# Optical Sum Rule in Strongly Correlated Systems

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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+$\Sigma$ 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. However, the optical integral itself is in general dependent on temperature and characteristic parameters, such as pseudogap width, correlation strength and disorder scattering, leading to effective "violation" of the optical sum rule, which may be observed in the experiments.

## I. INTRODUCTION

Many years ago Kubo [1] has proven the general sum rule for 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:

$$\frac{2}{\pi}\int_0^\infty Re\sigma(\omega)d\omega = \sum_r \frac{n_r e_r^2}{m_r} \qquad (1)$$

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

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

$$\int_0^\infty Re\sigma(\omega)d\omega = \frac{\omega_{pl}^2}{8} \qquad (2)$$

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

However, in any real experiment we are not dealing with an infinite range of frequencies. If one considers electrons in a crystal and limits himself 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]:

$$W = \int_0^{\omega_c} Re\sigma(\omega)d\omega = f(\omega_c)\frac{\pi e^2}{2}\sum_{\mathbf{p}}\frac{\partial^2\varepsilon_p}{\partial p_x^2}n_p \qquad (3)$$

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

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

where $n(\varepsilon)$ is the usual Fermi distribution. In Eq. (3) $\omega_c$ represents an ultraviolet cut-off, frequency, which 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 Drude spectral weight beyond $\omega_c$ [5] and is unity if we formally set $\omega_c$ to infinity while ignoring the interband transitions.

Although the general sum rule is certainly preserved, the optical integral $W(\omega_c, T)$ is not a conserved quantity since both $f(\omega_c)$ [5] and $n_p$ [4, 6] depend on 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 anomalies were observed both in c-axis and in-plane conductivity both in normal and superconducting states [8, 9, 10, 11, 12, 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, $\sigma(\omega) = (\omega_{pl}^2/4\pi)/(1/\tau - i\omega)$ and the sum rule can only be "violated" due to the presence of $f(\omega_c)$. Integrating over $\omega$ and expanding for $\omega_c\tau >> 1$, one can see that

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

For 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 one obtains a sum rule "violation" even if $\omega_{pl}$ is $T$ independent [5, 7]. Other aspects of cut-off dependence were discussed recently in detail in Ref. [2].

In the present study we neglect the cut-off effects in optical integral from the outset. Our goal is to study $W$ dependence on $T$ and a number of interaction parameters, determining the electronic properties of strongly correlated systems, such as cuprates. In this context we shall discuss the problem of a possible "violation" of the optical sum rule in the normal (non superconducting)

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state of strongly correlated electronic systems, using our recently proposed DMFT+$\Sigma$ approach [14, 15, 16], as applied to dynamic conductivity in two typical models of such systems: the "hot – spot" model of the pseudogap state [19] and disordered Anderson – Hubbard model [20]. Our aim is both to check the consistency of DMFT+$\Sigma$ approach as 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 such important characteristics as pseudogap width, disorder and correlation strength, making (single band) sum rule "violation" rather ubiquitous for any strongly correlated system, even neglecting the cut-off effects.

## II. OPTICAL SUM RULE IN THE GENERALIZED DMFT+$\Sigma$ APPROACH

Characteristic feature of the general sum rule as expressed by Eqs. (3), (4) is that the integral $W$ over frequency in the l.h.s. is calculated via two-particle property (dynamic conductivity, determined by two-particle Green's function, in general, with appropriate vertex corrections), while the r.h.s. is determined by the single-particle characteristics, such as 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 dynamical mean field theory (DMFT+$\Sigma$) approach [14, 15, 16], supplying the standard dynamical mean field theory (DMFT) [17, 18] with an additional "external" self-energy $\Sigma$ (due to any kind of interaction outside the scope of DMFT, which is exact only in infinite dimensions), provides an effective method to calculate both single- and two-particle properties [19, 20]. The consistency check of this new approach is obviously of great interest by itself. We shall also see, that it gives a kind of a new insight in the problem of sum-rule "violation".

### A. Pseudogap state, the "hot spots" model

Pseudogap phenomena in strongly correlated systems have essential spatial length scale dependence [21]. To merge pseudogap physics and strong electron correlations we have generalized the dynamical-mean field theory [17, 18] by inclusion of the dependence on correlation length of pseudogap fluctuations via additional (momentum dependent) self-energy $\Sigma_{\mathbf{p}}(\varepsilon)$. This self-energy $\Sigma_{\mathbf{p}}(\varepsilon)$ describes non-local dynamical 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 spots" 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 characteristic vector $\mathbf{Q} = (\pi/a, \pi/a)$ ($a$ 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: $\Delta$ (pseudogap amplitude), which characterizes the energy scale of the pseudogap, and $\kappa = \xi^{-1}$ – the inverse correlation length of short range SDW (CDW) fluctuations. Both parameters $\Delta$ and $\xi$, determining pseudogap behavior, can in principle be calculated from the microscopic model at hand [15].

Weakly doped one-band Hubbard model with repulsive Coulomb interaction $U$ on a square lattice with nearest and next nearest neighbour hopping was numerically investigated within this generalized DMFT+$\Sigma$ self-consistent approach, as described in detail in Refs. [14, 15, 16].

Briefly, the DMFT+$\Sigma$ self-consistent loop looks like 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 case a functional of $\Sigma(\varepsilon)$. Then neglecting interference effects between the self-energies (which in fact is the major assumption of our approach) we can set up and solve the lattice problem of DMFT [17, 18]. Finally we define effective Anderson single impurity problem which is to be solved by any "impurity solver" (we mostly use numerical renormalization group - NRG) to close DMFT+$\Sigma$ equations.

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

In Ref. [19] this DMFT+$\Sigma$ procedure was generalized to calculate two-particle properties, such as dynamic conductivity, using previously developed recursion procedure for vertex corrections due to pseudogap fluctuations [24], producing typical pseudogap anomalies of optical conductivity and dependence of these anomalies on correlation strength $U$. Below we use the approach of Ref. [19]
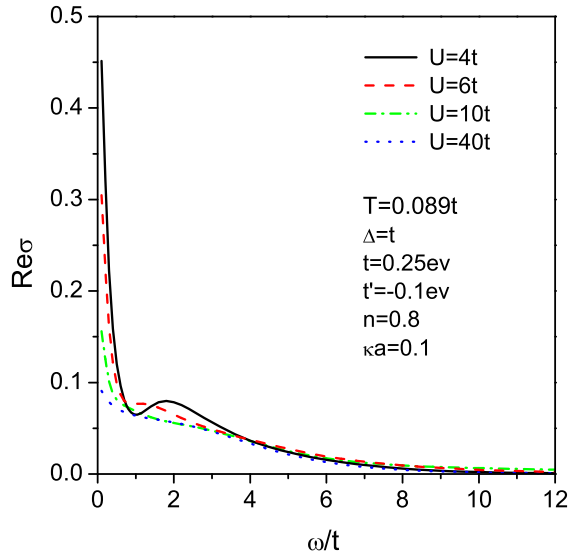
FIG. 1: Real part of optical conductivity for strongly correlated system in the pseudogap state ($t' = -0.4t$, $t = 0.25$ eV, $T = 0.089t$) in DMFT+$\Sigma_{\mathbf{p}}$ approximation — $U$ dependence. Band filling $n = 0.8$, pseudogap amplitude $\Delta = t$, correlation length $\xi = 10a$. Conductivity is given in units of $\sigma_0 = \frac{e^2}{\hbar}$.

to investigate the sum-rule in "hot spots" model.

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

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

In Fig. 2 we show the real part of optical conductivity for doped Mott insulator (fixed $U = 40t$, $t' = -0.4t$, $t = 0.25$ eV, band filling $n = 0.8$, $T = 0.089t$) for different values of pseudogap amplitude $\Delta = 0$, $\Delta = t$, $\Delta = 2t$. Correlation length is again $\xi = 10a$ and band filling factor $n = 0.8$. The "violation" of sum-rule here

TABLE I: Single-band optical sum rule check in the "hotspots" model. $U$ - dependence. Optical integral in units of $\frac{e^2}{\hbar}t$.

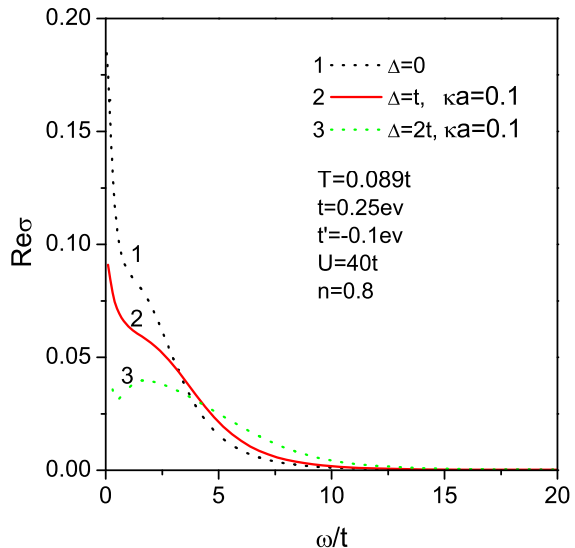| $U$ | $\frac{\pi e^2}{2} \sum_{\mathbf{p}} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n_p$ | $W = \int_0^\infty Re\sigma(\omega)d\omega$ |
|---|---|---|
| $U = 4t$ | 0.456 | 0.408 |
| $U = 6t$ | 0.419 | 0.387 |
| $U = 10t$ | 0.371 | 0.359 |
| $U = 40t$ | 0.323 | 0.306 |



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

is especially striking — optical integral obviously drops with the growth of $\Delta$. However, again the single band optical sum-rule (3) is strictly valid, as seen from Table II.

To study the details of sum-rule "violation", i.e. the dependence of the optical integral $W$ on the parameters of the model, we performed extensive calculations of the appropriate dependences of the r.h.s. of Eq. (3) and opti-

TABLE II: Single-band optical sum rule check in the "hot spots" model. $\Delta$ - dependence. Optical integral in units of $\frac{e^2}{\hbar}t$.

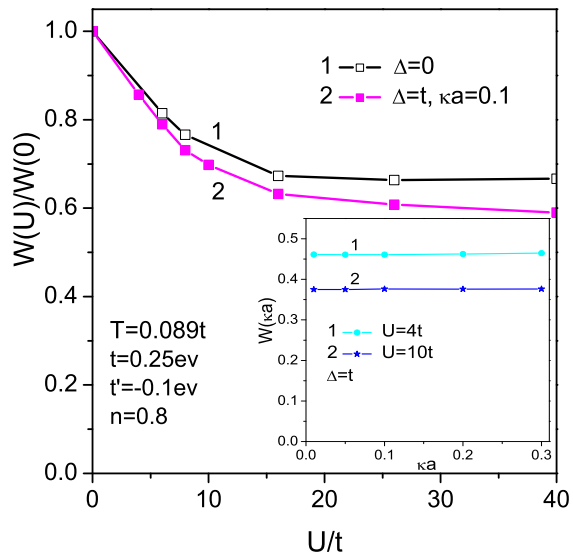| $\Delta$ | $\frac{\pi e^2}{2} \sum_{\mathbf{p}} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n_p$ | $W = \int_0^\infty Re\sigma(\omega)d\omega$ |
|---|---|---|
| $\Delta = 0$ | 0.366 | 0.36 |
| $\Delta = t$ | 0.314 | 0.304 |
| $\Delta = 2t$ | 0.264 | 0.252 |

FIG. 3: Dependence of normalized optical integral on correlation strength $U$ in the pseudogap state. All other parameters are listed in the figure. At the insert — correlation length dependence of optical integral in units of $\frac{e^2}{\hbar}t$.

cal integral $W$ on the temperature $T$, doping, pseudogap amplitude $\Delta$, correlation length of pseudogap fluctuations $\xi = \kappa^{-1}$ and correlation strength $U$. Some of the results are presented in Figs. 3 – 5.

Typical dependence of the (normalized) optical integral on correlation strength $U$ is shown in Fig. 3 for two values of $\Delta$. We can see rather significant drop of $W$ with the growth of $U$. As to correlation length dependence, which is shown at the insert Fig. 3, it was found to be very weak (practically negligible) in a whole region of realistic values of $\xi$, so that we shall not discuss it further. Dependence of $W$ on the pseudogap amplitude $\Delta$ (for several values of $U$) is shown in Fig. 4. Typical doping dependence, which reflects just the dependence of the square of the plasma frequency $\omega_{pl}^2$ on doping, is given in Fig. 5. In all cases other, the change of the relevant parameters of the model lead to rather significant drop in the values of $W$. As to the temperature dependence (shown in the insert on 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, so that the optical sum rule is significantly "violated", if we restrict ourselves with a single-band contribution.
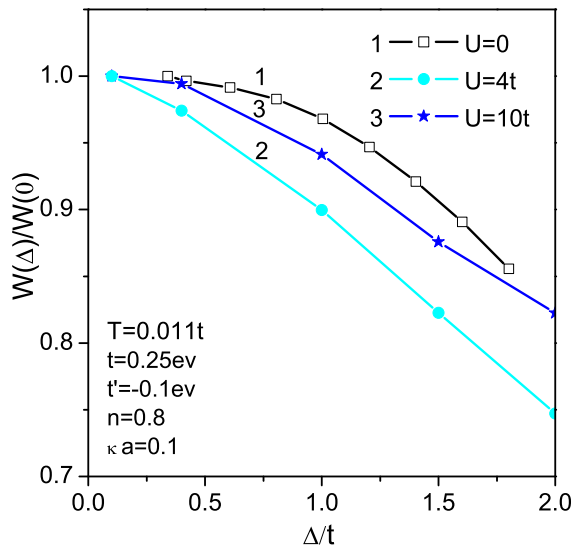


FIG. 4: Dependence of the normalized optical integral on the pseudogap amplitude $\Delta$. The other parameters are listed in the figure.

### B. Disordered Anderson – Hubbard model

In Ref. [20] we have applied DMFT+$\Sigma$ approximation to calculate the density of states, optical conductivity and phase diagram of strongly correlated and strongly disordered paramagnetic Anderson–Hubbard model, with Gaussian site disorder. Strong correlations were accounted by DMFT, while disorder was taken into account via the appropriate generalization of self-consistent theory of localization [25, 26, 27, 28]. We considered the three-dimensional system with semi-elliptic density of states. Correlated metal, Mott insulator and correlated Anderson insulator phases were identified via the evolution of density of states and dynamic conductivity, demonstrating both Mott-Hubbard and Anderson metal-insulator transitions and allowing the construction of complete zero-temperature phase diagram of Anderson–Hubbard model.

For "external" self-energy entering DMFT+$\Sigma$ loop we have 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 energies disorder takes the usual form:

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

where $\Delta$ denotes now the amplitude of site disorder.

Calculations of optical conductivity are considerably simplified [20] due to the fact, that there are no contributions to conductivity due to vertex corrections, determined by local Hubbard interaction. Finally, con-
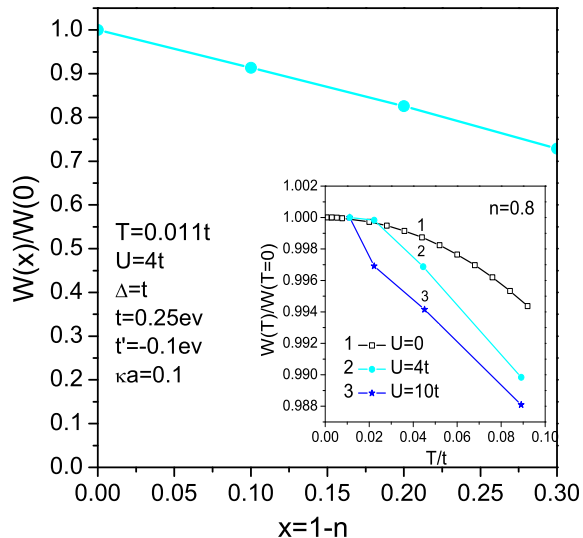
FIG. 5: Dependence of the normalized optical integral on hole doping in the pseudogap state. At the insert — temperature dependence. All other parameters are listed in the figure

TABLE III: Single-band optical sum rule check in Anderson – Hubbard model. $\Delta$ - dependence. Optical integral in units of $\frac{2e^2}{\hbar a}D$.

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

ductivity is essentially determined by the generalized diffusion coefficient, which is obtained from the appropriate generalization of self-consistent equation of Refs. [25, 26, 27, 28], which is to be solved in conjunction with DMFT+$\Sigma$ loop.

In Fig. 6 we show typical results for the real part of dynamic conductivity of a correlated metal described by the half–filled Anderson–Hubbard model (with bandwidth $2D$) for different degrees of disorder $\Delta$, and demonstrating continuous transition to correlated Anderson insulator with the growth of disorder.

Here again the direct check shows that the single band optical sum-rule (3) is obeyed within our numerical accuracy, as seen from Table III. At the same time, optical integral $W$ itself obviously changes with disorder.

Again, to study the details of this sum-rule "violation", i.e. the dependence of $W$ on the parameters of Anderson-Hubbard model, we performed detailed calculations of its dependences on the temperature $T$, disorder amplitude $\Delta$ and correlation strength $U$. Some of the results are
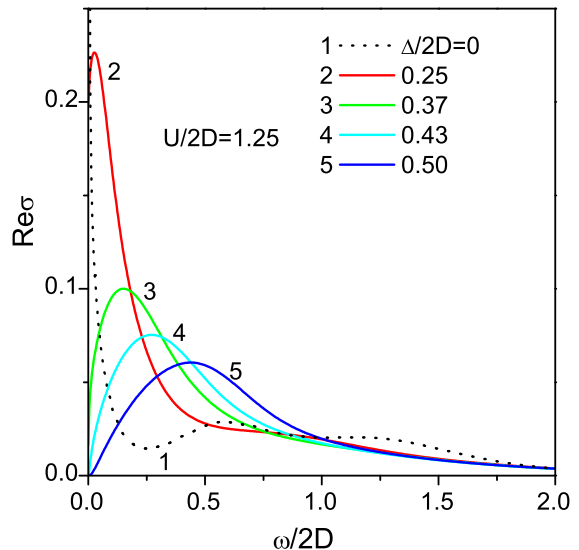


FIG. 6: Real part of dynamic conductivity for half–filled Anderson–Hubbard model for different degrees of disorder $\Delta$, and $U = 2.5D$, typical for correlated metal. Lines 1,2 are for metallic phase, line 3 corresponds to the mobility edge (Anderson transition), lines 4,5 correspond to correlated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

presented in Figs. 7 – 9.

In Fig. 7 we show the dependence of normalized optical integral on Hubbard $U$, for different degrees of disorder (both for strongly disordered metal and correlated Anderson insulator). It is seen that in all cases the growth of correlation strength leads to rather sharp drop of $W$ in metallic state, which becames mush slower in Mott insulator.

In Fig. 8 we present similar dependences on disorder strength $\Delta$. In metallic state optical integral generally drops with the growth of disorder, while an opposite behavior is observed if we start from Mott insulator (both obtained with the growth of $U$ from metallic state and under diminishing $U$ in hysteresis region of the phase diagram [20]). Note the absence of any significant changes in the immediate vicinity of critical disorder $\Delta_c/2D = 0.37$, corresponding to Anderson metal – insulator transition. At the same time it should be noted that the most significant growth of the optical integral takes place as the system transforms into disorder induced metallic state, obtained from Mott insulator, as observed in Ref.[20].

In Fig. 9 we show the temperature dependence of the normalized optical integral, for different degrees of disorder. In Anderson – Hubbard model it appears to be significantly stronger, than in "hot spots" model (see above), and decreases with the growth of disorder. Moreover, while in relatively weakly correlated state it is qualitatively the same – optical integral diminishes with the
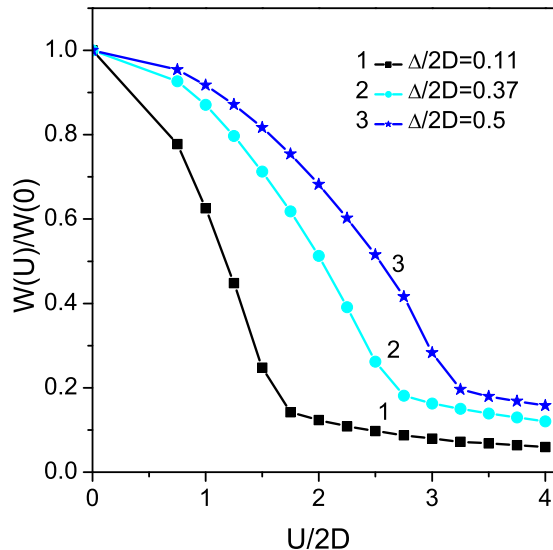
FIG. 7: Dependence of the normalized optical integral on correlation strength in Anderson-Hubbard model for different degrees of disorder $\Delta$ (1,2 – strongly disordered metal, 3 – correlated Anderson insulator).
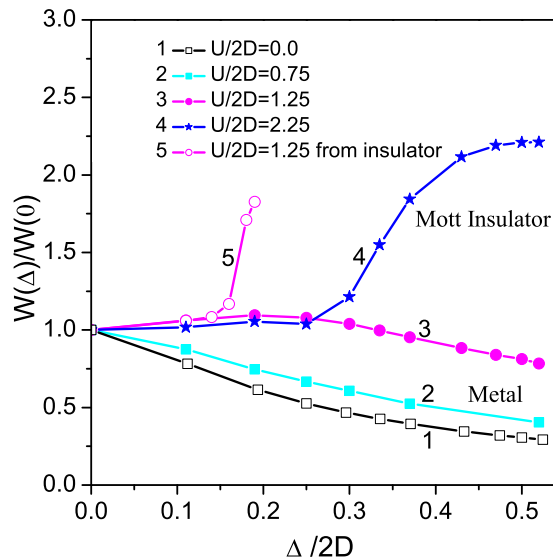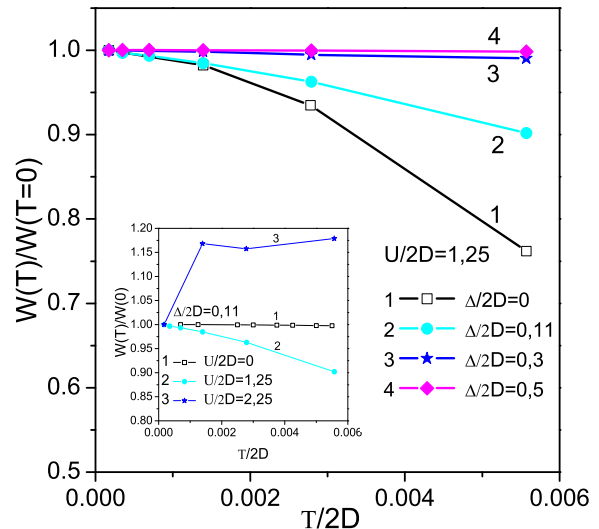


FIG. 9: Temperature dependence of normalized optical integral in Anderson-Hubbard model for different degrees of disorder. At the insert – similar dependence at fixed disorder, but for different values of Hubbard interaction $U$, line 3 here corresponds to disordered Mott insulator.

growth of $T$, it actually grows in disordered Mott insulator, as seen from line 3 at the insert in Fig. 9.

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



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.

## III. CONCLUSION

Based on DMFT+$\Sigma$ 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: (i) the "hot spots" model of the pseudogap state, which takes into account important non-local correlations due to AFM(CDW) short-range order fluctuations and (ii) Anderson-Hubbard model, which includes strong disorder effects, leading to disorder induced metal-insulator (Anderson) transition, alongside with Mott transition.

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

However, the optical integral $W = 2\int_0^\infty Re\sigma(\omega)d\omega$, entering the single band sum rule (3) is non universal and depends on the parameters of the model under consideration. Most of the previous studies addressed its (rela-

tively weak) temperature dependence. Here we have analyzed dependences on essential parameters of our models, showing that these may lead to rather strong "violations" of the optical sum rule. As 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.

## IV.   ACKNOWLEDGEMENTS

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