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OPTICAL SUM RULE IN STRONGLY CORRELATED SYSTEMS

E. Z. Kuchinskii, N. A. Kuleeva, I. A. Nekrasov, M. V. Sadovskii*

Institute for Electrophysics, Russian Academy of Sciences, Ural Branch
620016, Ekaterinburg, Russia

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We discuss the problem of a possible "violation" of the optical sum rule in the normal (nonsuperconducting) state of strongly correlated electronic systems, using our recently proposed DMFT+Σ approach applied to two typical models: the "hot spot" model of the pseudogap state and disordered Anderson–Hubbard model. We explicitly demonstrate that the general Kubo single-band sum rule is satisfied for both models. But the optical integral itself is in general dependent on temperature and characteristic parameters, such as the pseudogap width, correlation strength, and disorder scattering, leading to an effective "violation" of the optical sum rule, which may be observed in the experiments.

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1. INTRODUCTION

Many years ago, Kubo [1] proved the general sum rule for the diagonal dynamic (frequency-dependent) conductivity $\sigma(\omega)$, which holds for any system of charged particles irrespective of interactions, temperature, or statistics. This sum rule is usually written as

$$\frac{2}{\pi}\int\limits_0^\infty \mathrm{Re}\,\sigma(\omega)\,d\omega = \sum_r \frac{n_r e_r^2}{m_r}, \tag{1}$$

where r specifies the type of charged particles, and n_r and e_r are the respective densities and charges.

For the system of electrons in a solid, Eq. (1) takes the form

$$\int\limits_0^\infty \mathrm{Re}\,\sigma(\omega)\,d\omega = \frac{\omega_{pl}^2}{8}, \tag{2}$$

where n is the density of electrons and $\omega_{pl}^2 = 4\pi n e^2/m$ is the plasma frequency.

In any real experiment, however, we are not dealing with an infinite range of frequencies. If we consider electrons in a crystal and limit ourselves to the electrons in a particular (e.g., conduction) band, neglecting interband transitions, the general sum rule (2) reduces to the single-band sum rule of Kubo [1, 2]:

$$W = \int\limits_0^{\omega_c} \mathrm{Re}\,\sigma(\omega)\,d\omega = f(\omega_c)\frac{\pi e^2}{2}\sum_{\mathbf{p}} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n_p, \tag{3}$$

where ε_p is the bare dispersion defined by the effective single-band Hamiltonian, and n_p is the momentum distribution function (occupation number), which is in general defined by the interacting retarded electron Green's function $G^R(\varepsilon, \mathbf{p})$ [3, 4]:

$$n_p = -\frac{1}{\pi}\int\limits_{-\infty}^{\infty} d\varepsilon\, n(\varepsilon)\,\mathrm{Im}\,G^R(\varepsilon, \mathbf{p}), \tag{4}$$

where $n(\varepsilon)$ is the usual Fermi distribution. In Eq. (3), ω_c represents an ultraviolet cut-off, a frequency that is assumed to be larger than the bandwidth of the low-energy band but smaller than the gap to other bands. The function $f(\omega_c)$ accounts for the cut-off dependence, which arises from the presence of the Drude spectral weight beyond ω_c [5]; this fucntion is equal to unity if we formally set ω_c to infinity and ignore the interband transitions.

Although the general sum rule is certainly preserved, the optical integral $W(\omega_c, T)$ is not a conserved quantity because both $f(\omega_c)$ [5] and n_p [4, 6] depend on the temperature T and also on details of interactions [3]. This dependence of W on T and other parameters of the system under study has been termed the "sum rule violation". It was actively studied experimentally, especially in cuprates, where pronounced

*E-mail: sadovski@iep.uran.ru

anomalies were observed in both the c-axis and in-plane conductivity, in normal as well as superconducting states [8–13].

The finite cut-off effects were extensively studied in several theoretical papers on the T dependence of the optical integral [4, 5, 7]. In Refs. [5, 7], the effect of the cut-off was considered in the context of electrons coupled to phonons. In a simple Drude model,

$$\sigma(\omega) = \frac{\omega_{pl}^2}{4\pi} \Big/ \left(\frac{1}{\tau} - i\omega\right)$$

and the sum rule can only be "violated" due to the presence of $f(\omega_c)$. Integrating over ω and expanding for $\omega_c\tau \gg 1$, we can see that

$$f(\omega_c) = \left(1 - \frac{2}{\pi}\,\frac{1}{\omega_c\tau}\right). \qquad (5)$$

For the infinite cut-off, $f(\omega_c) = 1$ and $W = \omega_{pl}^2/8$, but for a finite cut-off, $f(\omega_c)$ contains the term proportional to $1/\omega_c\tau$. If $1/\tau$ changes with T, then we obtain a sum rule "violation" even if ω_{pl} is independent of T [5, 7]. Other aspects of the cut-off dependence were recently discussed in detail in Ref. [2].

In this paper, we neglect the cut-off effects in the optical integral from the outset. Our goal is to study the dependence of W on T and a number of interaction parameters determining the electron properties of strongly correlated systems, such as cuprates. In this context, we discuss the problem of a possible "violation" of the optical sum rule in the normal (non-superconducting) state of strongly correlated electronic systems, using our recently proposed DMFT+Σ approach [14–16] applied to dynamic conductivity in two typical models of such systems: the "hot spot" model of the pseudogap state [19] and the disordered Anderson–Hubbard model [20]. Our aim is to check the consistency of the DMFT+Σ approach applied to calculations of optical conductivity as well as to demonstrate rather important dependences of the optical integral W not only on T but also on important characteristics such as the pseudogap width, disorder, and correlation strength, which makes the (single-band) sum rule "violation" rather ubiquitous in strongly correlated systems, even if the cut-off effects are neglected.

2. OPTICAL SUM RULE IN THE GENERALIZED DMFT+Σ APPROACH

A characteristic feature of the general sum rule expressed by Eqs. (3) and (4) is that the integral W over frequency in the left-hand side is calculated based on a two-particle property (the dynamic conductivity, which is determined by the two-particle Green's function, with appropriate vertex corrections in general), but the right-hand side is determined by single-particle characteristics, such as the bare dispersion and occupation number (4) (determined by a single-particle Green's function). Thus, checking the validity of this sum rule, we are in fact thoroughly checking the consistency of any theoretical approach used in our model calculations.

Our generalized dynamic mean field theory (DMFT+Σ) approach [14–16], supplementing the standard dynamic mean field theory (DMFT) [17, 18] with an additional "external" self-energy Σ (due to any kind of interaction outside the scope of the DMFT, which is exact only in infinitely many dimensions), provides an effective method to calculate both single-particle and two-particle properties [19, 20]. The consistency check of this new approach is obviously of great interest by itself. We also see in what follows that it gives a kind of a new insight into the sum-rule "violation" problem.

A. Pseudogap state, the "hot spot" model

Pseudogap phenomena in strongly correlated systems have an essential spatial length scale dependence [21]. To merge pseudogap physics and strong electron correlations, we have generalized the DMFT [17, 18] by inclusion of the dependence on the correlation length of pseudogap fluctuations via an additional (momentum-dependent) self-energy $\Sigma_{\mathbf{p}}(\varepsilon)$. This self-energy $\Sigma_{\mathbf{p}}(\varepsilon)$ describes nonlocal dynamic correlations induced either by short-ranged collective SDW-like antiferromagnetic spin or CDW-like charge fluctuations [22, 23].

To calculate $\Sigma_{\mathbf{p}}(\varepsilon)$ in two-dimensional "hot spot" model [21] for an electron moving in the random field of pseudogap fluctuations (considered to be static and Gaussian) with dominant scattering momentum transfers of the order of the characteristic vector $\mathbf{Q} = (\pi/a, \pi/a)$ (where a is the lattice spacing), we used [15, 16] the recursion procedure proposed in Refs. [22, 23], which is controlled by two main physical characteristics of the pseudogap state: the pseudogap amplitude Δ, which characterizes the energy scale of the pseudogap, and the inverse correlation length $\kappa = \xi^{-1}$ of short-range SDW (CDW) fluctuations. Both parameters Δ and ξ, determining pseudogap behavior, can in principle be calculated from the relevant microscopic model [15].

The weakly doped one-band Hubbard model with a repulsive Coulomb interaction U on a square lattice with nearest and next-to-nearest neighbor hopping was numerically investigated within this generalized DMFT+Σ self-consistent approach, as described in detail in Refs. [14–16].

Briefly, the DMFT+Σ self-consistent loop is as follows. First, we guess some initial local (DMFT) electron self-energy $\Sigma(\varepsilon)$. Second, we compute the $\mathbf{p}$-dependent "external" self-energy $\Sigma_{\mathbf{p}}(\varepsilon)$, which is in general a functional of $\Sigma(\varepsilon)$. Then, neglecting interference effects between the self-energies (which is in fact the major assumption of our approach), we can set up and solve the lattice problem of DMFT [17, 18]. Finally, we define an effective Anderson single-impurity problem, which is to be solved by any "impurity solver" (we mostly use the numerical renormalization group, NRG) to close the DMFT+Σ equations.

The additive form of self-energy is in fact an advantage of our approach [14–16]. It allows preserving the set of self-consistent equations of the standard DMFT [17, 18]. But there are two distinctions from the conventional DMFT. During each DMFT iteration, we recalculate the corresponding $\mathbf{p}$-dependent self-energy $\Sigma_{\mathbf{p}}(\mu, \varepsilon, [\Sigma(\omega)])$ via an approximate scheme, taking interactions with collective modes or order parameter fluctuations into account, and the local Green function $G_{ii}(i\omega)$ is "dressed" by $\Sigma_{\mathbf{p}}(\varepsilon)$ at each step. When the input and output Green's functions (or self-energies) converge to each other (with prescribed accuracy), we consider the obtained solution selfconsistent. Physically, this corresponds to accounting for some "external" (e.g., pseudogap) fluctuations, characterized by an important length scale ξ, in the fermionic "bath" surrounding the effective Anderson impurity of the usual DMFT. The cases of strongly correlated metals and doped Mott insulators were considered in [15, 16]. Energy dispersions, quasiparticle damping, spectral functions, and ARPES spectra calculated within the DMFT+Σ scheme, all show a pseudogap effect close to the Fermi level of the quasiparticle band.

In Ref. [19], this DMFT+Σ procedure was generalized to calculate two-particle properties, such as the dynamic conductivity, using the previously developed recursion procedure for vertex corrections due to pseudogap fluctuations [24], producing typical pseudogap anomalies of the optical conductivity and a dependence of these anomalies on the correlation strength U. Below, we use the approach in Ref. [19] to investigate the sum-rule in the "hot spot" model.

To calculate the optical integral W, we have just used the conductivity data in Ref. [19] (extended to a wider frequency range needed to calculate W), while the right-hand side of (3) was recalculated using recursion relations for $\Sigma_{\mathbf{p}}(\varepsilon)$ and the whole self-consistency DMFT+Σ loop. All calculations were done for a tight-binding "bare" spectrum on the square lattice, with the nearest-neighbor transfer integral t and the next-to-nearest-neighbor transfer integral t'.

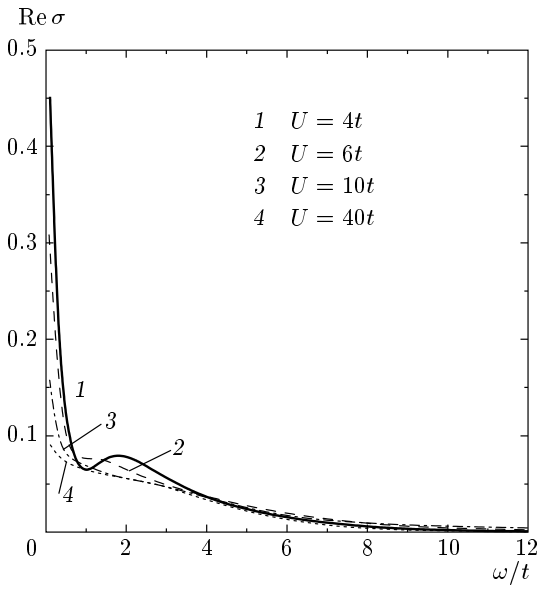

Fig. 1. Real part of the optical conductivity for a strongly correlated system in the pseudogap state ($t' = -0.4t$, $t = 0.25$ eV, and $T = 0.089t$) in the DMFT+$\Sigma_{\mathbf{p}}$ approximation, the U dependence. Band filling $n = 0.8$, pseudogap amplitude $\Delta = t$, correlation length $\xi = 10a$. Conductivity is given in units of $\sigma_0 = e^2/\hbar$

In Fig. 1, we present our typical data for the real part of conductivity (with $t' = -0.4t$, $t = 0.25$ eV, the band filling $n = 0.8$, and the temperature $T = 0.089t$) for different values of Hubbard interaction $U = 4t, 6t, 10t, 40t$ and a fixed pseudogap amplitude $\Delta = t$ (at the correlation length $\xi = 10a$). It is obvious from these data that the optical integral W is different for all of these curves; its value actually decreases with an increase in U (along with damping of pseudogap anomalies [19]). However, the single band optical sum-rule in (3) is satisfied within our numerical accuracy, as can be seen from Table 1. The small "deficiency" in the values of W in Table 1 is naturally due to a finite frequency integration interval over the conductivity data in Fig. 1.

In Fig. 2, we show the real part of the optical conductivity for a doped Mott insulator (at a fixed $U = 40t$, $t' = -0.4t$, $t = 0.25$ eV, and the band fill-

Table 1. Single-band optical sum rule check in the "hot spot" model, the U dependence. The optical integral is given in units of $e^2t/\hbar$

U	$\frac{\pi e^2}{2}\sum_{\mathbf{p}}\frac{\partial^2\varepsilon_p}{\partial p_x^2}n_p$	$W=\int_0^\infty \mathrm{Re}\,\sigma(\omega)\,d\omega$
$4t$	0.456	0.408
$6t$	0.419	0.387
$10t$	0.371	0.359
$40t$	0.323	0.306

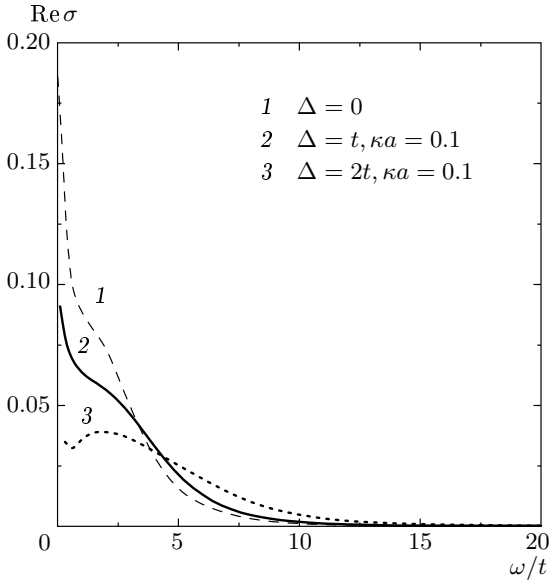

Fig. 2. Real part of the optical conductivity for a doped Mott insulator ($U = 40t$, $t' = -0.4t$, $t = 0.25$ eV, and $T = 0.089t$) in the DMFT+$\Sigma_{\mathbf{p}}$ approximation for different values of the pseudogap amplitude $\Delta = 0$, $\Delta = t$, and $\Delta = 2t$. Correlation length $\xi = 10a$, band filling factor $n = 0.8$

ing $n = 0.8$, $T = 0.089t$) for different values of the pseudogap amplitude $\Delta = 0$, $\Delta = t$, and $\Delta = 2t$. The correlation length is again $\xi = 10a$ and the band filling factor $n = 0.8$. The "violation" of the sum rule here is especially striking: the optical integral obviously decreases with an increase in Δ. However, again, the single-band optical sum rule in (3) is strictly valid, as can be seen from Table 2.

To study the details of the sum-rule "violation", i.e., the dependence of the optical integral W on the parameters of the model, we performed extensive calculations

Table 2. Single-band optical sum rule check in the "hot spot" model, the Δ dependence. The optical integral is given in units of $e^2t/\hbar$

Δ	$\frac{\pi e^2}{2}\sum_{\mathbf{p}}\frac{\partial^2\varepsilon_p}{\partial p_x^2}n_p$	$W=\int_0^\infty \mathrm{Re}\,\sigma(\omega)\,d\omega$
0	0.366	0.36
t	0.314	0.304
$2t$	0.264	0.252

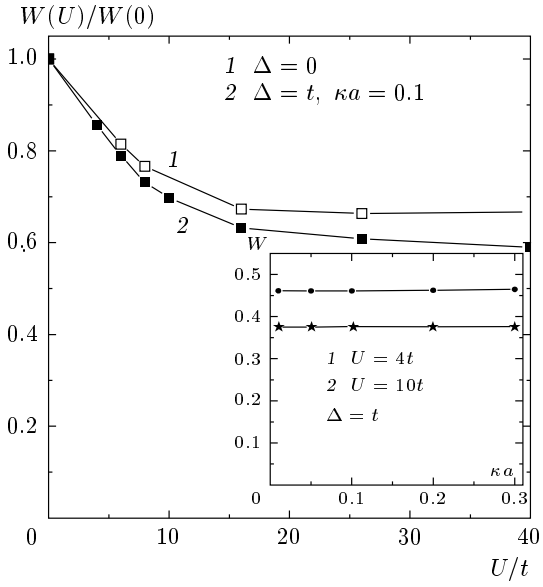

Fig. 3. Dependence of the normalized optical integral on the correlation strength U in the pseudogap state ($T = 0.089t$, $t = 0.25$ eV, $t' = -0.1$ eV, $n = 0.8$). Inset: the correlation length dependence of the optical integral in units of the $e^2t/\hbar$

of the appropriate dependences of the right-hand side of Eq. (3) and the optical integral W on the temperature T, doping, the pseudogap amplitude Δ, the correlation length of pseudogap fluctuations $\xi = \kappa^{-1}$, and the correlation strength U. Some of the results are presented in Figs. 3–5.

A typical dependence of the (normalized) optical integral on the correlation strength U is shown in Fig. 3 for two values of Δ. We can see a rather significant decrease in W with an increase in U. As regards the correlation length dependence, which is shown in the inset to Fig. 3, it was found to be very weak (practically negligible) in the whole region of realistic values of ξ, and we therefore do not discuss it further. The

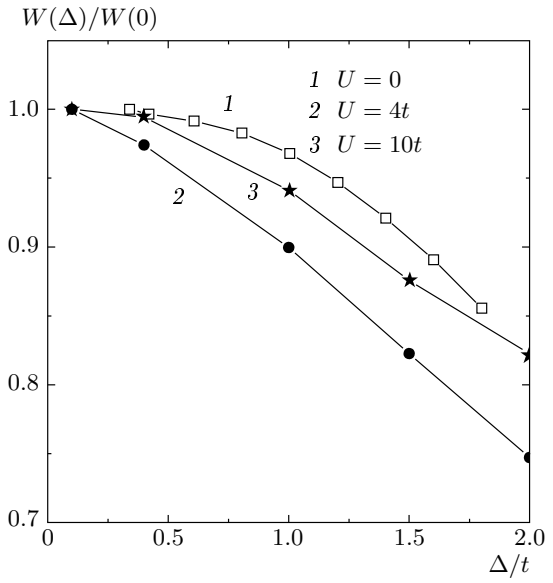

Fig. 4. Dependence of the normalized optical integral on the pseudogap amplitude Δ ($T = 0.011t$, $t = 0.25$ eV, $t' = -0.1$ eV, $n = 0.8$, $\kappa a = 0.1$)

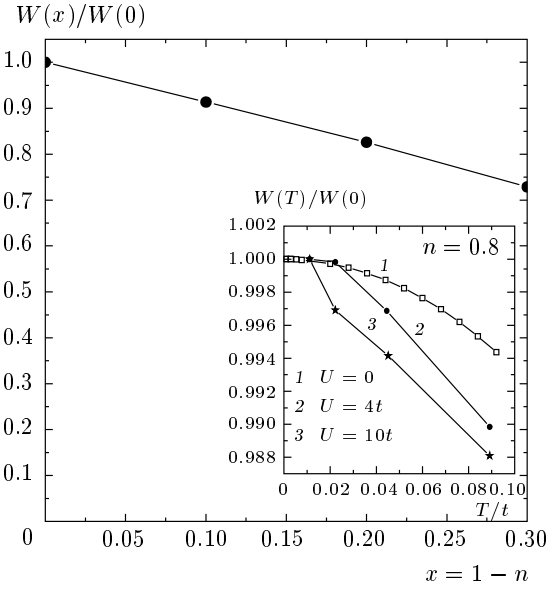

Fig. 5. Dependence of the normalized optical integral on hole doping in the pseudogap state. Inset: the temperature dependence ($T = 0.011t$, $U = 4t$, $\Delta = t$, $t = 0.25$ eV, $t' = -0.1$ eV, $\kappa a = 0.1$)

dependence of W on the pseudogap amplitude Δ (for several values of U) is shown in Fig. 4. A typical doping dependence, which reflects just the dependence of the square of the plasma frequency ω_{pl}^2 on doping, is given in Fig. 5. In all other cases, the change of the relevant parameters of the model leads to a rather significant decrease in the values of W. As regards the temperature dependence (shown in the inset to Fig. 5), it is rather weak, quadratic in T and quite similar to that found in Refs. [4].

Basically, these results show that the value of the optical integral depends on all the major parameters of the model and, in this sense, its value is not universal and hence the optical sum rule is significantly "violated" if we restrict ourselves to a single-band contribution.

B. Disordered Anderson–Hubbard model

In Ref. [20], we used the DMFT+Σ approximation to calculate the density of states, the optical conductivity, and the phase diagram of a strongly correlated and strongly disordered paramagnetic Anderson–Hubbard model, with a Gaussian site disorder. Strong correlations were taken into account by the DMFT, while disorder was taken into account via the appropriate generalization of the self-consistent theory of localization [25–28]. We considered the three-dimensional system with a semi-elliptic density of states. The correlated metal, Mott insulator, and correlated Anderson insulator phases were identified via the evolution of the density of states and dynamic conductivity, demonstrating both Mott–Hubbard and Anderson metal–insulator transitions and allowing the construction of the complete zero-temperature phase diagram of the Anderson–Hubbard model.

For the "external" self-energy entering the DMFT+Σ loop, we used the simplest possible approximation (neglecting "crossing" diagrams for disorder scattering), i.e., just the self-consistent Born approximation, which in the case of Gaussian site-energy disorder takes the usual form

$$\Sigma(\varepsilon) = \Delta^2 \sum_{\mathbf{p}} G(\varepsilon, \mathbf{p}), \tag{6}$$

where Δ now denotes the amplitude of site disorder.

Calculations of the optical conductivity are considerably simplified [20] because there are no contributions to conductivity due to vertex corrections determined by a local Hubbard interaction. The conductivity is essentially determined by the generalized diffusion coefficient, which is obtained from the appropriate generalization of the self-consistency equation in Refs. [25–28], which is to be solved in conjunction with the DMFT+Σ loop.

In Fig. 6, we show typical results for the real part of the dynamic conductivity of a correlated metal de-

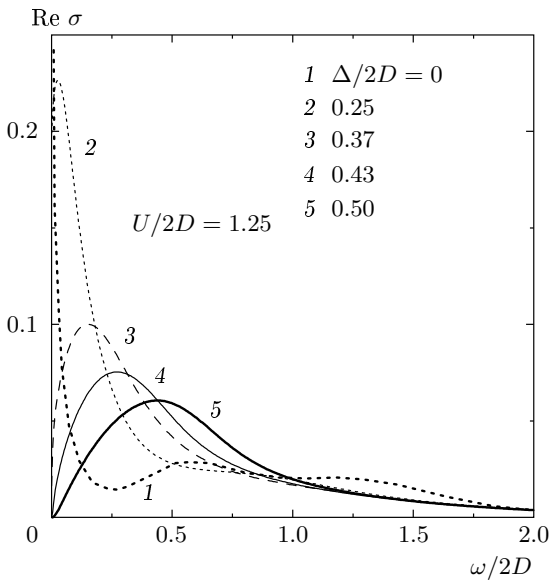

Fig. 6. Real part of the dynamic conductivity for the half-filled Anderson–Hubbard model for different degrees of disorder Δ and $U = 2.5D$, typical for a correlated metal. Lines *1* and *2* are for the metallic phase, line *3* corresponds to the mobility edge (Anderson transition), and lines *4* and *5* correspond to the correlated Anderson insulator. The conductivity is in units of $e^2/\hbar a$

Table 3. Single-band optical sum rule check in the Anderson–Hubbard model, the Δ dependence. The optical integral is in units of $2e^2D/\hbar a$

$\Delta/2D$	$\frac{\pi e^2}{2}\sum_{\mathbf{p}}\frac{\partial^2\varepsilon_p}{\partial p_x^2}n_p$	$W=\int_0^\infty \mathrm{Re}\,\sigma(\omega)\,d\omega$
0	0.063	0.064
0.25	0.068	0.07
0.37	0.06	0.056
0.5	0.049	0.05

scribed by the half-filled Anderson–Hubbard model (with the bandwidth $2D$) for different degrees of disorder Δ and $U = 2.5D$; the results demonstrate a continuous transition to the correlated Anderson insulator as disorder increases.

Again, the direct check shows that the single-band optical sum rule in (3) is satisfied within our numerical accuracy, as can be seen from Table 3. At the same time, the optical integral W itself obviously changes with disorder.

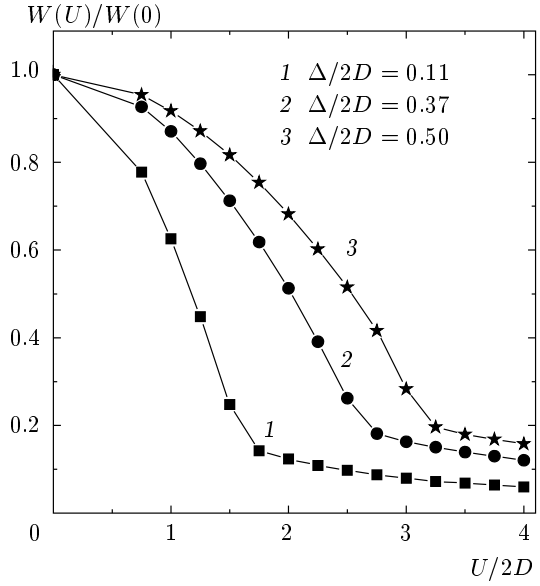

Fig. 7. Dependence of the normalized optical integral on the correlation strength in the Anderson–Hubbard model for different degrees of disorder Δ (*1* and *2*, strongly disordered metal; *3*, correlated Anderson insulator)

Again, to study the details of this sum rule "violation", i.e., the dependence of W on the parameters of the Anderson–Hubbard model, we performed detailed calculations of its dependences on the temperature T, the disorder amplitude Δ, and the correlation strength U. Some of the results are presented in Figs. 7–9.

In Fig. 7, we show the dependence of the normalized optical integral on U, for different degrees of disorder (for both a strongly disordered metal and a correlated Anderson insulator). It is seen that in all cases, an increase in the correlation strength leads to a rather sharp decrease in W in the metallic state; this decrease is much slower in the Mott insulator.

In Fig. 8, we present similar dependences on the disorder strength Δ. In the metallic state, the optical integral generally decreases as disorder increases, but the opposite behavior is observed if we start from the Mott insulator (obtained either with an increase in U from the metallic state or for a reduced U in the hysteresis region of the phase diagram [20]). We note the absence of any significant changes in the immediate vicinity of the critical disorder $\Delta_c/2D = 0.37$, corresponding to the Anderson metal–insulator transition. At the same time, we note that the most significant increase in the optical integral occurs as the system transforms into the disorder-induced metallic state obtained from the Mott insulator, as observed in Ref. [20].

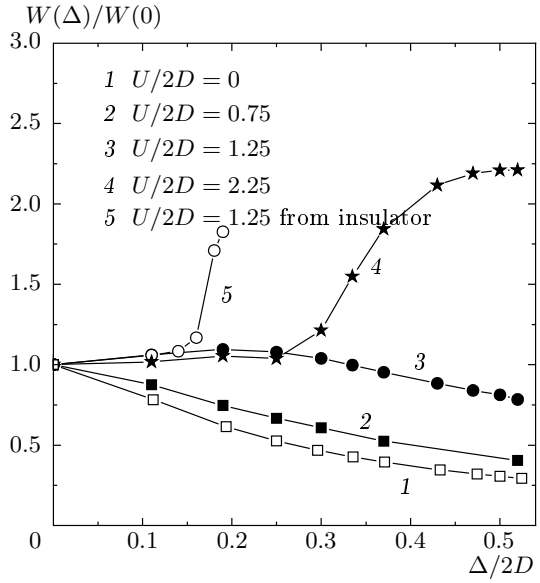

Fig. 8. Disorder dependence of the normalized optical integral in Anderson-Hubbard model for different values of Hubbard interaction U. Lines *1, 2, 3* — correlated metal, transforming into Anderson insulator. Line *4* — Mott insulator state obtained with the growth of U from correlated metal, line *5* — Mott insulator obtained with diminishing U in hysteresis region of the phase diagram

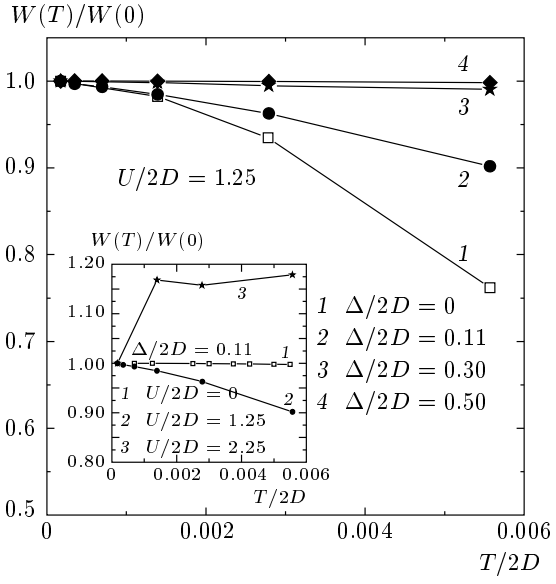

Fig. 9. Temperature dependence of the normalized optical integral in the Anderson–Hubbard model for different degrees of disorder. Inset: a similar dependence at a fixed disorder but for different values of the Hubbard interaction U; line *3* here corresponds to a disordered Mott insulator

In Fig. 9, we show the temperature dependence of the normalized optical integral, for different degrees of disorder. In the Anderson–Hubbard model, it appears to be significantly stronger than in the "hot spots" model (see above), and decreases as disorder increases. Moreover, in a relatively weakly correlated state, the situation is qualitatively the same, the optical integral decreases as T increases, but in a disordered Mott insulator, the integral increases, as can be seen from line 3 in the inset to Fig. 9.

Again, as in the case of the pseudogap "hot spot" model, these results for the Anderson–Hubbard model clearly demonstrate that the value of the optical integral is not universal and depends on all the major parameters of the model, and therefore the single-band optical sum rule is strongly "violated".

3. CONCLUSION

Based on the DMFT+Σ approach, we have studied the single-band optical sum rule for two typical strongly correlated systems, which are outside the scope of the standard DMFT scheme: (i) the "hot spot" model of the pseudogap state, which takes important nonlocal correlations due to AFM(CDW) short-range order fluctuations into account and (ii) the Anderson–Hubbard model, which includes strong disorder effects leading to the disorder-induced metal–insulator (Anderson) transition alongside with the Mott transition.

We have explicitly demonstrated that the single-band optical sum rule in (3) is satisfied for both models, confirming the self-consistency of the DMFT+Σ approach for calculation of two-particle properties.

However, the optical integral

$$W = 2\int\limits_0^\infty \mathrm{Re}\,\sigma(\omega)\,d\omega$$

entering single-band sum rule (3) is nonuniversal and depends on the parameters of the model under consideration. Most of the previous studies addressed its (relatively weak) temperature dependence. Here, we have analyzed dependences on the essential parameters of our models, showing that these may lead to rather strong "violations" of the optical sum rule. Because most of the parameters under discussion may be varied in different kinds of experiments, these dependences should be taken into account in the analysis of optical experiments on strongly correlated systems.

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