecting only the *d*-wave channel in the self-energy (2.7), the result (3.15)

could not be obtained. Indeed, a single-channel separable potential makes the interaction term of the Hamiltonian *not* gauge invariant, and then it would contribute to both the current operator and diamagnetic term, as we will discuss in the next section within the context of the reduced model. However, once that the result (2.26) has been established, and all the intermediate steps have been performed in respecting GI requirements, we can definitely select from the self-energy (2.7) only the *d*-wave channel. As a consequence, if $\Sigma(\mathbf{p})$ is approximated as in Eq. (3.3), the result (3.15) follows.

The Eq. (3.15) can also be obtained from the generalized WI (2.23). Indeed, at small $\mathbf{q}$ the difference $G^{-1}(p)-G^{-1}(p+q)$, where G is defined in Eq. (3.4), is given by

$$q_\mu \Gamma_\mu = G^{-1}(k) - G^{-1}(k+q) = -i\Omega_m \sigma_0 + v_{\mathbf{k}}^F \cdot \mathbf{q}\sigma_3 + v_{\mathbf{k}}^D \sigma_2. \tag{3.16}$$

Since, according to the definitions (2.16), the bare vertex satisfies $q_\mu \gamma_\mu = -i\Omega_m \sigma_0 + v_{\mathbf{k}}^F \cdot \mathbf{q}\sigma_3$, for $\Omega_m = 0$ we can find again that the static vertex (3.15) satisfies the WI (2.23). Note that from the WI (3.16) one can be tempted to generalize the result (3.15) for all $\Omega_m, \mathbf{q} \approx 0$: however, one cannot exclude that an additional term with zero space-time divergence can be added to the solution (3.15), still satisfying Eq. (3.16).

According to the discussion of Sec. II D one can try to use the result (3.15) by evaluating the optical conductivity with the symmetric bubble (2.33). In the specific case of the DDW order, this would correspond to evaluating the following current-current correlation functions:

$$\Pi_{ij}^{\mathrm{DDW}}(\mathbf{q}, i\Omega_m) = -2\frac{T}{N}\sum_{\mathbf{k}, i\omega_n}^{\mathrm{RBZ}} \mathrm{Tr}[G(\mathbf{k}_-, i\omega_n + i\Omega_m) V_i(\mathbf{k}) G(\mathbf{k}_+, i\omega_n) V_j(\mathbf{k})]. \tag{3.17}$$

As it was explained in Sec. II D the ansatz (3.17) guarantees the correctness of the dc conductivity, and in general can be used to study the low-frequency conductivity. Nevertheless, one can check that the bubble $\Pi_{ii}^{\mathrm{DDW}}(0)$ is not compatible with the diamagnetic tensor (3.7), violating again the GI condition (2.20) checked above for $\Pi_{ii}^{(\gamma)}$. The origin of this violation is obvious, viz. instead of the asymmetric bubble (2.22) with one full and one bare vertex that would maintain the GI condition (2.20), we used the symmetric correlation function (2.33). Thus the issue arises whether the diamagnetic tensor $\langle \tau \rangle$ can also be modified to become compatible with the bubble (3.17). As we shall see in the next section, the diamagnetic tensor and sum rule corresponding to the approximate bubble (3.17) can be obtained without further assumptions by analyzing the properties of the reduced Hamiltonian (3.2).

IV. THE REDUCED MODEL

An approach often proposed in the literature to deal with the DDW state is that to consider directly the mean-field Hamiltonian (3.2) as the starting point.[31,34–40] The idea is that at low energy the reduced model (3.2) captures the important physics of the system, so that one can consider it as a starting microscopic Hamiltonian, describing noninteracting quasiparticles. In this case the Green's function (3.4) does not provide any more an approximation, but it is the correct one for the solvable, quadratic model (3.2). Since this Hamiltonian describes noninteracting quasiparticles, it can be solved exactly and the corresponding conductivity is given by the bare bubble. This point of view was taken in Ref. 31 where an unusual form of the optical-conductivity sum rule was obtained. One can notice that any distinction in the Hamiltonian (3.2) in the total energy between a kinetic and a potential part, as can be done for the Hamiltonian (2.1), becomes somehow ambiguous, so that the result of Ref. 31 is not surprising.

In what follows we compare this picture with the traditional one, and show that since the dc conductivity calculated in both approaches appears to be the same, one can also estimate the low-energy sum rule of the microscopic model (2.1) by considering the one realized in the reduced model (3.2).

A. The diamagnetic tensor, current operator and the sum rule for the reduced model

Let us now consider the Hamiltonian (3.2) as the starting microscopic model and analyze how all the considerations made in Sec. II can be applied in this case. Since the Hamiltonian (3.2) describes noninteracting quasiparticles, it is straightforward to calculate the current-current correlation function and the electrical conductivity, because in the absence of an interaction term the Eq. (2.24) for the vertex has a trivial solution $\Gamma_\mu(p_+, p_-) = \tilde{\gamma}_\mu(p_+, p_-)$, where $\tilde{\gamma}_\mu(p_+, p_-)$ is the bare vertex for the model DDW Hamiltonian (3.2). Nevertheless, one should be careful and take into account that this vertex is different from the bare vertex (2.16) for the Hamiltonian (2.1). This can be understood by deriving the particle current operator compatible with the conservation law (2.17) and with the equations of motion for the operators c and $c^\dagger$,[36,37,39,40]

$$\mathbf{j}(\mathbf{q}, t) = \frac{1}{N}\sum_{\mathbf{k},\sigma} (v_{\mathbf{k}}^F c_{\mathbf{k}-\mathbf{q}/2\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}/2\sigma} - i v_{\mathbf{k}}^D c_{\mathbf{k}-\mathbf{q}/2\sigma}^\dagger c_{\mathbf{k}+\mathbf{Q}+\mathbf{q}/2\sigma}), \tag{4.1}$$

The first term of the previous expression relates as usual the particle current to the band velocity $v_{\mathbf{k}}^F$. The second term, which only appears for nonvanishing D_0, takes into account the contribution of the orbital currents to the electrical conductivity, arising when the DDW order is established. Observe that in the reduced model (3.2) the term proportional to D_0 appears as an additional, temperature dependent band, which couples $\mathbf{k}$ and $\mathbf{k}+\mathbf{Q}$ electrons, and as a consequence a corresponding term appears in the definition of the current. By rewriting the electric current operator (4.1) using the spinors (2.2), one has

$$\mathbf{j}_i(\mathbf{0},t) = \frac{1}{N}\sum_{\mathbf{k}\sigma}^{\mathrm{RBZ}} \chi^{\dagger}_{\mathbf{k}\sigma} V_i(\mathbf{k}) \chi_{\mathbf{k}\sigma} \tag{4.2}$$

and, accordingly, the bare vertex reads:[39]

$$\tilde{\gamma}_{\mu}(\mathbf{k}-\mathbf{q}/2,\mathbf{k}+\mathbf{q}/2) = (V_i(\mathbf{k}),\sigma_0), \quad \mathbf{q}\to 0, \tag{4.3}$$

where $V_i(\mathbf{k})$ is the generalized velocity defined in Eq. (3.15). Substituting the bare vertex (4.3) and the Green's function (3.4) in the Ward identity (2.25) one can easily see that it is satisfied. Moreover, since for noninteracting quasiparticles the full and bare vertex functions coincide, the correlation function $\Pi^{(\tilde{\gamma})}$ of Eq. (2.21), evaluated with the bare vertex $\tilde{\gamma}$ of Eq. (4.3), has two properties, (i) it is the *exact* one for the quadratic model (3.2); (ii) it coincides with Π^{DDW}_{ij} in Eq. (3.17), which is an *approximation* for the full model (2.1). As a consequence, the sum rule corresponding to the bubble Π^{DDW}_{ij} can be obtained by the knowledge of the stress tensor for the reduced system. Observe that the current operator (4.1) is also obtained when the Peierls substitution is performed directly in the reduced model (3.2). As we discussed in Sec. II A, after the Peierls substitution both the current operator and the diamagnetic tensor can be derived from $H(A)$, according to Eq. (2.10). As a consequence, in the reduced model not only the current operator but also the diamagnetic tensor τ_{ii} is modified, containing an extra term for $D_0 \neq 0$,[31]

$$\langle \tau_{ii} \rangle = -\frac{1}{2N}\sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} \langle c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle + iD_{\mathbf{k}} \langle c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{Q}\sigma}\rangle). \tag{4.4}$$

When the operator averages are evaluated, or analogously Eq. (2.18) is used, one finds that the sum rule for the reduced model is

$$\frac{W^{\mathrm{DDW}}(D,T)}{(\pi e^2 a^2/V)} = -\frac{1}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} E_{\mathbf{k}}[f(\xi_{+,\mathbf{k}}) - f(\xi_{-,\mathbf{k}})], \tag{4.5}$$

where $E_{\mathbf{k}}$ and $\xi_{\pm,\mathbf{k}}$ were already defined after Eq. (3.6). Equation. (4.5) was derived using the fact that $\partial_{x,y} v^F_{\mathbf{k}} = 2ta^2 \cos k_{x,y} a$ [and $\partial_{x,y} v^D_{\mathbf{k}} = \pm (D_0/2) a^2 \cos k_{x,y} a$], and it reduces to Eq. (1.3) for $D_0 = 0$.

Once more, the result (4.4) is consistent with the GI for the reduced model. Indeed, if the bubbles $\Pi^{\mathrm{DDW}}(\mathbf{q}, i\Omega_m)$ (3.17) are evaluated in the static limit, instead of the result (3.14) for $\Pi^{(\gamma)}$ one has

$$\Pi^{\mathrm{DDW}}_{ii}(\mathbf{0},0) = -\frac{2}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} \frac{(v^F_i D + v^D_i \varepsilon)^2}{E^3}[f(\xi_+) - f(\xi_-)] + \frac{(v^F_i \varepsilon - v^D_i D)^2}{E^2}[f'(\xi_+) + f'(\xi_-)]. \tag{4.6}$$

If now one integrates by parts the second term of Eq. (4.6) one finds that

$$\begin{aligned} &-\frac{2}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} \frac{(v^F_i \varepsilon - v^D_i D)^2}{E^2}[f'(\xi_+) + f'(\xi_-)] \\ &= \frac{2}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} [f(\xi_+) - f(\xi_-)] \frac{\partial}{\partial \mathbf{k}} \frac{(v^F_i \varepsilon - v^D_i D)}{E} \\ &= \frac{2}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} \frac{(v^F_i D + v^D_i \varepsilon)^2}{E^3}[f(\xi_+) - f(\xi_-)] \\ &\quad - \frac{1}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} E[f(\xi_+) - f(\xi_-)], \end{aligned}$$

and as a consequence the GI relation $\Pi^{\mathrm{DDW}}_{ii}(\mathbf{0},0) = \langle \tau_{ii} \rangle$ with $\langle \tau_{ii} \rangle$ given by Eq. (4.4) is satisfied, as expected when the exact vertex Γ in included in the bubble.

A comment is in order now about a third possible approach proposed in the literature[38] for the analysis of the reduced model (3.2). By rewriting the quadratic Hamiltonian (3.2) as $H = \Sigma^{\mathrm{RBZ}}_{\mathbf{k},\sigma} \chi^{+}_{\mathbf{k}\sigma} \hat{H}_{\mathbf{k}} \chi_{\mathbf{k}\sigma}$ the matrix $\hat{H}_{\mathbf{k}}$ can be diagonalized by means of an unitary transformation $U_{\mathbf{k}}$, $\hat{H} = U_{\mathbf{k}} \Lambda_{\mathbf{k}} U^{+}_{\mathbf{k}}$ where $\Lambda_{\mathbf{k}} = \mathrm{diag}(\xi_+, \xi_-)$. According to our definition (4.1), the current is derived from $\hat{H}_{\mathbf{k}}(\mathbf{A})$, so that it corresponds to $j_{\mathrm{DDW}} = (1/N)\Sigma^{\mathrm{RBZ}}_{\mathbf{k}\sigma} \chi^{+}_{\mathbf{k}\sigma} (\partial_{\mathbf{k}} \hat{H}_{\mathbf{k}}) \chi_{\mathbf{k}\sigma} = (1/N)\Sigma^{\mathrm{RBZ}}_{\mathbf{k}\sigma} \chi^{+}_{\mathbf{k}\sigma} \partial_{\mathbf{k}} (U_{\mathbf{k}} \Lambda_{\mathbf{k}} U^{+}_{\mathbf{k}}) \chi_{\mathbf{k}\sigma}$ (see also Ref. 40). Let us introduce the spinors $\psi_{\mathbf{k}\sigma} = U^{+}_{\mathbf{k}} \chi_{\mathbf{k}\sigma}$ which diagonalize the Hamiltonian matrix $\hat{H}$, $H = \Sigma^{\mathrm{RBZ}}_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma} \Lambda_{\mathbf{k}} \psi_{\mathbf{k}\sigma}$. Then, by making the assumption that the gauge field couples by Peierls ansatz not to $\chi_{\mathbf{k}\sigma}$ but to the new quasiparticle operators $\psi_{\mathbf{k}\sigma}$, one would calculate the current starting from $\Lambda_{\mathbf{k}}(\mathbf{A})$, so that the current, the diamagnetic term and the static limit of the current-current bubble would be defined as:[38]

$$j_{QP} = \frac{1}{N}\sum_{\mathbf{k}\sigma}^{\mathrm{RBZ}} \psi_{\mathbf{k}\sigma} \partial_{\mathbf{k}} \Lambda_{\mathbf{k}} \psi_{\mathbf{k}\sigma} = \frac{1}{N}\sum_{\mathbf{k}\sigma}^{\mathrm{RBZ}} \chi^{+}_{\mathbf{k}\sigma} U_{\mathbf{k}} (\partial_{\mathbf{k}} \Lambda) U^{+}_{\mathbf{k}} \chi_{\mathbf{k}\sigma},$$

$$\langle \tau_{ii,QP} \rangle = \frac{1}{N}\sum_{\mathbf{k}\sigma}^{\mathrm{RBZ}} \left(\frac{\partial^2 \xi_+}{\partial k_i^2} f(\xi_+) + \frac{\partial^2 \xi_-}{\partial k_i^2} f(\xi_-) \right),$$

$$\Pi_{ii,QP}(\mathbf{0},0) = -\frac{1}{N}\sum_{\mathbf{k}\sigma}^{\mathrm{RBZ}} \left[\left(\frac{\partial \xi_+}{\partial k_i} \right)^2 f'(\xi_+) + \left(\frac{\partial \xi_-}{\partial k_i} \right)^2 f'(\xi_-) \right].$$

Observe that this approximation is still GI in the sense that it is easy to see that $\tau_{ii,QP}$ and $\Pi_{ii,QP}(0)$ defined above satisfy the condition (2.20). However, this approximation has no relation with the microscopic starting model, in the way we explained in Sec. II. For this reason, we do not comment further on this approach, and we analyze instead the result obtained with the current operator (4.1) and the bubbles (3.17), whose correspondence with the microscopic model we established above.

B. Temperature dependence of the spectral weight

Once that we clarified the different approximations used in deriving the two sum rules (3.7) and (4.5), let us discuss

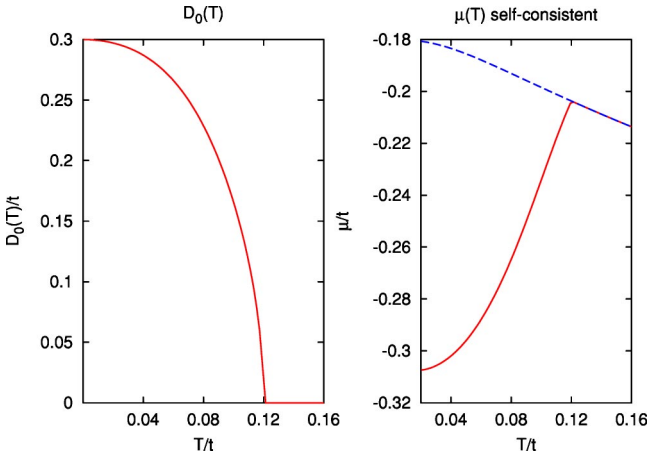

FIG. 1. (Color online) Left panel, Temperature dependence of the DDW gap according to the function $g(x)$ defined in the text. Right panel, $\mu(T)$ in the normal state (dashed line) and in the DDW state (solid line), obtained solving the self-consistency equation (3.6) for the particle number (with $D_0=0$ for the normal state).

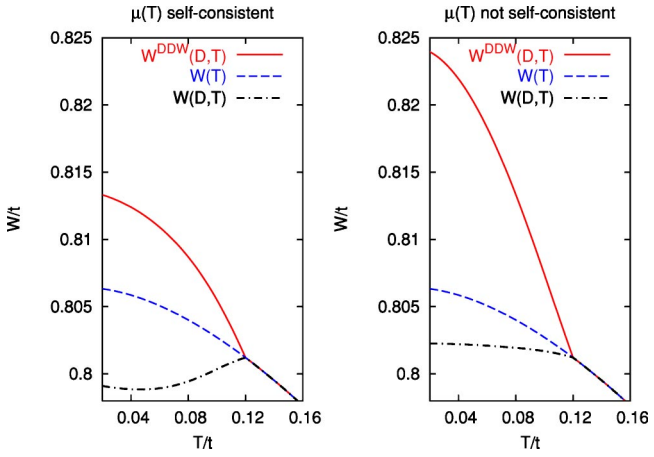

FIG. 2. (Color online) Spectral weight $W^{\mathrm{DDW}}(D,T)$, $W(D,T)$, and $W(T)$, according to Eqs. (4.5), (3.7), and (1.4), respectively, in units of $e^2\pi a^2/V$. We used here $D(0)=2.5T_{\mathrm{DDW}}=0.3t$ and $\delta=0.1$. Left panel, results obtained using the chemical potential obtained solving the self-consistency equation (3.6) for the particle number with $D_0\neq 0$ [for $W^{\mathrm{DDW}}(D,T)$ and $W(D,T)$ and $D_0=0$ (for $W(T)$)], respectively, see Fig. 1. Right panel, evaluation of $W^{\mathrm{DDW}}(D,T)$ and $W(D,T)$ using the chemical potential of the normal state.

the outcomes of these two approaches as far as the temperature dependence of the spectral weight is concerned. Two observations should be kept in mind, (i) the overall variations of the spectral weight in the DDW state are not expected in general to be large if quite small gap values $D(0)/t\ll 1$ are considered; (ii) in Eqs. (3.7) and (4.5) the temperature variation of both the gap and the chemical potential μ contribute to the shape of $W(T)$. In the case of free electrons, the variation of $\mu(T)$ is almost negligible compared to the temperature variation of the occupation number, given by the Fermi function. Indeed, even considering the temperature variation of $\mu(T)$ the result (1.4) is only modified by terms of order T^4. In the case of Eqs. (3.7) and (4.5) also the band structure is varying in temperature, and it is important to keep track of this by solving at each temperature the self-consistent equation for the chemical potential. Here, instead of solving explicitly Eq. (3.5), we adopt a general mean-field temperature dependence for $D_0(T)=D(0)g(T/T_{\mathrm{DDW}})$, with $g(x)=(1-x^4/3)\sqrt{1-x^4}$, as shown in the left panel of Fig. 1. In the right panel of Fig. 1 we also present the temperature dependence of the chemical potential in the DDW state, as one can see, below T_{DDW} there is an inversion of tendency of $\mu(T)$ due to the opening of the gap. The temperature dependence of the spectral weight in the DDW state according to Eq. (3.7) $[W(D,T)]$ and (4.5) $[W^{\mathrm{DDW}}(D,T)]$ is reported in Fig. 2, where also the tight-binding spectral weight (1.4) $[W(T)]$ is shown for comparison. Here we used a small gap value, $D(0)=2.5T_{\mathrm{DDW}}=0.3t$, and doping $\delta=0.1$. The influence of the chemical-potential variation are evident comparing the right panel of Fig. 2, where $W(D,T)$ and $W^{\mathrm{DDW}}(D,T)$ are evaluated keeping μ constant (at the value it has in the normal state), and the left panel, where the density is constant. In addition, we see that for this value of $D(0)$ the overall spectral-weight variations are small in the DDW state. However, it is found that the definition (3.7) leads to a smooth decrease of the spectral weight below T_{DDW}, in analogy with the results for a SC transition, while the definition (4.5) gives an increase. Such variations are quantitatively (but not qualitatively) modified if the temperature variations of the chemical potential are not properly taken into account, see right panel of Fig. 2. Observe that the relative variations of $W(T)$ between $T=0.16t$ and $T=0$ are never larger than $\sim 1.2\%$, and cannot be appreciated on the scale of the figure reported in Ref. 40.

Even though a detailed description of cuprates is not the main aim of our paper, we find nevertheless useful to compare our results for a choice of parameters appropriated for HTSC. Since on this respect different attitudes are present in the literature, we briefly recall here the phase diagram analyzed in Ref. 26 within the more general attitude of investigating the consequences of describing the pseudogap state with a k-space modulated charge density wave. In Ref. 26 it was shown that one outcome of this description is the possibility to interpret the leading-edge shift observed in photoemission experiments as due to a particle-hole gap. In particular, for a band dispersion with a next-nearest-neighbors hopping term $t'=0$ the hole-pockets Fermi surface formed by doping the DDW system with respect to half-filling is a simplification intended to reproduce the arcs of Fermi surface observed experimentally. A simple calculation shows that in such a case the gap measured by ARPES at the M points corresponds approximately to $D_0-|\mu|$. As a consequence, $D_0(0)$ and T_{DDW} do not correspond directly to the maximum gap value and the T^* temperature measured by ARPES, but both are quite larger, as shown in Ref. 26 where the values of the DDW gap and of the temperature T_{DDW} were chosen to properly reproduce the phase diagram of Bi2212 compounds.

In agreement with Ref. 31 we keep here this attitude and use a doping and temperature dependent DDW gap $D_0(T,\delta)=cT_{\mathrm{DDW}}(\delta)g(T/T_{\mathrm{DDW}})$, where $T_{\mathrm{DDW}}(\delta)=0.16t[1-(\delta/\delta_0)^4]$ vanishes at the critical doping $\delta_0=0.2$ for DDW formation, and $c=7$ is a fitting parameter.[26] Since the result-

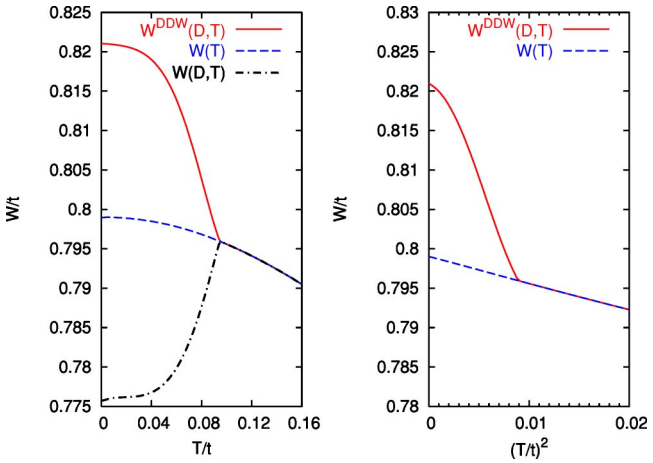

FIG. 3. (Color online) Left panel, spectral weight $W^{\mathrm{DDW}}(D,T)$, $W(T)$, and $W(D,T)$ in units of $e^2\pi a^2/V$ for a choice of parameter values appropriate for cuprates (see the discussion in the text). Here we show the results for $\delta=0.16$, corresponding approximately to optimal doping, and we calculate the chemical potential self-consistently. Right panel, spectral weight plotted as a function of $(T/t)^2$: one can see that a T^2 temperature dependence is still recovered for $W^{\mathrm{DDW}}(D,T)$ in a wide range of temperatures.

ing temperature dependence of the sum rule (4.5) was already shown in Ref. 31, we just report here for comparison the behavior of the two sum rules $W(D,T)$ in Eq. (3.7) and $W^{\mathrm{DDW}}(D,T)$ in Eq. (4.5) for this choice of parameters at $\delta=0.16$. As it can be seen in Fig. 3, the relative variation of the spectral weight below T_{DDW} is made now more pronounced, enhancing the differences between the two possible approaches followed in deriving the sum rule. It is then clear that the standard sum-rule derivation leading to $W(D,T)$ in Eq. (3.7) cannot be consistent with the experiments, since no decrease of the spectral weight has been observed in the pseudogap phase of cuprates. The result $W^{\mathrm{DDW}}(D,T)$ in Eq. (4.5) is instead resembling more closely the experimental findings, in particular if we consider that at this doping level the room temperature below which the data in Refs. 1, 2, and 4 are reported corresponds to $T/t\sim 0.1$, so that the overall measured temperature dependence of $W(T)$ would correspond in our picture to the DDW result (4.5). Indeed, as we show in the right panel of Fig. 3, the $W^{\mathrm{DDW}}(D,T)$ evaluated according to Eq. (4.5) still displays a T^2 temperature dependence, but with a larger slope, as observed experimentally. This approach would allow one to understand why the spectral-weight increase looks like a "standard" free tight-binding model, but with a much larger slope. However, as we shall see in the next section, the comparison with the experiments is made much more involved when the optical conductivity corresponding to the sum rule (4.5) is evaluated. Finally, one can in principle extend this analysis to the case where also SC is added, but since also the experimental situation is not clear on this respect we refer to Ref. 31 for a discussion about the SC state.

C. The role of a next-nearest-neighbors hopping term

Up to now we did not consider the possibility of a next-neighbors hopping term t' in the bare band dispersion $\varepsilon_{\mathbf{k}}$. Indeed, from one side we wanted to simplify the notation while discussing the issue of the relation between gauge invariance and sum rule, and from the other side we believe that even when comparing with cuprates the case $t'=0$ is enough to reproduce phenomenologically the arc of Fermi surface observed in the pseudogap phase (see discussion above). However, for the sake of completeness, we report here briefly the modifications induced in the sum rule when a t' term is included in the band dispersion, so that

$$\varepsilon_{\mathbf{k}} = s_{\mathbf{k}} + p_{\mathbf{k}},$$

$$s_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a),$$

$$p_{\mathbf{k}} = 4t' \cos k_x a \cos k_y a. \tag{4.7}$$

In the DDW state the perfect nesting condition is lost due to the t' term, so that $\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{k}+\mathbf{Q}}=2p_{\mathbf{k}}, \varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{Q}}=2s_{\mathbf{k}}$ and the two quasiparticle branches in the DDW state become $\xi_{\pm,\mathbf{k}}=p_{\mathbf{k}}-\mu\pm E_{\mathbf{k}}$, where $E_{\mathbf{k}}=\sqrt{s_{\mathbf{k}}^2+D_{\mathbf{k}}^2}$. As a consequence, given the relation (2.13) between the sum rule and the diamagnetic tensor, and the definitions (2.15) and (4.4) of the diamagnetic tensor for the original and the reduced model, respectively, it is easy to see that Eqs. (1.4), (3.7), and (4.5) get modified as

$$\frac{W(T)}{(\pi e^2 a^2/V)} = -\frac{1}{N}\sum_{\mathbf{k}} (\varepsilon + p) f(\xi), \tag{4.8}$$

$$\frac{W(D,T)}{(\pi e^2 a^2/V)} = -\frac{1}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} \left(\frac{s^2}{E}[f(\xi_+) - f(\xi_-)] + 2p[f(\xi_+) + f(\xi_-)] \right), \tag{4.9}$$

$$\frac{W^{\mathrm{DDW}}(D,T)}{(\pi e^2 a^2/V)} = -\frac{1}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} \{E[f(\xi_+) - f(\xi_-)] + 2p[f(\xi_+) + f(\xi_-)]\}, \tag{4.10}$$

where the explicit dependence on $\mathbf{k}$ is omitted. In Fig. 4 we compare again the temperature dependence of the spectral weight in the different cases, for $t'=0.3t$, $\delta=0.1$, $T_{\mathrm{DDW}}=0.12t$ and $D(0)=4T_{\mathrm{DDW}}$. Even though the introduction of the t' term modifies the temperature dependence of the chemical potential in the normal and DDW state (due to the shift of the Van Hove singularity which is now below the Fermi level at $\delta=0.1$), the general trend of Figs. 2 and 3 is confirmed. Indeed, $W^{\mathrm{DDW}}(D,T)$ is larger than $W(T)$ below T_{DDW}, while $W(D,T)$ is smaller. In particular, it is worth noting that apart from possible quantitative differences with respect to the case $t'=0$, the exact form of the band dispersion is irrelevant as far as the main issue discussed in the preceding sections, i.e., the fact that different approximations for the current-current correlation functions lead to different results for the optical-conductivity sum rule. For this reason, we do not discuss further in the following the role of a t' term, and remind the reader for example to Refs. 40 and 41, where this issue is investigated in more details.

D. The optical conductivity of the reduced model

As we discussed in the preceding sections, one would expect that our result (4.5) for $W^{\mathrm{DDW}}(D,T)$ is only valid at low energy scales, possibly below the plasma frequency, which can be thought as a general cutoff for any tight-binding based description of the system. In principle one could also expect that the low-energy theory (3.2) is valid at even lower energy scales, but since at the plasma energy one still finds experimentally strong variation with respect to the naive estimate (1.4), it is plausible that a quite larger cutoff holds here for the tight-binding model itself. To analyze the dependence of the result (4.5) on the cutoff frequency we need an explicit calculation of the optical conductivity obtained with the bubble (3.17).

By using the spectral representation of the Green's functions the current-current correlation function Π_{ii}^{DDW} (3.17) can be evaluated in analogy with $\Pi_{ii}^{(\gamma)}$ in Eq. (3.12), with the bare vertices γ_i substituted by the full one $\Gamma_i(k,k)$ of Eq. (3.15). To take into account the effect of disorder we make the simplest ansatz of substituting the delta functions associated to a quasiparticle pole in the spectral representation (3.11) with a Lorentzian of finite width w [$w=1/(2\tau_{tr})$, where τ_{tr} is the transport time],

$$\delta(z) \rightarrow M(z) = \frac{1}{\pi}\frac{w}{z^2+w^2}. \tag{4.11}$$

As a consequence, after analytical continuation in Eq. (3.12), we obtain

$$\begin{aligned}\sigma^{\mathrm{DDW}}(\omega) &= -\frac{2\pi e^2}{V}\sum_{\mathbf{k}}^{\mathrm{RBZ}}\int dz \frac{f(z+\omega)-f(z)}{\omega}\Bigg(\frac{(\varepsilon v^F - D v^D)^2}{E^2} \\ &\times[M(z+\omega-\xi_+)M(z-\xi_+)+M(z+\omega-\xi_-)(z-\xi_-)] \\ &+\frac{(\varepsilon v^D + D v^F)^2}{E^2}[M(z+\omega-\xi_+)M(z-\xi_-) \\ &+M(z+\omega-\xi_-)M(z-\xi_+)]\Bigg),\end{aligned} \tag{4.12}$$

where v^F and v^D refers to the component in a given x or y direction.

As already observed in Ref. 37, and more recently in Refs. 40 and 41, the optical conductivity is composed of two contributions, due to the splitting of the original single band $\varepsilon_{\mathbf{k}}$ in two new bands $\xi_{\pm}$ after the gap opening. In Eq. (4.12) the first line describes intraband excitations (corresponding to the product of two M functions evaluated at the same quasiparticle branch), while the second line takes into account interband processes. It is easy to see that this second contribution is only possible when $\omega > 2|\mu|$ (at low temperatures). Indeed, when the system is doped with respect to half-filling ($|\mu| \neq 0$) the smallest energy difference between occupied and unoccupied states in different branches is equal to $2|\mu|$, and it is realized at the points $(\pm\pi/2, \pm\pi/2)$ where the energy $E_{\mathbf{k}}$ vanishes and the two bands merge. The first contribution has instead a Drude-type shape, as it is shown in Fig. 5, where we report the optical conductivity at $T=0$ for a system with and without DDW gap. Here we used the set of parameters discussed above for cuprates, at $\delta=0.13$. When compared with the free-electron conductivity at the same temperature, one can see that the Drude peak is smaller in the DDW state, because part of the spectral weight has been transferred to the interband processes. To quantify this transfer of spectral weight we integrate numerically the optical conductivity $\sigma^{\mathrm{DDW}}(\omega)$ (4.12), and its analogous $\sigma(\omega)$ at $D_0=0$, evaluating for a given cutoff frequency ω the quantity,

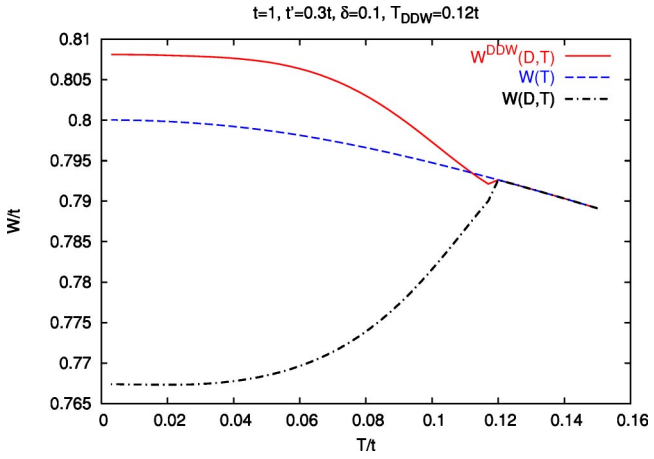

FIG. 4. (Color online) Spectral weight in the presence of a t' term in the band dispersion. Here we show $W^{\mathrm{DDW}}(D,T)$, $W(D,T)$, and $W(T)$, according to Eqs. (4.10), (4.9), and (4.8), respectively, in units of $e^2\pi a^2/V$. We used here $t'=0.3t$, $T_{\mathrm{DDW}}=0.12t$, $D(0)=4T_{\mathrm{DDW}}$, and $\delta=0.1$. The chemical potential is evaluated self-consistently at each temperature by solving Eq. (3.6) in the presence of a t' term in the band dispersion. Observe that near T_{DDW} a small decrease of W^{DDW} with respect to $W(T)$ is observed, due to the change of chemical potential near T_{DDW}.

$$N^{(\mathrm{DDW})}(\omega) = 2\int_0^{\omega}\sigma^{(\mathrm{DDW})}(\omega')d\omega', \tag{4.13}$$

which verifies $N^{\mathrm{DDW}}(\omega\rightarrow\infty)=W^{\mathrm{DDW}}(D,T=0)$ and $N(\omega\rightarrow\infty)\rightarrow W(T=0)$ for the DDW and normal state, respectively.

In the inset of Fig. 5 we show $N^{\mathrm{DDW}}(\omega)$ and $N(\omega)$ at $T=0$ corresponding to the calculated optical conductivities. As we can see, at low energy the formation of a DDW state leads to an overall decrease of spectral weight, since intraband processes are partly suppressed. However, at higher energy interband excitations are allowed and the spectral weight lost in the Drude peak is over-compensated, giving rise to an overall increase of $W^{\mathrm{DDW}}(D,T=0)$ in the DDW state compared to $W(T=0)$ in the normal state. For a value of $t\sim 0.25$ eV one sees that in the case of Fig. 5 the crossing of $N^{\mathrm{DDW}}(\omega)$ with respect to $N(\omega)$ is already satisfied at cutoff frequencies smaller than the plasma frequency ($\approx 4t$), even though N^{DDW} saturates at higher frequencies. Of course it is evident that the determination of the exact frequency at which the sum rule $W(T)$ or $W^{\mathrm{DDW}}(T)$ are exhausted depends on the choice of parameters. For example, at smaller doping or smaller D_0 (which both lead to a smaller value of $|\mu|$ in

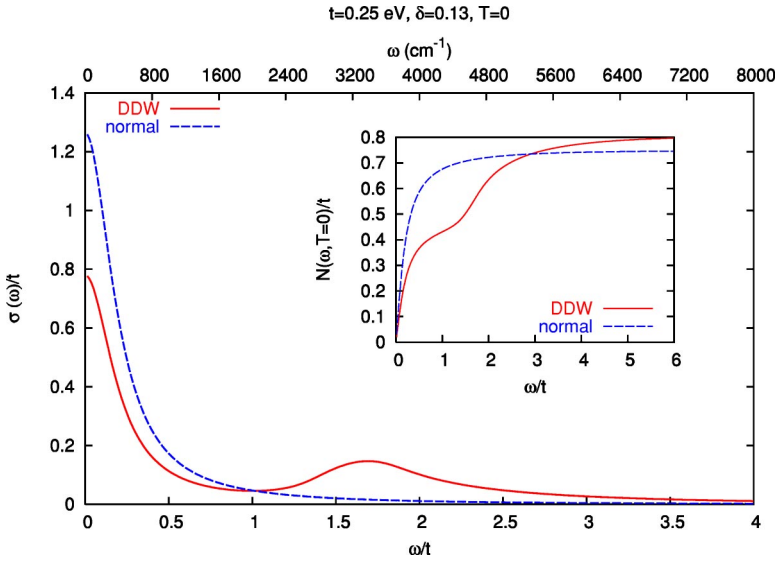

FIG. 5. (Color online) Optical conductivity in units of $e^2\pi a^2/V$ at zero temperature for a free tight-binding system and for the DDW state at $\delta=0.13$ ($\mu=-0.69t$ at $T=0$ in the DDW state, $w=0.1t$ were used). For convenience we also report the frequencies in cm^{-1}, as it is customary in the experiments. Inset, frequency variation of $N(\omega)$ according to Eq. (4.13). Observe that at low cutoff energy the spectral weight in the DDW state is smaller than in the normal state.

the DDW state, see Fig. 1) the intraband processes occur at lower energy, so that $N^{\mathrm{DDW}}(\omega)>N(\omega)$ will be satisfied at lower cutoff energy ω. In Fig. 5 we report one of the cases when the cutoff frequency is larger, because the chemical potential shifts from $\mu=-0.28t$ in the normal state to $\mu=-0.69t$ in the DDW state, due to the large value of the DDW parameter ($D_0=0.92t$), pushing interband processes at relatively high energies. It is interesting to observe that the optical conductivity in the DDW state reported in Fig. 5, which was evaluated with the ansatz (3.17) for the current-current correlation function, has the same *qualitative* behavior of the optical conductivity reported in Ref. 41, where the bare bubble approximation (2.21) was considered for the correlation function. Indeed, in the bare bubble approximation the optical conductivity has the same structure of Eq. (4.12) (i.e., a Drude term plus interband processes), but with $v_D=0$. However, the two approaches lead to two *quantitatively* different temperature dependences of the sum rule. Indeed in the absence of the v_D term in Eq. (4.12), coming from the vertex corrections, the spectral weight lost in the Drude term when the DDW state is formed would not be compensated any more by the interband processes, so that the total spectral weight $N^{\mathrm{DDW}}(\omega\to\infty)$ in the DDW state would be always lower than the spectral weight $N(\omega\to\infty)$ in the normal state, as observed in Ref. 41.

In Fig. 6 we report the optical conductivity in the DDW state at several temperature between $T=0$ and $T_{\mathrm{DDW}}=0.13t$ at the doping $\delta=0.13$. As one can see, when the temperature increases the interband processes shift to lower frequency, due to the decrease of the absolute value of the chemical potential (see right panel of Fig. 1). As a consequence, the spectral weight is transferred again towards the Drude peak, and the overall balance of spectral weight leads to a decrease of $W^{\mathrm{DDW}}(D,T)$. In the inset of Fig. 6 we show also the integrated spectral weight $N^{\mathrm{DDW}}(\omega_M)$ and $N(\omega_M)$ at the same temperatures of the main panel, with a cutoff frequency $\omega_M=6t$. Even though this estimate of the spectral weight is much less accurate than the direct evaluation of Eq. (4.5), due to lower numerical accuracy of this procedure, we find the same behavior discussed in the preceding sections while computing directly Eq. (4.5). Indeed, we can see that the spectral weight increases in the DDW state with respect to

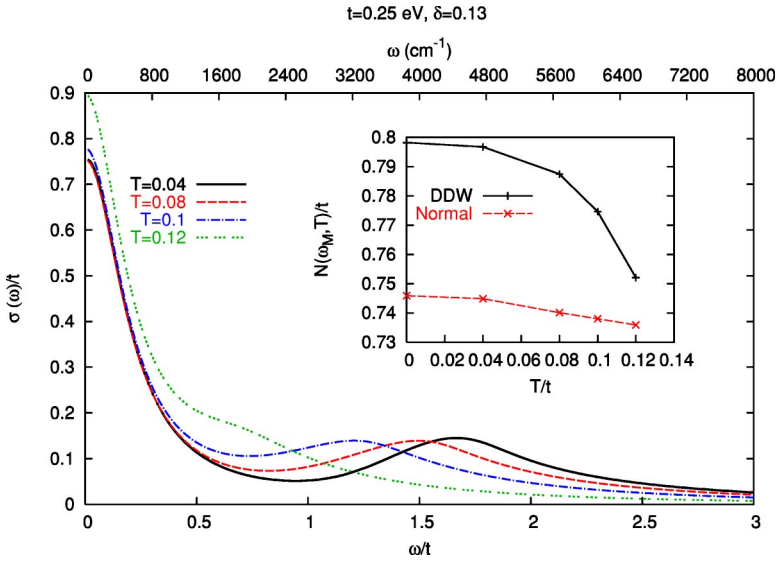

FIG. 6. (Color online) Optical conductivity in units of $e^2\pi a^2/V$ at various temperature for the DDW state at $\delta=0.13$, $T_{\mathrm{DDW}}=0.13t$. In the upper x-axis the frequencies are reported in cm^{-1}. Inset, comparison between the temperature dependence of the integrated spectral weight $N^{\mathrm{DDW}}(\omega_M)$ and $N(\omega_M)$ for the DDW and normal state, respectively. The cutoff is $\omega_M=6t$.

the normal state, even though the relative contribution of the Drude term is lower in the DDW state than in the normal state.

A comment is in order now about the role of disorder. In the preceding sections we reported the numerical results obtained for clean systems, but to amplify the differences between the conductivity of a noninteracting system and of the DDW state we used in Figs. 5 and 6 a quite large value of the inverse scattering time $w=0.1t$, as appropriate, for example, to reproduce qualitatively the large Drude peak observed in BSCCO samples at about 100 K.[2,4] As a consequence, also the self-consistency equation (3.6) for the particle number and the sum rules $W^{\mathrm{DDW}}(D,T)$ and $W(T)$ should be evaluated in the presence of disorder for a given doping. The main difference is only in the absolute value of the spectral weight, while the relative difference between the case with or without DDW is the same. In the Appendix B we discuss the modifications to the particle number and spectral weight equations in the presence of disorder, that we used in computing the optical conductivity in Figs. 5 and 6.

V. DISCUSSION

In the present paper we analyzed a possible approach to determine a GI approximation for the optical conductivity in a system which displays a transition to a *d*-wave modulated CDW or flux phase. As we explained in detail in Sec. II the requirement of GI of a theory fixes the relation (2.20) between the current-current correlation function and the diamagnetic term. To understand better the expected domain of applicability the sum rule $W^{\mathrm{DDW}}(D,T)$ (4.5) let us summarize the assumptions that led us to this rule. We have checked in Sec. III B [Eq. (3.13)] that the bubble $\Pi^{(\gamma)}$ of Eq. (2.21), evaluated with the mean-field DDW Green's function (3.4) and the bare vertex γ, does not satisfy the GI condition (2.20) when the standard diamagnetic term (3.7) is considered. As discussed in Sec. II C, this situation is quite standard, and considering the WI (2.26) this violation of the gauge invariance can be attributed to the $\mathbf{k}$-dependent character of the DDW gap $D_{\mathbf{k}}$, which makes necessary the use of the full vertex $\Gamma(k,k)$ instead of the bare one $\gamma(\mathbf{k},\mathbf{k})$.

In general the vertex function is determined by solving the integral equation (2.24), but in the static limit it reduces to the expression (2.26). Since we do not know an analytical solution at finite frequencies and momenta of the vertex $\Gamma(k_+,k_-)$, corresponding to the microscopic many-body Hamiltonian (2.1), we can try to use our knowledge of its static limit to give a better approximation than Eq. (2.21) for the current-current correlation function. More precisely, we showed in Sec. II D that the dc conductivity derived from the symmetric bubble Π_{ij}^{sym} (2.33), where two full vertex functions in the static limit appear, coincides with the exact result at $T=0$.[39,45] Even though this procedure allows us to correctly reproduce the optical conductivity in the low-frequency limit, it does not solve the problem of knowing *a priori* the sum rule corresponding to this approximated optical conductivity. Indeed, since this symmetric bubble is not exact for the full model (2.1), and in contrast to the bubble (2.22) contains two full vertices, one cannot expect that the optical conductivity calculated using this bubble would satisfy the usual sum rule corresponding to the diamagnetic tensors (2.15) or (3.7).

However, this last issue can be solved exactly by applying the same GI arguments to the reduced quadratic model (3.2). Indeed, the static limit $\Gamma_i \equiv \gamma_i + V_i(\mathbf{k})$ of the full vertex function, obtained from the original interacting model, can also be considered as a bare vertex $\tilde{\gamma}$ for the DDW Hamiltonian (3.2). Moreover, since this Hamiltonian describes noninteracting quasiparticles, the bare and the full vertex coincide, so that the symmetric correlator Π^{DDW} in Eq. (3.17) is the *exact* one for this model. As a consequence, the diamagnetic term (4.4) of the reduced model gives the sum rule $W^{\mathrm{DDW}}(D,T)$ (4.5) for the symmetric current operator (3.17), which is the exact one within the quadratic theory (3.2) and at the same time provides us with a good approximation for the optical conductivity of the true interacting system, at least at low energy.

The last issue we addressed in the present paper is to analyze to which extent the sum rule (4.5) can be related to the behavior of the microscopic Hamiltonian (2.1). In general, it is believed that in the presence of interactions the restricted sum rule (1.3), derived for the electrons within the lowest conducting tight-binding band, is still valid, provided that the occupation number $n_{\mathbf{k}\sigma}$ takes into account the effect of the interactions. In this case, we should rely on the estimate $W(D,T)$ in Eq. (3.7) for the sum rule in the DDW state. However, this approach has two disadvantages, (i) we cannot derive the optical-conductivity which would lead to this sum rule; (ii) no general argument holds to justify why this attitude is the correct one to estimate, at mean-field level, the sum rule for the interacting microscopic model. Motived by these observations we argued that in the case of interactions leading to a DDW formation a better mean-field approach to the transport properties is provided by the calculation of the optical conductivity by means of the bubbles Π^{DDW}. Thus, to obtain the correct mean-field approximation for the spectral-weight behavior is not sufficient to modify the occupation number $n_{\mathbf{k}\sigma}$ below T_{DDW}, but it is more likely that a proper redefinition of the diamagnetic tensor is needed. As a consequence, the sum rule should be estimated by means of Eq. (4.5) instead of Eq. (3.7), leading to an *increase* of spectral weight below T_{DDW}. However, this assumption would require also that the integrated spectral weight $N^{\mathrm{DDW}}(\omega)$ in the DDW state becomes larger than the $N(\omega)$ for the noninteracting system at some "low" frequency ω_M. As we discussed in Sec. IV D, such cutoff frequency ω_M turns out to be in general lower than the plasma edge, but its precise value depends crucially on the parameters of the DDW transition (doping, order parameter at $T=0$, etc.). Moreover, it is not clear yet if a ω_M below the plasma frequency is a sufficiently low-energy scale for the interacting tight-binding model, since no universal definition exists of the frequency itself below which the restricted sum rule should be applicable.

Finally, a comment is in order now about the comparison between our results and the experimental optical data for cuprates. A first issue is related to the fact that the most recent experiments show that the temperature variation of the spectral weight is larger than expected in a tight-binding es-

timate also in optimally doped and overdoped compounds[4,6] (see also Appendix A), i.e., eventually at doping larger than the critical doping $\delta_0=0.2$ for the charge ordering phenomenon. This could mean that a more general effect of the strong correlations present in these materials can be responsible for the large temperature variation of $W(T)$. This possibility has been indeed investigated recently in Ref. 50, where $W(T)$ has been evaluated by means of the DMFT (dynamical mean field theory) approach to the Hubbard model, which seems to reproduce the large temperature variations of $W(T)$ observed in the experiments. A second issue arises about the lack, in the experiments, of a clear signature of an interband conductivity as the one reported in Fig. 4. In particular, BSCCO compounds, that were used as a paradigm for the choice of DDW parameter values in cuprates,[26] exhibit in general a quite featureless conductivity, with a slowly decaying high-frequency tail. However, in different families of cuprates, displaying a similar spectral-weight behavior, clear signatures of charge ordering have been indeed observed in the optical spectra, even though located at much lower energy scales with respect to the one obtained here using the parameter values for BSCCO compounds. This is the case of LSCO and YBCO, where far-infrared features, well separated from the Drude peak, have been measured recently.[47] In both Refs. 48 and 49 these features were actually interpreted as due to a charge-ordering phenomenon, described by means of some different theoretical approaches which did not allow one to discuss at the same time the issue of the spectral-weight behavior. For these reasons, even though the analysis presented here cannot be conclusive as far as the optical spectra of HTSC are concerned, we believe that a deeper investigation of the role of charge degrees of freedom can eventually lead to a better understanding of the conductivity of cuprates. At the same time, the analysis presented here could be extended to other systems like 2*H*-$TaSe_2$, where a *k*-space modulated CDW forms[30] and where clear signatures of a Drude response accompanied by a mid-infrared peak have been observed in the optical spectra.[29]

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APPENDIX A: FAILURE OF THE TIGHT-BINDING ESTIMATE

As we noticed in the Introduction, even though a T^2 temperature decrease of $W(T)$ is observed in the experiments, the measured slope is quite larger than the one expected within the simple noninteracting tight-binding estimate (1.4). To quantify this discrepancy in the most accurate way, we evaluate explicitly the spectral weight for the tight-binding model by including also a next-nearest-neighbors term in the band dispersion, see Eq. (4.7). As a consequence, $W(T)$ is given by Eq. (4.8).

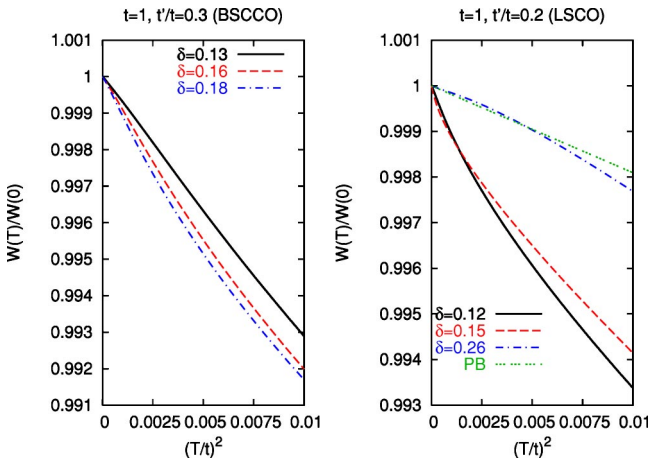

FIG. 7. (Color online) Spectral weight $W(T)/W(0)$ according to Eq. (4.8) for $t'=0.3t$ [left panel, appropriate for BSCCO (Refs. 2 and 4)] and $t'=0.2t$ [right panel, appropriate for LSCO (Ref. 6)] at various doping. In the right panel we also report the result obtained with the estimate (1.4) and the parabolic band (PB) approximation for $c(\mu)=1/4\pi t$, using the value $W(0)=0.682t$ at $\delta=0.26$.

To correctly reproduce the Fermi surface of BSCCO and LSCO compounds we will assume $t=0.3eV$ and $t'=rt$, where $r=0.3$ for BSCCO and $r=0.2$ for LSCO (where the Fermi surface changes topology in the overdoped region, becoming electronlike at about $\delta=0.2$ doping[51]). The results of $W(T)/W(0)$ as a function of $(T/t)^2$ from Eq. (4.8) are reported in Fig. 7 for several doping (by fixing as usual the correct chemical potential at each doping and temperature from the self-consistency equation for the particle number). In the left panel we report the estimate for BSCCO, that should be compared to the experimental data (for underdoped, optimally doped, and overdoped samples) of Refs. 1, 2, and 4. Observe that in Refs. 2 and 4 the variation of $W(T)/W(0)$ between room temperature and $T=0$ of the order of 20%–5% when measured at various cutoff frequencies, while the tight-binding estimate in Fig. 7 never exceed the 0.6% [for $t=0.3$ eV, $T=300$ K corresponds to $(T/t)^2=0.0074$]. Analogous considerations hold for the comparison between the measured spectral weight in LSCO (Ref. 6) and the estimate (4.8) reported in the right panel of Fig. 7. A comment is in order now about the role of the Van Hove singularity (VHS) in the density of states. Indeed, according to Eq. (1.4), where the $t'=0$ case was considered, the coefficient $c(\mu)=\mu N'(\mu)+N(\mu)$ could increase considerably by approaching the VHS. This effect is indeed seen in the curves at $\delta=0.12$ and $\delta=0.16$, where the initial slope of $W(T)$ is quite large. However, as soon as the temperature increases the effect of the VHS is washed out very rapidly and the overall variation in the range of T between $0-0.1t$ attains the same values found for the case $t'=0.3t$. Moreover, for the overdoped case $\delta=0.26$ the slope of $W(T)/W(0)$ agrees very well with the approximation $c(\mu)=1/4\pi t$ of the parabolic band dispersion (PB in the figure), which would give the value $\pi^2 c(\mu)/6=0.13/t$ for the coefficient in Eq. (1.4). For these reasons one can conclude that the t' term in

the band dispersion (4.7) has a minor role in determining the spectral-weight variations, and indeed it was only briefly discussed in Sec. IV C of the present work.

APPENDIX B: SUM RULE IN THE PRESENCE OF DISORDER

As we did in Sec. IV D we will take into account the effect of disorder by using the substitution (4.11) in the spectral representation (3.10) of the Green's function. To see how Eq. (3.6) is modified we rewrite it in terms of the spectral function,

$$n = \frac{2T}{N}\sum_{\mathbf{k},i\omega_n}^{\mathrm{RBZ}} \mathrm{Tr}[G(\mathbf{k},i\omega_n)]e^{i\omega_n 0^+} = \frac{2}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} \int dz[M(z-E)+M(z+E)]f(z-\mu). \quad \text{(B1)}$$

Analogously, the definition (4.4) of the diamagnetic tensor in the DDW state can be expressed as

$$\langle \tau_{ii}\rangle = -\frac{T}{N}\sum_{\mathbf{k},i\omega_n}^{\mathrm{RBZ}} \{\varepsilon_{\mathbf{k}}\mathrm{Tr}[G(\mathbf{k},i\omega_n)\sigma_3] - D_{\mathbf{k}}\mathrm{Tr}[G(\mathbf{k},i\omega_n)\sigma_2]\}e^{i\omega_n 0^+} = -\frac{1}{N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} E_{\mathbf{k}}\int dz[M(z-E)-M(z+E)]f(z-\mu). \quad \text{(B2)}$$

Observe that if one sets $M(z)=\delta(z)$ the results (3.6) and (4.5) can be recovered, and for $D_0=0$ one finds the corresponding expressions for the normal state. At $T=0$, which is the case considered in Fig. 5, the previous equations simplify. Indeed, since the Fermi functions reduce to a step function, one has

$$\int_{-\infty}^{\infty} dzM(z-E)f(z-\mu) = \int_{-\infty}^{\mu} dz\frac{1}{\pi}\frac{w}{z^2+w^2} = \frac{1}{\pi}\left(\arctan\frac{\mu-E}{w}+\frac{\pi}{2}\right) \quad \text{(B3)}$$

so that the self-consistency equation for the particle number and the equation for the spectral weight can be written as

$$n-1 = \frac{2}{\pi N}\sum_{\mathbf{k}}^{\mathrm{RBZ}}\left(\arctan\frac{\mu-E}{w}+\arctan\frac{\mu+E}{w}\right), \quad \text{(B4)}$$

$$\frac{W^{\mathrm{DDW}}(D,T=0)}{(\pi e^2a^2/V)} = -\frac{1}{\pi N}\sum_{\mathbf{k}}^{\mathrm{RBZ}} E_{\mathbf{k}}\left(\arctan\frac{\mu-E}{w}-\arctan\frac{\mu+E}{w}\right). \quad \text{(B5)}$$

Observe that here we did not consider the effect of the DDW formation on the transport scattering time, which can be present. For a detailed discussion of impurity scattering in the DDW state see Ref. 35.

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