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ORIGINAL PAPER

Attractive Hubbard Within the Generalized DMFT: Normal State Properties, Disorder Effects and Superconductivity

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Abstract Using the generalized DMFT+Σ approach, we have studied disorder influence on the density of states, optical conductivity of the normal phase, superconducting transition temperature, and Ginzburg–Landau coefficients in the attractive Hubbard model. The wide range of attractive potentials U was studied—from the weak coupling region, where both the instability of the normal phase and superconductivity are well described by the BCS model, to the strong coupling region, where superconducting transition is due to the Bose–Einstein condensation (BEC) of preformed Cooper pairs. For semi-elliptic "bare" density of states of conduction band, the disorder influence on all single-particle properties (e.g., density of states) is universal for arbitrary strength of electronic correlations and is due only to the general disorder widening of conduction band. Using the combination of DMFT+Σ and Nozieres–Schmitt-Rink approximations, we have studied the disorder influence upon superconducting transition temperature T_c for the range of characteristic values of U and disorder including the BCS-BEC crossover region. Disorder can either suppress T_c (in the weak coupling region) or significantly increase T_c (in strong coupling region). However, in all cases, the generalized Anderson theorem is valid and all changes of superconducting critical temperature are essentially due only to the general disorder widening of the conduction band.

Keywords Attractive Hubbard model · BCS-BEC crossover · Anderson theorem

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The problem of strong coupling superconductivity was studied for a long time, starting with pioneering papers by Eagles and Leggett [1, 2]. Significant progress here was achieved by Nozieres and Schmitt-Rink [3], who suggested an effective method to study the transition temperature crossover from weak coupling BCS-like behavior towards Bose–Einstein condensation (BEC) scenario in the strong coupling region. One of the simplest models allowing the study of BCS-BEC crossover is the Hubbard model with attractive on site interaction. The most successive approach to the solution of Hubbard model, both in the case of repulsive interaction and for the studies of BCS-BEC crossover in case of attraction, is the dynamical mean field theory (DMFT) [4–6]. Attractive Hubbard model was studied within DMFT in a number of recent papers [7–11]. However, up to now there are only few studies of disorder influence on the properties of normal and superconducting phases in this model, especially in the region of BCS-BEC crossover.

In recent years, we have developed the so called generalized DMFT+Σ approach [12–18], which is very convenient for the inclusion of different additional interactions into the Hubbard model. This approach is also well suited to analyze two-particle properties, such as optical (dynamic) conductivity [16, 18]. Here, we shall concentrate on the

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discussion of disorder effects in the attractive Hubbard model.

The Hamiltonian of disordered Hubbard model can be written as:

$$H = -t \sum_{\langle ij \rangle \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $t > 0$ is the transfer integral between nearest sites of the lattice, U is the on site interaction (in the case of attraction $U < 0$), $n_{i\sigma} = a^{\dagger}_{i\sigma} a_{i\sigma}$ is the operator of the number of electrons on the lattice site i, and $a_{i\sigma}$ ($a^{\dagger}_{i\sigma}$) is the annihilation (creation) operator for electron with spin σ on site i. The local energy levels ϵ_i are assumed to be independent random variables at different lattice sites with Gaussian distribution:

$$\mathcal{P}(\epsilon_i) = \frac{1}{\sqrt{2\pi}\,\Delta} \exp\left(-\frac{\epsilon_i^2}{2\Delta^2}\right) \tag{2}$$

Parameter Δ represents here is the measure of disorder and this Gaussian random field (with "white noise" correlation on different lattice sites) generates the "impurity" scattering leading to the standard diagram technique for the calculation of the ensemble averaged Green's functions [19, 20].

Generalized DMFT+Σ approach [12–15] extends the standard DMFT [4–6] introducing an additional self-energy $\Sigma_{\mathbf{p}}(\varepsilon)$ (in general case momentum dependent), which is due to some interaction mechanism outside the DMFT. It gives an effective procedure to calculate both single- and two-particle properties [16, 18]. The single-particle Green's function is then written in the following form:

$$G(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon + \mu - \varepsilon(\mathbf{p}) - \Sigma(\varepsilon) - \Sigma_{\mathbf{p}}(\varepsilon)}, \tag{3}$$

where $\varepsilon(\mathbf{p})$ is the "bare" electronic dispersion, while the total self-energy completely neglects the interference between the Hubbard and additional interaction and is given by the additive sum of the local self-energy $\Sigma(\varepsilon)$ of DMFT and "external" self-energy $\Sigma_{\mathbf{p}}(\varepsilon)$. This conserves the standard structure of DMFT equations [4–6].

As an effective Anderson impurity solver in our DMFT calculations, we have used here the numerical renormalization group (NRG) [21], which allows to perform calculations at pretty low temperatures.

For the self-energy due to disorder scattering produced by the Hamiltonian (1), we use the simplest self-consistent Born approximation neglecting the diagrams with "intersecting" interaction lines:

$$\Sigma_{\mathbf{p}}(\varepsilon) \to \Delta^2 \sum_{\mathbf{p}} G(\varepsilon, \mathbf{p}), \tag{4}$$

where $G(\varepsilon, \mathbf{p})$ is the single-particle Green's function (3).

In the following, we shall consider the three-dimensional system with the "bare" semi-elliptic density of states (per unit cell and one spin projection), with the total bandwidth $2D$, which is given by:

$$N_0(\varepsilon) = \frac{2}{\pi D^2} \sqrt{D^2 - \varepsilon^2}. \tag{5}$$

In this case, one can directly demonstrate that in DMFT+Σ approximation disorder influence upon single-particle properties of disordered Hubbard model (both repulsive and attractive) is completely described by effects of general band widening by disorder scattering. Actually, in the system of self-consistent DMFT+Σ equations [13, 15, 16], both the "bare" band spectrum and disorder scattering enter only at the stage of calculations of the local Green's function:

$$G_{ii} = \sum_{\mathbf{p}} G(\varepsilon, \mathbf{p}), \tag{6}$$

where the full Green's function $G(\varepsilon, \mathbf{p})$ is determined by (3), while the self-energy due to disorder, in the self-consistent Born approximation, is given by (4). Then, the local Green's function takes the following form:

$$G_{ii} = \int_{-D}^{D} d\varepsilon' \frac{N_0(\varepsilon')}{\varepsilon + \mu - \varepsilon' - \Sigma(\varepsilon) - \Delta^2 G_{ii}}. \tag{7}$$

In the case of semi-elliptic density of states (5), this integral can be calculated in analytic form and the local Green's function can be written as [22]:

$$G_{ii} = \int_{-D_{\mathrm{eff}}}^{D_{\mathrm{eff}}} d\varepsilon' \frac{\tilde{N}_0(\varepsilon')}{\varepsilon + \mu - \varepsilon' - \Sigma(\varepsilon)}, \tag{8}$$

where we have introduced D_{eff}, an effective half-width of the band (in the absence of electronic correlations, i.e., for $U = 0$) widened by disorder scattering:

$$D_{\mathrm{eff}} = D\sqrt{1 + 4\frac{\Delta^2}{D^2}} \tag{9}$$

and

$$\tilde{N}_0(\varepsilon) = \frac{2}{\pi D_{\mathrm{eff}}^2} \sqrt{D_{\mathrm{eff}}^2 - \varepsilon^2} \tag{10}$$

represents the density of states in the absence of interaction U widened by disorder. The density of states in the presence of disorder remains semi-elliptic, so that all effects of disorder scattering on single-particle properties of disordered Hubbard model in DMFT+Σ approximation are reduced only to disorder widening of conduction band, i.e., to the replacement $D \to D_{\mathrm{eff}}$.

As we noted above, DMFT+Σ approach is also well suited to analyze the optical (dynamic) conductivity [16, 18], though in this case the disorder influence cannot be reduced to this simple replacement.

Below, we discuss the typical case of quarter-filled band ($n = 0.5$). In Fig. 1, we present the evolution of the density of states and optical conductivity with changing disorder.

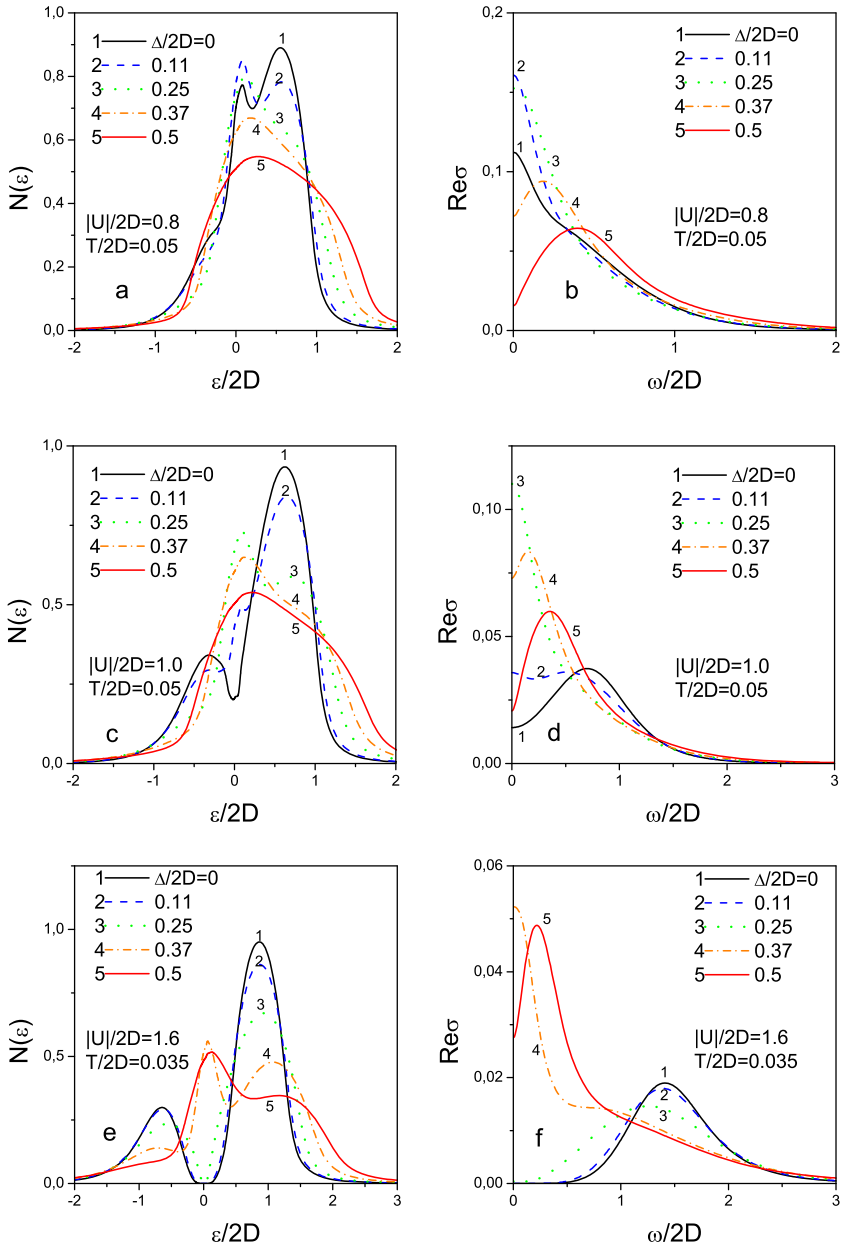

Fig. 1 Evolution of the density of states (*left panels*) and optical conductivity (*right panels*) with disorder for different values of U ($|U|/2D = 0.8$ (**a** and **b**); $|U|/2D = 1$ (**c** and **d**); $|U|/2D = 1.6$ (**e** and **f**))

At relatively weak attraction ($|U|/2D = 0.8$, Fig. 1a), the growth of disorder just widens the density of states. Disorder effectively masks peculiarities of the density of states due to correlation effects. In particular, quasiparticle peak and the "wings" due to upper and lower Hubbard bands present in Fig. 1a in the absence of disorder completely vanish at strong enough disorder. The evolution of optical conductivity with the growth of disorder Δ, shown in Fig. 1b, is in general agreement with the evolution of density of states. Weak enough disordering (curves 1 and 2 in Fig. 1b), leads to some growth of static conductivity, which is connected with the suppression of correlation effects at the Fermi level (curves 1–3 in Fig. 1a. Further growth of disorder leads to significant widening of the band and the drop of the density of states (curve 4 in Fig. 1a,b), which leads to the drop of static conductivity. Finally, the growth of disorder leads to Anderson localization which takes place at $\Delta/2D = 0.37$ for $T = 0$ [16]. However, here, we consider the case of high enough temperature $T/2D = 0.05$, so that static conductivity (see curve 5 in Fig. 1b) always remains finite, though the localization behavior is also clearly seen. At larger value of attractive interaction $|U|/2D = 1$, the evolution of the density of states and optical conductivity is more or less similar (Fig. 1c,d). However, in the absence of disorder, we observe here the Cooper pairing pseudogap in the density of states, while disorder suppresses it, leading both to the growth of the density of states at the Fermi level and related

growth of static conductivity. Finally, at still larger attraction $|U|/2D = 1.6$ (Fig. 1e,f) in the absence of disorder, there is the real Cooper pairing gap in the density of states. This gap is also evident in optical conductivity. With growth of disorder Cooper pairing gap both in the density of states and conductivity becomes narrower (curves 2 and 3). Further growth of disorder leads to complete suppression of this gap and restoration of metallic state with finite density of states at the Fermi level and finite static conductivity. This closure of Cooper gap is obviously related to the effective growth of the conduction bandwidth $2D_{\text{eff}}$, which leads to the lowering of $|U|/2D_{\text{eff}}$ ratio, which actually controls the formation of Cooper gap. The situation here is similar to the closure of Mott gap by disorder in repulsive Hubbard model [16]. However, at large disorder (curve 5 in Fig. 1f), we clearly observe localization behavior, so that the growth of disorder at $T = 0$ will first lead to metallic state (the closure of Cooper pairing gap), while the further growth of disorder will induce Anderson metal-insulator transition. Similar picture is observed for large positive U at half-filling ($n = 1$) [16], where the growth of disorder leads to Mott insulator-correlated metal-Anderson insulator transition.

Cooper instability, determining T_c is related to divergence of two-particle loop in the Cooper channel. In the weak coupling limit, when superconductivity is due to the appearance of Cooper pairs at T_c, disorder only slightly influences superconductivity with s-wave pairing [23, 24]. This is the essence of the so called Anderson theorem, and changes of T_c are due only to the relatively small changes of the density of states at the Fermi level induced by disorder.

In the region of BCS-BEC crossover and in the strong coupling region the Nozieres–Schmitt-Rink approach [3] assumes that corrections due to strong pairing attraction significantly change the chemical potential of the system, while possible correction due to this interaction to Cooper instability condition can be neglected, so that we can always use the weak coupling (ladder) approximation. Then the condition of Cooper instability in disordered Hubbard model takes the form:

$$1 = -|U|\chi_0(q = 0, \omega_m = 0) \tag{11}$$

where $\chi_0(q = 0, \omega_m = 0)$ represents the two-particle loop (susceptibility) in the Cooper channel "dressed" only by disorder scattering ($\omega_m = 2\pi mT$ are the usual Boson Matsubara frequencies).

Using the exact Ward identity, derived in Ref. [18], after the standard summation over Matsubara frequencies [19, 20], we get [22]:

$$\chi_0(q = 0, \omega_m = 0) = -\int_{-\infty}^{\infty} d\varepsilon \frac{\tilde{N}_0(\varepsilon)}{2\varepsilon} th\frac{\varepsilon}{2T}, \tag{12}$$

where $\tilde{N}_0(\varepsilon)$ is the density of states ($U = 0$), renormalized by disorder scattering (10). In (12), the energy ε origin is at the chemical potential. If the origin of energy is shifted to the middle of conduction band, we have to replace $\varepsilon \to \varepsilon - \mu$, and the condition of Cooper instability (11) leads to the following equation for T_c:

$$1 = \frac{|U|}{2}\int_{-\infty}^{\infty} d\varepsilon \tilde{N}_0(\varepsilon)\frac{th\frac{\varepsilon-\mu}{2T_c}}{\varepsilon-\mu}, \tag{13}$$

The chemical potential of the system at different values of U and Δ now should be determined from DMFT+Σ calculations, i.e., from the standard equation for the number of electrons (band-filling), determined by Green's function given by (3), which allows us to find T_c for the wide range of model parameters, including the BCS-BEC crossover and strong coupling regions, as well as for different levels of disorder. This is the gist of Nozieres–Schmitt-Rink approximation—in the weak coupling region, superconducting transition temperature is controlled by the equation for Cooper instability (13), while in the strong coupling limit it is determined by the temperature of Bose–Einstein condensation, which is controlled by chemical potential. Then the joint solution of (13) and equation for the chemical potential guarantees the correct interpolation for T_c through the region of BCS-BEC crossover. In the absence of disorder, this combination of Nozieres–Schmitt-Rink approximation with DMFT produces the results for the critical temperature, which is almost quantitatively close [11] to exact results, obtained by direct numerical DMFT calculations [7, 8, 10, 11], but demands much less numerical efforts.

Equation (13) demonstrates that Cooper instability depends on disorder only through the disorder dependence of the density of states $\tilde{N}_0(\varepsilon)$, which is the main statement of Anderson theorem. Within Nozieres–Schmitt-Rink approach, Eq. (13) is conserved also in the region of strong coupling, when the critical temperature is determined by BEC condition for compact Cooper pairs. However, the chemical potential μ, entering (13), may significantly depend on disorder. In DMFT+Σ approximation, this dependence of chemical potential (as well as any other single-particle characteristic) in the model with semi-elliptic density of states is only due to disorder widening of conduction band. In this sense, both in BCS-BEC crossover region and in the strong coupling limit, a kind of generalized Anderson theorem actually holds and (13) leads to universal dependence of T_c on disorder, due to the change of $D \to D_{\text{eff}}$. Such universality is fully confirmed by direct numerical calculations of T_c in this model, performed in Ref. [25].

In Fig. 2a, we present the dependence of T_c (normalized by the critical temperature in the absence of disorder

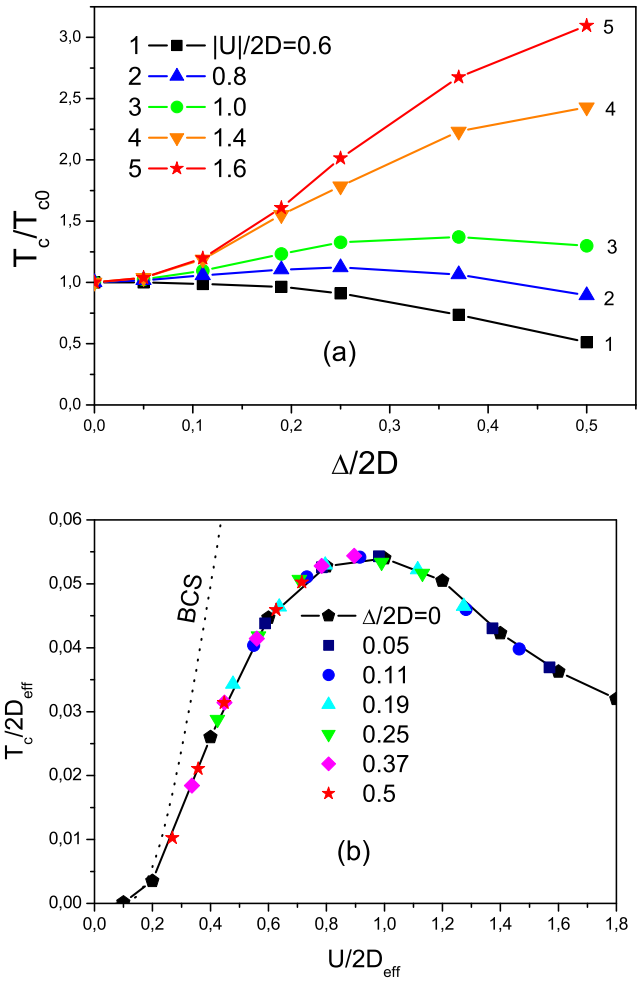

Fig. 2 Dependence of superconducting critical temperature on Hubbard attraction U for different disorder levels: **a** explicit results for T_c normalized by its value T_{c0} in the absence of disorder ($\Delta = 0$) on $U/2D$; **b** universal U dependence of T_c normalized by $2D_{\text{eff}}$ on $U/2D_{\text{eff}}$ (*black curve* corresponds to the case of $\Delta = 0$)

$T_{c0} = T_c(\Delta = 0)$) on disorder for different values of pairing interaction U. In the weak coupling limit ($U/2D \ll 1$), disorder slightly suppresses T_c (curve 1). At intermediate couplings ($U/2D \sim 1$), weak disorder increases T_c, while the further growth of disorder suppresses the critical temperature (curve 3). In the strong coupling region ($U/2D \gg 1$), the growth of disorder leads to significant increase of the critical temperature (curves 4 and 5). However, this rather complicated dependence of T_c on disorder is actually completely determined simply by disorder widening of the initial ($U = 0$) conduction band, demonstrating the validity of the generalized Anderson theorem for all values of U. This is illustrated in Fig. 2b, where the black curve with octagons shows the dependence of the critical temperature $T_c/2D$ on coupling strength $U/2D$ in the absence of disorder ($\Delta = 0$). In the weak coupling region, superconducting transition temperature is well described by BCS model (in Fig. 2b, the dashed curve represents the result of the solution of BCS model, with T_c determined by (13), with chemical potential independent of U, and determined by quarter-filling of the "bare" band), while in the strong coupling region the critical temperature is determined by Bose–Einstein condensation of Cooper pairs and drops $\sim t^2/U$ with the growth of U (inversely proportional to the effective mass of the pair), passing through the maximum, at $U/2D_{\text{eff}} \sim 1$. The other symbols in Fig. 2b show the results for T_c obtained by the combination of DMFT+Σ and Nozieres–Schmitt-Rink approximations for the case of semi-elliptic band. We can see that all data (expressed in normalized units of $U/2D_{\text{eff}}$ and $T_c/2D_{\text{eff}}$) ideally fit the universal curve, obtained in the absence of disorder.

Universal dependence on disorder is also observed for the coefficients of A and B of Ginzburg–Landau expansion:

$$F_s - F_n = A|\Delta_{\mathbf{q}}|^2 + q^2C|\Delta_{\mathbf{q}}|^2 + \frac{B}{2}|\Delta_{\mathbf{q}}|^4, \tag{14}$$

where $\Delta_{\mathbf{q}}$ is the spatial Fourier component of the amplitude of superconducting order parameter. Actually, these coefficients of homogeneous part of this expansion are related to loop diagrams with Cooper-channel vertices with the sum of incoming (outgoing) momenta $q = 0$. In particular, the coefficient A is given by [19, 20]:

$$A(T) = \chi_0(q = 0, T) - \chi_0(q = 0, T_c), \tag{15}$$

where $\chi_0(q = 0, T)$ is Cooper susceptibility (12) and subtraction of $\chi_0(q = 0, T_c)$ guarantees the zero value of $A(T = T_c)$. Using (11) to determine $\chi_0(q = 0, T_c)$, we get:

$$A(T) = \frac{1}{|U|} - \int_{-\infty}^{\infty} d\varepsilon \tilde{N}_0(\varepsilon) \frac{th\frac{\varepsilon-\mu}{2T}}{2(\varepsilon-\mu)}. \tag{16}$$

so that the coefficient $A(T)$ reduces to zero for $T \to T_c$ and is written as:

$$A(T) = a(T - T_c). \tag{17}$$

For the case of the "bare" band with semi-elliptic density of states, the dependence of a on disorder is again related only to the general widening of the band by disorder, i.e., is completely described by the replacement $D \to D_{\text{eff}}$. Thus, in the presence of disorder, we obtain the universal dependence of a on U (normalized by D_{eff}).

Ginzburg–Landau coefficient B is determined by the "loop" diagram with four Cooper vertices [19, 20]. After rather complicated analysis [26], which is based on some generalizations of Ward identity derived in Ref. [18], it can be shown exactly, that B is given by:

$$B = \int_{-\infty}^{\infty} \frac{d\varepsilon}{4(\varepsilon-\mu)^3} \left(th\frac{\varepsilon-\mu}{2T} - \frac{(\varepsilon-\mu)/2T}{ch^2\frac{\varepsilon-\mu}{2T}} \right) \tilde{N}_0(\varepsilon) \tag{18}$$

Thus, the dependence of coefficient B on disorder, similarly to A, is determined only by the density of states $\tilde{N}_0(\varepsilon)$ renormalized (widened) by disorder and the chemical potential μ. Then, in the case of semi-elliptic density of states, the dependence of B on disorder is reduced to the simple replacement $D \to D_{\text{eff}}$, so that in the presence of disorder we obtain again the universal dependence of B on U.

It should be noted that (16) and (18) for coefficients A and B were obtained using the exact Ward identities and remain valid also in the limit of strong disorder (Anderson localized phase), when both A and B depend on disorder also only via the effective bandwidth D_{eff}.

This universal dependence on disorder (due only to the replacement $D \to D_{\text{eff}}$) is reflected in the specific heat discontinuity at the transition temperature, which is determined by coefficients a and B:

$$C_s(T_c) - C_n(T_c) = T_c \frac{a^2}{B} \tag{19}$$

This universal behavior is illustrated in Fig. 3.

To determine the coefficient C of the gradient term of Ginzburg–Landau expansion, we need the knowledge of nontrivial of q-dependence of Cooper vertex [19, 20], which is essentially changed by disorder scattering. In particular, the behavior of coefficient C is qualitatively changed at Anderson localization transition [23]. Thus, the coefficient C is basically determined by two-particle characteristics of the system and does not demonstrate the universal dependence on disorder due only to changes of the effective bandwidth.

In this paper, in the framework of DMFT+Σ generalization of dynamical mean field theory [15], we have studied disorder effects in BCS-BEC crossover region of attractive Hubbard model. We performed extensive calculations of the densities of states and dynamic (optical) conductivity for the wide range of interactions U and at different disorder levels Δ. We have shown analytically for the case of conduction band with semi-elliptic density of states (which is a good approximation for three-dimensional case) in DMFT+Σ approximation disorder influences all single-particle properties (e.g., density of states) in a universal way—all changes of these properties are due only to disorder widening of the conduction band. Similar universal dependences on disorder are also reflected in superconducting critical temperature and the coefficients of homogeneous Ginzburg–Landau expansion for attractive Hubbard model, where the combination of DMFT+Σ and Nozieres–Schmitt-Rink approximations demonstrates the validity of the generalized Anderson theorem both in BCS-BEC crossover and strong coupling regions.

Naturally, no universal dependences on disorder were obtained for the two-particle properties like optical conductivity, where vertex corrections due to disorder scattering become very important, leading to new physics, like that of Anderson transition.

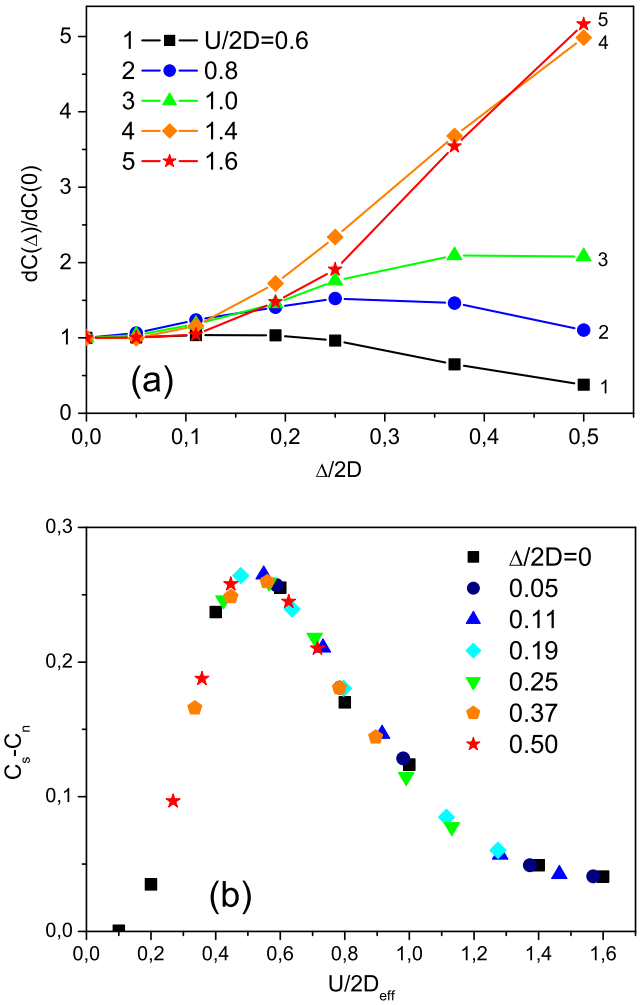

Fig. 3 Dependence of specific heat discontinuity at critical temperature $dC \equiv C_s - C_n$ on disorder for different values of Hubbard attraction U (**a**) and universal dependence of this discontinuity on U for different values of disorder (**b**)

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