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Disordered Hubbard Model: DMFT+Sigma Approximation

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RUSSIAN ACADEMY OF SCIENCES URALS DIVISION

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Basic Models for Metal-Insulator Transition

Anderson model

P.W.Anderson (1958)







+ 1.17 Potential energy used by Anderson (1958): (a) without a random potential and (b) with such a potential. The density of states is also shown.



: 1.18 Wave function ψ of an electron when $l \sim a$: (a) extended states; (b) weakly localized states.

At small disorder dc conductivity of a metal at T = 0 is determined by Drude expression:

$$\tau_0 = \frac{ne^2}{m}\tau = \frac{ne^2}{p_F}l$$
(2.2)

where τ — is the mean free time, n — is electron density and e — its charge. Usual kinetic theory can be applied if

$$\frac{p_F l}{\hbar} \gg 1 \text{ or } \frac{E_F \tau}{\hbar} \gg 1$$
 (2.3)

which is a condition of weak scattering (disorder). From Eq. (2.2) and Eq. (2.3), taking into account $n = p_F^3/(3\pi^2\hbar^3)$, we can estimate the lower limit of conductivity for which Drude approximation is still valid:

$$\sigma_0 = \frac{e^2 p_F}{3\pi^2 \hbar^2} \left(\frac{p_F l}{\hbar}\right) \gg \frac{e^2 p_F}{3\pi^2 \hbar^2} \tag{2.4}$$

The conductivity value:

$$\sigma_c \approx \frac{e^2 p_F}{3\pi^2 \hbar^2} \tag{2.5}$$

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is usually called the "minimal metallic conductivity" [Mott N.F. (1974)

Self - Consistent Theory of Localization



These "maximally crossed" diagrams lead to the following quantum correction to diffusion coefficient:

$$\frac{\delta D(\omega)}{D_0} = -\frac{1}{\pi N(E)} \sum_{|\mathbf{k}| < k_0} \frac{1}{-i\omega + D_0 k^2} \qquad (\$)$$

Appropriate correction to relaxation kernel can be expressed via the correction to diffusion coefficient as:

$$\delta M_E(\omega) = -i\frac{2E_F}{dm}\frac{\delta D(\omega)}{D(\omega)^2} = -\frac{M_E(\omega)}{D(\omega)}\delta D(\omega)$$

Considering the usual Drude metal as the zeroth approximation we get:

$$\delta M_E(\omega) = -\frac{M_0}{D_0} \delta D(\omega)$$

The central point of the self-consistent theory of localization [Götze W. (1979)] reduces to the replacement of Drude diffusion coefficient D_0 in the diffusion pole of (\$) by the generalized one $D(\omega)$.



$$M_E(\omega) = 2i\gamma \left\{ 1 + \frac{1}{\pi N(E)} \sum_{|\mathbf{k}| < k_0} \frac{i}{\omega + \frac{2E}{dm} \frac{k^2}{M_E(\omega)}} \right\}$$

or the equivalent equation for the generalized diffusion coefficient itself:

$$\frac{D_0}{D_E(\omega)} = 1 + \frac{1}{\pi N(E)} \sum_{|\mathbf{k}| < k_0} \frac{1}{-i\omega + D_E(\omega)k^2} \qquad k_0 \approx Min\{p_F, l^{-1}\}$$

$$\sigma(\omega) = \frac{ne^2}{m} \frac{i}{\omega + M_E(\omega)} \to e^2 D_E(\omega) N(E) \text{ for } \omega \to 0$$

$$\sigma = \frac{ne^2}{m} \frac{1}{2\gamma} \left\{ 1 - \left(\frac{E_c}{E}\right)^{\frac{4-d}{2}} \right\}; \qquad 2 < d < 4$$

$$E_{sc} = m^{\frac{d}{4-d}} (\Delta^2)^{\frac{2}{4-d}}$$

$$E_c = \left\{ \frac{d}{d-2} \frac{x_0^{d-2}}{\Gamma\left(\frac{d}{2}\right)} (2\pi)^{-\frac{d}{2}} \right\}^{\frac{2}{4-d}} E_{sc} \qquad \sigma \approx \frac{ne^2}{m} \frac{1}{2\gamma(E_c)} \left(\frac{4-d}{2}\right) \left(\frac{E-E_c}{E_c}\right) \sim \frac{E-E_c}{E_c}$$

A.V.Myasnikov, M.V.Sadovskii; D.Vollhardt, P.Woelfle 1982

Basic Models for Metal-Insulator Transition



DMFT

Anderson - Hubbard Model

Our aim is to consider non-magnetic disordered Anderson-Hubbard model (mainly) at half-filling for arbitrary interaction and disorder strengths. Mott-Hubbard and Anderson MITs will be investigated on an equal footing. The Hamiltonian of the model under study is written as:

is written as:

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

where t > 0 is the amplitude for hopping between nearest neighbors, U is the on-site repulsion, $n_{i\sigma} = a_{i\sigma}^{\dagger}a_{i\sigma}$ is the local electron number operator, $a_{i\sigma}$ $(a_{i\sigma}^{\dagger})$ is the annihilation (creation) operator of an electron with spin σ , and the local ionic energies ϵ_i at different lattice sites are considered to be independent random variables. To simplify diagrammatics in following we assume Gaussian probability distribution for ϵ_i :

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

Here the parameter Δ is just a measure of disorder strength, and Gaussian ("white" noise) random field of energy level ϵ_i at lattice cites produces "impurity" scattering, leading to the standard diagram technique for calculation on the averaged Green's functions¹⁹.

Basics of DMFT+ Σ

• **DMFT**+Σ:

M.V.Sadovskii, I.A.Nekrasov, E.Z.Kuchinskii, Th.Pruschke, V.I.Anisimov (2005)

$$G_{\mathbf{k}}(i\omega) = \frac{1}{i\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(i\omega) - \Sigma_{\mathbf{k}}(i\omega)}$$



DMFT+Σ calculation scheme



Σ for impurity scattering

Self-consistent Born approximation

$$\Sigma_{\mathbf{p}}(i\varepsilon) = \Delta^2 \sum_{\mathbf{p}} G(i\varepsilon, \mathbf{p}) \equiv \Sigma_{imp}(i\varepsilon)$$

$$\Sigma_{imp}^{R,A}(\varepsilon) = \Delta^2 \sum_{\mathbf{p}} G^{R,A}(\varepsilon, \mathbf{p}) = \operatorname{Re}\Sigma_{imp}(\varepsilon) \pm i\gamma(\varepsilon)$$

Semi - elliptic DOS:

$$\gamma(\varepsilon) = \pi \Delta^2 N(\varepsilon)$$

$$N(\varepsilon) = \frac{2}{\pi D^2} \sqrt{D^2 - \varepsilon^2} \qquad W = 2D \qquad \Longrightarrow \qquad W_{eff} = W \sqrt{1 + 16 \frac{\Delta^2}{W^2}}$$

Dynamic conductivity in DMFT+ Σ

E.Z.Kuchinskii, I.A.Nekrasov, M.V.Sadovskii (2006)

A. Basic expressions for optical conductivity

To calculate dynamic conductivity we use the general expression relating it to retarded density – density correlation function $\chi^{R}(\omega, \mathbf{q})^{17,18}$:

$$\sigma(\omega) = -\lim_{q \to 0} \frac{i e^2 \omega}{q^2} \chi^R(\omega, \mathbf{q})$$

where e is electronic charge.

Consider full polarization loop graph in Matsubara representation which is conveniently (with explicit frequency summation) written as:

$$\Phi(i\omega, \mathbf{q}) = \sum_{\varepsilon\varepsilon'} \Phi_{i\varepsilon i\varepsilon'}(i\omega, \mathbf{q}) \equiv \sum_{\varepsilon} \Phi_{i\varepsilon}(i\omega, \mathbf{q})$$

and contains all possible interactions of our model, described by the full vertex part

Retarded density–density correlation function is determined by appropriate analytic continuation of this loop and can be written as:

$$\chi^{R}(\omega,\mathbf{q}) = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i} \left\{ \left[f(\varepsilon_{+}) - f(\varepsilon_{-}) \right] \Phi_{\varepsilon}^{RA}(\mathbf{q},\omega) + f(\varepsilon_{-}) \Phi_{\varepsilon}^{RR}(\mathbf{q},\omega) - f(\varepsilon_{+}) \Phi_{\varepsilon}^{AA}(\mathbf{q},\omega) \right\}$$



Dynamic conductivity:

$$\begin{split} \sigma(\omega) &= \lim_{q \to 0} \left(-\frac{e^2 \omega}{2\pi q^2} \right) \int_{-\infty}^{\infty} d\varepsilon \left\{ \left[f(\varepsilon_+) - f(\varepsilon_-) \right] \left[\Phi_{\varepsilon}^{RA}(\mathbf{q},\omega) - \Phi_{\varepsilon}^{RA}(0,\omega) \right] + f(\varepsilon_-) \left[\Phi_{\varepsilon}^{RR}(\mathbf{q},\omega) - \Phi_{\varepsilon}^{RR}(0,\omega) \right] - f(\varepsilon_+) \left[\Phi_{\varepsilon}^{AA}(\mathbf{q},\omega) - \Phi_{\varepsilon}^{AA}(0,\omega) \right] \right\}. \end{split}$$



$$\phi(i\omega) \equiv \lim_{q \to 0} \frac{\Phi(i\omega, \mathbf{q}) - \Phi(i\omega, 0)}{q^2} = \sum_{\varepsilon} \gamma_{i\varepsilon}^2 (i\omega, \underline{q} = 0) \phi_{i\varepsilon}^0 (i\omega)$$

$$\phi^0_{i\varepsilon}(i\omega) \equiv \lim_{q \to 0} \frac{\Phi^0_{i\varepsilon}(i\omega,\mathbf{q}) - \Phi^0_{i\varepsilon}(i\omega,0)}{q^2}$$

Only impurity scattering here!

$$\gamma_{\varepsilon}(\omega \mathbf{q=0}) = \mathbf{1} + \mathbf{\Gamma} \mathbf{U} + \gamma_{i\varepsilon}(i\omega, \mathbf{q=0}) = \mathbf{1} + \sum_{\varepsilon'\varepsilon''} U_{i\varepsilon i\varepsilon''}(i\omega) \Phi_{i\varepsilon'' i\varepsilon'}(i\omega, \mathbf{q=0})$$



 $= 1 + \underbrace{\varepsilon'_{+}}_{\varepsilon'_{-}} \underbrace{\varepsilon''_{+}}_{\varepsilon''_{-}} \underbrace{\varepsilon''_{+}}_{\varepsilon''_{-}} \underbrace{\varepsilon''_{+}}_{\varepsilon'_{-}} \underbrace{\varepsilon''_{+}}_{\varepsilon''_{-}} \underbrace{\varepsilon''_{+}}_{\varepsilon'_{-}} \underbrace{\varepsilon''_{+}} \underbrace{\varepsilon''_{+}}_{\varepsilon'_{-}} \underbrace{\varepsilon''_{+}}_{\varepsilon'_{-}} \underbrace{\varepsilon''_{+}}_{\varepsilon'_{-}} \underbrace{\varepsilon''_{+}} \underbrace{\varepsilon'''$

Ward •

$$\gamma_{i\varepsilon}(i\omega, q=0) = 1 - \frac{\Delta\Sigma(i\omega)}{i\omega}$$

$$\Delta\Sigma(i\omega) = \Sigma(i\varepsilon + i\omega) - \Sigma(i\varepsilon)$$
$$\phi(i\omega) = \sum_{\varepsilon} \phi_{i\varepsilon}^{0}(i\omega) \left[1 - \frac{\Delta\Sigma(i\omega)}{i\omega}\right]^{2}$$

Dynamic Conductivity in DMFT+ Σ

E.Z. Kuchinskii, I. A. Nekrasov, M.V. Sadovskii (2006)

$$\begin{split} Re\sigma(\omega) &= \frac{e^2\omega}{2\pi} \int_{-\infty}^{\infty} d\varepsilon \left[f(\varepsilon_-) - f(\varepsilon_+) \right] Re \left\{ \phi_{\varepsilon}^{0RA}(\omega) \left[1 - \frac{\Sigma^R(\varepsilon_+) - \Sigma^A(\varepsilon_-)}{\omega} \right]^2 - \right. \\ &\left. - \phi_{\varepsilon}^{0RR}(\omega) \left[1 - \frac{\Sigma^R(\varepsilon_+) - \Sigma^R(\varepsilon_-)}{\omega} \right]^2 \right\} \end{split}$$

$$\begin{split} \phi_{\varepsilon}^{0RA}(\omega) &= \lim_{q \to 0} \frac{\Phi_{\varepsilon}^{0RA}(\omega, \mathbf{q}) - \Phi_{\varepsilon}^{0RA}(\omega, 0)}{q^2} \\ \phi_{\varepsilon}^{0RR}(\omega) &= \lim_{q \to 0} \frac{\Phi_{\varepsilon}^{0RR}(\omega, \mathbf{q}) - \Phi_{\varepsilon}^{0RR}(\omega, 0)}{q^2} \\ \Phi_{\varepsilon}^{0RA}(\omega, \mathbf{q}) &= \sum_{\mathbf{p}} G^R(\varepsilon_+, \mathbf{p}_+) G^A(\varepsilon_-, \mathbf{p}_-) \Gamma^{RA}(\varepsilon_-, \mathbf{p}_-; \varepsilon_+, \mathbf{p}_+) \\ \Phi_{\varepsilon}^{0RR}(\omega, \mathbf{q}) &= \sum_{\mathbf{p}} G^R(\varepsilon_+, \mathbf{p}_+) G^R(\varepsilon_-, \mathbf{p}_-) \Gamma^{RR}(\varepsilon_-, \mathbf{p}_-; \varepsilon_+, \mathbf{p}_+) \end{split}$$

 \mathbf{p}



Does not contain vertex corrections on the U

 $\Phi^{\text{RA}} \leftarrow$ the generalization of the self-consistent theory of localization

Self - consistent equations for diffusion coefficient

The most important block $\Phi_{\varepsilon}^{0RA}(\omega, \mathbf{q})$ can be calculated using the basic approach of self-consistent theory of localization with appropriate extensions, taking into account the role of the local Hubbard interaction using DMFT+ Σ approach. The only important difference with the standard approach is that equations of self-consistent theory are now

derived using

$$G^{R,A}(\varepsilon,\mathbf{p}) = \frac{1}{\varepsilon + \mu - \epsilon(\mathbf{p}) - \Sigma^{R,A}(\varepsilon) - \Sigma^{R,A}_{imp}(\varepsilon)}$$

containing DMFT contributions $\Sigma^{\overline{R},A}(\varepsilon)$, not only impurity scattering contained in:

$$\Sigma_{imp}^{R,A}(\varepsilon) = \Delta^2 \sum_{\mathbf{p}} G^{R,A}(\varepsilon, \mathbf{p}) = \operatorname{Re}\Sigma_{imp}(\varepsilon) \pm i\gamma(\varepsilon)$$

where $\gamma(\varepsilon) = \pi \Delta^2 N(\varepsilon)$ and $N(\varepsilon)$ is the density of states renormalized by Hubbard interaction, accounted via DMFT+ Σ .

Following all the usual steps of standard derivation we obtain diffusion like (singular at small ω and q) contribution to $\Phi_{\varepsilon}^{0RA}(\omega, \mathbf{q})$ as:

$$\Phi_{\varepsilon}^{0RA}(\mathbf{q},\tilde{\omega}) = \frac{2\pi i N(\varepsilon)}{\tilde{\omega} + i D(\omega)q^2}$$

where the important difference with the single-particle case is contained in

$$\tilde{\omega} = \varepsilon_{+} - \varepsilon_{-} - \Sigma^{R}(\varepsilon_{+}) + \Sigma^{A}(\varepsilon_{-}) = \omega - \Sigma^{R}(\varepsilon_{+}) + \Sigma^{A}(\varepsilon_{-}) \equiv \omega - \Delta\Sigma^{RA}(\omega)$$

$$\Delta\Sigma^{RA}(\omega = 0) = 2i\mathrm{Im}\Sigma(\varepsilon) \sim Max\{T^{2}, \varepsilon^{2}\},$$
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$$\operatorname{Re}\sigma(\omega) = \frac{e^2\omega}{2\pi} \int_{-\infty}^{\infty} d\varepsilon \left[f(\varepsilon_{-}) - f(\varepsilon_{+}) \right] \operatorname{Re}\left\{ \frac{i\sum_{\mathbf{p}} \Delta G_{\mathbf{p}} D(\omega)}{\omega^2} - \phi_{\varepsilon}^{0RR}(\omega) \left[1 - \frac{\Delta \Sigma^{RR}(\omega)}{\omega} \right]^2 \right\}$$

The second term here was taken in the "ladder" approximation:

$$\begin{split} \Phi_{\varepsilon}^{0RR}(\omega,\mathbf{q}) &= \frac{\sum_{\mathbf{p}} G^{R}(\varepsilon_{+},\mathbf{p}_{+})G^{R}(\varepsilon_{-},\mathbf{p}_{-})}{1 - \Delta^{2}\sum_{\mathbf{p}} G^{R}(\varepsilon_{+},\mathbf{p}_{+})G^{R}(\varepsilon_{-},\mathbf{p}_{-})}\\ D(\omega) &= \frac{\langle v \rangle^{2}}{d} \frac{i}{\tilde{\omega} + M(\omega)} \end{split}$$

$$M(\omega) = -\Delta \Sigma_{imp}^{RA}(\omega) + \Delta^4 \sum_{\mathbf{p}} (\Delta G_{\mathbf{p}})^2 \sum_{\mathbf{q}} \frac{1}{\tilde{\omega} + iD(\omega)q^2}$$

$$\langle v \rangle = \frac{\sum_{\mathbf{p}} |\mathbf{v}_{\mathbf{p}}| \Delta G_{\mathbf{p}}}{\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}}; \ \mathbf{v}_{\mathbf{p}} = \frac{\partial \epsilon(\mathbf{p})}{\partial \mathbf{p}} \qquad \qquad \Delta G_{\mathbf{p}} = G^{R}(\varepsilon_{+}, \mathbf{p}) - G^{A}(\varepsilon_{-}, \mathbf{p})$$

$$D(\omega) = i \frac{\langle v \rangle^2}{d} \left\{ \tilde{\omega} - \Delta \Sigma_{imp}^{RA}(\omega) + \Delta^4 \sum_{\mathbf{p}} (\Delta G_{\mathbf{p}})^2 \sum_{\mathbf{q}} \frac{1}{\tilde{\omega} + iD(\omega)q^2} \right\}^{-1}$$
$$q < k_0 = Min\{l^{-1}, p_F\}$$

Density of States

E.Z.Kuchinskii, I.A.Nekrasov, M.V.Sadovskii JETP **106**, 581 (2008); arXiv:0706.2618





The disorder restores the metallic phase

$$\frac{U_{c1,c2}(\Delta)}{W_{eff}} = \frac{U_{c1,c2}}{W}$$
$$W_{eff} = W\sqrt{1 + 16\frac{\Delta^2}{W^2}}$$

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DISORDER INFLUENCE ON SINGLE – PARTICLE PROPERTIES FOR THE CASE OF SEMI–ELLIPTIC DENSITY OF STATES

E.Z.Kuchinskii, N.A.Kuleeva, M.V.Sadovskii JETP **120**, 1055 (2015); arXiv:1411.1547

$$G_{ii} = \int_{-D}^{D} d\varepsilon' \frac{N_0(\varepsilon')}{\varepsilon + \mu - \varepsilon' - \Sigma(\varepsilon) - \Delta^2 G_{ii}} = \int_{-D}^{D} d\varepsilon' \frac{N_0(\varepsilon')}{E_t - \varepsilon'},\tag{8}$$

where we have introduced the notation $E_t = \varepsilon + \mu - \Sigma(\varepsilon) - \Delta^2 G_{ii}$. In the case of semi – elliptic \leftarrow usity of states (5) this integral is easily calculated in analytic form, so that the local Green's function is written as:

$$G_{ii} = 2 \frac{E_t - \sqrt{E_t^2 - D^2}}{D^2}.$$
(9)

It is easily seen that Eq. (9) represents one of the roots of quadratic equation:

$$G_{ii}^{-1} = E_t - \frac{D^2}{4} G_{ii},\tag{10}$$

corresponding to the correct limit of $G_{ii} \to E_t^{-1}$ for infinitely narrow $(D \to 0)$ band. Then

$$G_{ii}^{-1} = \varepsilon + \mu - \Sigma(\varepsilon) - \Delta^2 G_{ii} - \frac{D^2}{4} G_{ii} = \varepsilon + \mu - \Sigma(\varepsilon) - \frac{D_{eff}^2}{4} G_{ii}, \tag{11}$$

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:

$$D_{eff} = D\sqrt{1+4\frac{\Delta^2}{D^2}}.$$
(12)

Eq. (10) was obtained from (8), thus comparing (11) and (10), we obtain:

$$G_{ii} = \int_{-D_{eff}}^{D_{eff}} d\varepsilon' \frac{\tilde{N}_0(\varepsilon')}{\varepsilon + \mu - \varepsilon' - \Sigma(\varepsilon)}, \qquad (13)$$

Here

$$\tilde{N}_0(\varepsilon) = \frac{2}{\pi D_{eff}^2} \sqrt{D_{eff}^2 - \varepsilon^2}$$
(14)

single-particle properties is universal for all U and are reduced to the replacement $D \rightarrow D_{eff}$

disorder influence on all

Universality of DOS dependence on disorder



Conductivity and Metal-Insulator Transition



Phase Diagram (T=0)



As a rule of thumb Gaussian value of Δ_c should be multiplied by $\sqrt{12}$ to obtain the critical disorder value for rectangular distribution. This gives $\Delta_c \approx 1.28$ in rather good agreement with $\Delta_c(U=0) \approx 1.35W$ value of K. Byczuk, W. Hofstetter, D. Vollhardt.

Disorder-induced Mott Insulator to Metal Transition



Phase Diagram d=2

E.Z.Kuchinskii, N.A.Kuleeva, I.A.Nekrasov, M.V.Sadovskii JETP **110**, 325 (2010); arXiv:0908.3747





Infinite two-dimensional systems are localized for arbitrarily weak disorder, however R_{loc} is exponentially large for small Δ . In finite systems, the Anderson transition occurs - localization length R_{loc} diverges ! at some critical disorder $\Delta_c(L)$. Qualitative criterion of Anderson transition: $R_{loc}(L \rightarrow \infty) \sim L$



Dashed stripe – region of the effective Anderson transition between Δ_c (L = 10⁵a) and Δ_c (L = 10⁸a)

$$U_c^*(\Delta) = U_c(0) \frac{W_{eff}(\Delta)}{W} = U_c(0) \left(\frac{2\Delta^2}{W^2} ln\left(\frac{c+1}{c-1}\right) + c\right)$$
$$c = \sqrt{4\left(\frac{\Delta}{W}\right)^2 + 1}.$$

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN Vol. 12, No. 6, JUNE, 1957

Statistical-Mechanical Theory of Irreversible Processes. I. General Theory and Simple Applications to Magnetic and Conduction Problems

By Ryogo Kubo

General sum rule for optical conductivity !

Thus we have proved the sum rule

$$\frac{2}{\pi} \int_0^\infty \operatorname{Re} \, \sigma^s{}_{\mu\nu}(\omega) d\omega = \sum_r \frac{e^2{}_r n_r}{m_r} \,\delta_{\mu\nu} \tag{8.8}$$

$$\lim_{\omega \to \infty} \omega \operatorname{Im} \sigma^{s}{}_{\mu\nu} = -\sum_{r} \frac{e^{2}{}_{r} n_{r}}{m_{r}} \delta_{\mu\nu} \qquad (8.9)$$

which hold for any system irrespective of the interaction of particles, the temperature, the statistics and even in the presence of magnetic field. This is the most general form of the sum rule.

For a system of electrons, Eqs. (8.8) and (8.9) are written as

$$\frac{2}{\pi} \int_{0}^{\infty} \operatorname{Re} \, \sigma^{s}{}_{\mu\nu}(\omega) d\omega = \frac{ne^{2}}{m} \delta_{\mu\nu} \qquad (8.10)$$
$$\operatorname{Im} \, \sigma^{s}{}_{\mu\nu}(\omega) \to -\frac{e^{2}n}{m\omega} \delta_{\mu\nu} \quad (\omega \to \infty) \; . \qquad (8.11)$$

Here we should remember that m is the true mass of electrons. The integration of $\sigma(\omega)$ has to be carried over all range of frequencies.

One band sum rule:

If one considers electrons in a crystal and confines himself to the electrons in a particular band neglecting interband transitions, the sum rule has to be modified to

$$\begin{split} & \frac{2}{\pi} \int_{0}^{\infty} \operatorname{Re} \, \sigma^{s}{}_{\mu\nu}(\omega) \, d\omega \\ &= -\lim_{\omega \to \infty} \omega \, \operatorname{Im} \, \sigma^{s}{}_{\mu\nu}(\omega) \\ &= e^{2} \, \operatorname{Tr} \left\{ \rho \cdot \partial^{2} E(p) / \partial p_{\nu} \partial p_{\mu} \right\} \,. \end{split} \tag{8.12}$$

This holds if the electron system is described by the Hamiltonian

$$\mathscr{H} = \sum_{i} E(p_i) + V(r_1, \cdots r_N) \qquad (8.13)$$

where E(p) is the energy of an electron with the crystal moments p. Also one has to omit the interband elements of the potential V.



E.Z.Kuchinskii, N.A.Kuleeva, I.A.Nekrasov, M.V.Sadovskii JETP **107**, 281 (2008); arXiv:0803.3869

$$\int_{-\infty}^{\infty} d\omega Re\sigma_{xx}(\omega) = \pi e^2 \sum_{\mathbf{p},\sigma} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n(\varepsilon_p)$$
$$n(\varepsilon_p) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) Im G^R(\varepsilon, \mathbf{p})$$

This should be valid in any reasonable model of optical conductivity!

Dependence of the r.h.s. on temperature and any other parameter is sometimes called "sum rule violation".

Check of the general optical sum rule:

$$\int_{-\infty}^{\infty} d\omega Re\sigma_{xx}(\omega) = \pi e^2 \sum_{\mathbf{p},\sigma} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n(\varepsilon_p)$$



$\Delta/2D$	$\int_{-\infty}^{\infty}d\omega Re\sigma_{xx}(\omega)$	$\pi e^2 \sum_{\mathbf{p},\sigma} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n(\varepsilon_p)$
0	0,063	0,064
0,25	0,068	0.07
0,37	0,06	0.061
0,43	0,056	0.056
0,50	0,049	0.05

Sum rule "violation":





Superconductivity of disordered systems

Weak coupling (BCS), weak disorder (p_Fl>>1)

The theory of "dirty" superconductors A.A. Abrikosov, L.P. Gor'kov. JETP **35**, **36**, **39** (1958-1960)

Anderson's theorem on Tc P.W. Anderson J. Phys. Chem. Solids **11** (1959)

Weak coupling (BCS), strong disorder (p_Fl~1)

Superconductivity near the Anderson transition L.N.Bulaevskii, M.V. Sadovskii. JETP Letters **39** (1984); J.Low.Temp.Phys. **59** (1985) Qualitative change in the coefficient C before the gradient term of the GL expansion and the temperature behavior of Hc2

Strong coupling (crossover BCS -BEC) weak disorder(p_F l>>1); strong disorder (p_F l~1) ?

BCS-BEC crossover

A. J. Leggett (Springer, Berlin 1980),

P. Nozieres and S. Schmitt-Rink, J. Low Temp. Phys. 59, 195 (1985)

Weak coupling – (BCS)

Very strong coupling (BEC)

- loose Cooper pairs ($\xi >>a$)
- Cooper pairs are formed in the condensate (q=0)
- $\circ T_{\rm c} \sim \Delta(0)$

 compact pairs (ξ<a)
 pairs are formed at T*~ Δ(0)>>T_c (q≠0)
 T_c ← BEC

Attractive Hubbard Model (DMFT)

Attractive Hubbard Model with Disorder

We consider the disordered nonmagnetic Anderson – Hubbard model with attraction described by the Hamiltonian:

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

where t > 0 is transfer integral between nearest neighbors, U is the Hubbard attraction on the lattice site, $n_{i\sigma} = a_{i\sigma}^{\dagger}a_{i\sigma}$ – number of electrons operator on the site, $a_{i\sigma}$ ($a_{i\sigma}^{\dagger}$) – annihilation (creation) operator for an electron with spin σ , and local energies ϵ_i are assumed to be independent random variables on different lattice sites. For the validity of the standard "impurity" diagram technique [33, 34] we assume the Gaussian distribution for energy levels ϵ_i :

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

Distribution width Δ serves as a measure of disorder and the Gaussian random field of energy levels (independent on different lattice sites – "white noise" correlations) induces the "impurity" scattering, which is considered within the standard approach, based on calculations of the averaged Green's functions [34].

Density of States $(T>T_c; \Delta=0)$

N.A.Kuleeva, E.Z.Kuchinskii, M.V.Sadovskii JETP 119, 264 (2014); arXiv:1401.2295



Spectral Density (T>Tc; Δ =0) $A(\varepsilon, \mathbf{p}) = -\frac{1}{\pi} Im G^{R}(\varepsilon, \mathbf{p})$





Disorder Effects: DOS and Dynamic Conductivity T>T_c

N.A.Kuleeva, E.Z.Kuchinskii, M.V.Sadovskii JETP **119**, 264 (2014); arXiv:1401.2295

Anderson transition at Δ =0.37 (T=0)

 $U_c(\Delta)/2D_{eff} = U_c(0)/2D$

Critical Temperature T_c ($\Delta=0$)

N.A.Kuleeva, E.Z.Kuchinskii, M.V.Sadovskii JETP 119, 264 (2014); arXiv:1401.2295



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 $T_c \sim t^2/|U|$ for $|U| >> t \sim D$

DISORDER INFLUENCE ON SUPERCONDUCTING TRANSITION

In general, Nozieres – Schmitt-Rink approach 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 here the weak coupling (ladder) approximation. In such approximation the condition of Cooper instability in disordered Hubbard model takes the form:

$$1 = U\chi_0(q = 0, \omega_m = 0) \tag{15}$$

where

$$\chi_0(q=0,\omega_m=0) = T \sum_n \sum_{\mathbf{pp}'} \Phi_{\mathbf{pp}'}(\varepsilon_n)$$
(16)

represents the two – particle loop (susceptibility) in Cooper channel "dressed" only by disorder scattering, and $\Phi_{\mathbf{pp}'}(\varepsilon_n)$ is the averaged two – particle Green's function in Cooper channel ($\omega_m = 2\pi mT$ and $\varepsilon_n = \pi T(2n+1)$ are the usual Boson and Fermion Matsubara frequencies).

To obtain $\sum_{\mathbf{pp}'} \Phi_{\mathbf{pp}'}(\varepsilon_n)$ we use the exact Ward identity

$$G(\varepsilon_n, \mathbf{p}) - G(-\varepsilon_n, -\mathbf{p}) = -\sum_{\mathbf{p}'} \Phi_{\mathbf{p}\mathbf{p}'}(\varepsilon_n) (G_0^{-1}(\varepsilon_n, \mathbf{p}') - G_0^{-1}(-\varepsilon_n, -\mathbf{p}')), \quad (17)$$

Here $G(\varepsilon_n, \mathbf{p})$ is the impurity averaged (but not containing Hubbard interaction corrections!) single – particle Green's function. Using the obvious symmetry $\varepsilon(\mathbf{p}) = \varepsilon(-\mathbf{p})$ and $G(\varepsilon_n, -\mathbf{p}) = G(\varepsilon_n, \mathbf{p})$, we obtain from the Ward identity (17):

$$\sum_{\mathbf{p}\mathbf{p}'} \Phi_{\mathbf{p}\mathbf{p}'}(\varepsilon_n) = -\frac{\sum_{\mathbf{p}} G(\varepsilon_n, \mathbf{p}) - \sum_{\mathbf{p}} G(-\varepsilon_n, \mathbf{p})}{2i\varepsilon_n},$$
(18)

so that for Cooper susceptibility (16) we have:

$$\chi_0(q=0,\omega_m=0) = -T\sum_n \frac{\sum_{\mathbf{p}} G(\varepsilon_n, \mathbf{p}) - \sum_{\mathbf{p}} G(-\varepsilon_n, \mathbf{p})}{2i\varepsilon_n} = -T\sum_n \frac{\sum_{\mathbf{p}} G(\varepsilon_n, \mathbf{p})}{i\varepsilon_n}.$$
 (19)

Performing now the standard summation over Matsubara frequencies we obtain:

$$\chi_0(q=0,\omega_m=0) = -\frac{1}{4\pi i} \int_{-\infty}^{\infty} d\varepsilon \frac{\sum_{\mathbf{p}} G^R(\varepsilon,\mathbf{p}) - \sum_{\mathbf{p}} G^A(\varepsilon,\mathbf{p})}{\varepsilon} th \frac{\varepsilon}{2T} = \int_{-\infty}^{\infty} d\varepsilon \frac{\tilde{N}(\varepsilon)}{2\varepsilon} th \frac{\varepsilon}{2T},$$
(20)

where $\tilde{N}(\varepsilon)$ is the density of states (U = 0) "dressed" by disorder scattering. In Eq. (20) the energy ε is reckoned from the chemical potential and if we reckon it from the center of conduction band we have to replace $\varepsilon \to \varepsilon - \mu$, so that the condition of Cooper instability (15) leads to the following equation for T_c :

$$1 = \frac{U}{2} \int_{-\infty}^{\infty} d\varepsilon \tilde{N}_0(\varepsilon) \frac{th \frac{\varepsilon - \mu}{2T_c}}{\varepsilon - \mu},\tag{21}$$

where $\tilde{N}_0(\varepsilon)$ is again the density of states (calculated for U = 0) "dressed" by disorder scattering. At the same time, the chemical potential of the system at different values of Uand Δ 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 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.

T_c and the Generalized Anderson Theorem

E.Z.Kuchinskii, N.A.Kuleeva, M.V.Sadovskii JETP Lett. 100, No.3, 213 (2014); arXiv:1406.5603



-DOS in the absence of interaction U "dressed" by disorder



Coefficient A

$$A(T) = \chi_0(q = 0, T) - \chi_0(q = 0, T_c)$$

where

$$\chi_0(q=0,T) = -T\sum_n \sum_{\mathbf{pp'}} \Phi_{\mathbf{pp'}}(\varepsilon_n)$$

is the two – particle loop in Cooper channel "dressed" only by disorder scattering

Ward identity
$$\longrightarrow \qquad \chi_0(q=0,T) = -\int_{-\infty}^{\infty} d\varepsilon \frac{\tilde{N}(\varepsilon)}{2(\varepsilon-\mu)} th \frac{\varepsilon-\mu}{2T}$$

Cooper instability of the normal phase, determining superconducting transition temperature

$$1 = -U\chi_0(q=0,T_c)$$

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

For $T \to T_c$ coefficient A(T) takes the usual form: $A(T) \equiv \alpha(T - T_c)$

In BCS weak coupling limit we obtain the standard expressions $\alpha_{BCS} = \frac{\tilde{N}_0(\mu)}{T_c}$

Coefficient B

Coefficients A,B and specific heat discontinuity

E.Z.Kuchinskii, N.A.Kuleeva, M.V.Sadovskii JETP 122, No.2, 375 (2016); arXiv:1507.07649



Coefficient C

 $C = -T \lim_{q \to 0} \sum_{n, \mathbf{p}, \mathbf{p}'} \frac{\Psi_{\mathbf{p}\mathbf{p}'}(\varepsilon_n, \mathbf{q}) - \Psi_{\mathbf{p}\mathbf{p}'}(\varepsilon_n, 0)}{q^2}$



$$\begin{split} & \underset{\text{susceptibility:}}{\text{Cooper susceptibility:}} & \chi(\mathbf{q}) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\varepsilon Im \Phi^{RA}(\omega = 2\varepsilon, \mathbf{q}) th \frac{\varepsilon}{2T} \\ & \bullet \partial^{-2\pi i N(0)} \\ & \Phi^{RA}(\omega = 2\varepsilon, \mathbf{q}) = -\underbrace{\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}(\varepsilon)}_{\omega + i D(\omega) q^2} & \varepsilon \rightarrow 0 \\ & \text{rge } \Delta G_{\mathbf{p}}(\varepsilon) = G^{R}(\varepsilon, \mathbf{p}) - G^{A}(-\varepsilon, \mathbf{p}) \end{split}$$

$$\begin{split} C &= \lim_{q \to 0} \frac{\chi(\mathbf{q}) - \chi(\mathbf{q} = 0)}{q^2} = -\frac{1}{8\pi} \int_{-\infty}^{\infty} d\varepsilon \frac{th\frac{\varepsilon}{2T}}{\varepsilon} Im\left(\frac{iD(2\varepsilon)\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}(\varepsilon)}{\varepsilon + i\delta}\right) = \\ &= -\frac{1}{8\pi} \int_{-\infty}^{\infty} d\varepsilon \frac{th\frac{\varepsilon}{2T}}{\varepsilon^2} Re(D(2\varepsilon)\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}(\varepsilon)) - \frac{1}{16T} Im(D(0)\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}(0)) \end{split}$$

Coefficient C

E.Z.Kuchinskii, N.A.Kuleeva, M.V.Sadovskii JETP **125**, 111 (2017); arXiv:1702.05247





Physical properties



the **slope of the upper critical filed** close to T_c :

$$H_{c2} = \frac{\Phi_0}{2\pi\xi^2(T)} = -\frac{\Phi_0}{2\pi}\frac{A}{C}$$
$$\left|\frac{dH_{c2}}{dT}\right| = \frac{\Phi_0}{2\pi}\frac{\alpha}{C}$$

Coherence length

E.Z.Kuchinskii, N.A.Kuleeva, M.V.Sadovskii JETP **125**, 111 (2017); arXiv:1702.05247

unfilled symbols and dashed curves – ladder approximation



BCS limit: $\xi \sim l^{1/2}$



Penetration depth and Ginzburg - Landau parameter κ=λ/ξ

E.Z.Kuchinskii, N.A.Kuleeva, M.V.Sadovskii JETP **125**, 111 (2017); arXiv:1702.05247



BCS limit: $\lambda \sim l^{-1/2}$, $\kappa \sim l^{-1}$





Slope of the upper critical field

E.Z.Kuchinskii, N.A.Kuleeva, M.V.Sadovskii JETP **125**, 111 (2017); arXiv:1702.05247



BCS limit: $dH_{c2} \sim 1/\sigma$





Relations for H_{c2}

condition for Cooper instability

$$1 = -U\chi(\mathbf{q}) \longrightarrow 1 = -U\chi(q^2 = q_0^2)$$

 $\mathbf{q} \to \mathbf{q} - \frac{2e}{c}\mathbf{A}$

As we assume isotropic electron spectrum, Cooper susceptibility $\chi(\mathbf{q})$ depends on \mathbf{q} only via q^2 . The minimal eigenvalue of $(\mathbf{\hat{q}} - \frac{2e}{c}\mathbf{A})^2$, determining (orbital)¹ upper critical magnetic field $H = H_{c2}$ is given by [30]

$$\begin{split} q_0{}^2 &= 2\pi \frac{H}{\Phi_0}, \end{split} \text{ where } \Phi_0 = \frac{ch}{2e} = \frac{\pi\hbar}{e} \text{ is magnetic flux quantum.} \\ \text{Cooper susceptibility:} \\ \chi(q_0{}^2) &= -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\varepsilon Im \Phi^{RA}(\omega = 2\varepsilon, q_0{}^2) th \frac{\varepsilon}{2T} \\ \Phi^{RA}(\omega = 2\varepsilon, q_0{}^2) &= -\frac{\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}(\varepsilon)}{\omega + iD(\omega)q_0{}^2}, \qquad \text{rge } \Delta G_{\mathbf{p}}(\varepsilon) \\ \Phi^{RA}(\omega = 2\varepsilon, q_0{}^2) &= -\frac{\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}(\varepsilon)}{\omega + iD(\omega)q_0{}^2}, \qquad \text{rge } \Delta G_{\mathbf{p}}(\varepsilon) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) = \Phi_{\mathbf{p},\mathbf{p}'}(\omega_m = 2\varepsilon_n, \mathbf{q}) \\ \Phi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) &= \Phi_{\mathbf{p},\mathbf{p}'}(\omega_m = 2\varepsilon_n, \mathbf{q}) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) &= \Phi_{\mathbf{p},\mathbf{p}'}(\omega_m = 2\varepsilon_n, \mathbf{q}) \\ \Phi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) &= \Phi_{\mathbf{p},\mathbf{p}'}(\omega_m = 2\varepsilon_n, \mathbf{q}) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) &= \Phi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) &= \Phi_{\mathbf{p},\mathbf{p}'}(\omega_m = 2\varepsilon_n, \mathbf{q}) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) &= \Phi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) &= \Phi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q}) \\ \Psi_{\mathbf{p},\mathbf{p}'}(\varepsilon_n, \mathbf{q})$$

$$1 = -\frac{U}{2\pi} \int_{-\infty}^{\infty} d\varepsilon Im \left(\frac{\sum_{\mathbf{p}} \Delta G_{\mathbf{p}}(\varepsilon)}{2\varepsilon + iD(2\varepsilon)2\pi \frac{H_{c2}}{\Phi_0}} \right) th \frac{\varepsilon}{2T}$$

orbital



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a - lattice parameter





$H_{c2}(T)$ disorder influence

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0,06 2та²H_{c2}/Ф₀ Weak coupling, 0,04 **BCS** limit 0.0 0,00

Intermediate coupling, BCS - BEC crossover region

BEC limit

unfilled symbols and dashed curves – ladder approximation







Приведен результат численного расчета непосредственно из уравнения (9) в отсутствие влияния поля на диффузию для величины $h = \omega_H / T_c^{2g} E^{1g}$ от T/T_c в металлической фазе при различных значениях ω_c / T_c : 1. 100; 2. 10; 3. 2π ; 4. 3; 5. 1; 6. О — точка андерсоновского перехода.

На вставке:

Низкотемпературная часть зависимости $h = \omega_H / T_c^{2/3} E^{1/3}$ от T/T_c в окрестности Андерсоновского перехода.

(1) Точка Андерсоновского перехода ($\omega_e/T_e = 0$). С учетом влияния поля на диффузию.

Металлическая фаза, ω_c/T_c = 0,1. В отсутствие влияния поля на диффузию.

3. Точка Андерсоновского перехода ($\omega_c/T_c = 0$). В отсутствие влияния поля на диффузию.

Диэлектрическая фаза, ω_c / T_c = 0,1. В отсутствие влияния поля на диффузию.

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Thank you very much!

Doped Mott insulator (T=0)



No Mott-Hubbard Insulator! Correlated Metal and Anderson Insulator!

Universality of DOS dependence on disorder:



Dependence of the density of states on disorder in the model with semi – elliptic band.



Universal dependence of the density of states on disorder: (a) — the model of semi – elliptic "bare" density of states; (b) — the model of flat "bare" density of states.

T_c and the Generalized Anderson Theorem



FIG. 3: Dependence of superconducting transition temperature on disorder for different values of Hubbard attraction U: (a) — semi – elliptic band; (b) — flat band.



FIG. 4: Universal dependence of superconducting critical temperature on Hubbard attraction U for different disorder levels: (a) — semi – elliptic[tic band. Dashed curve represent BCS dependence in the absence of disorder. (b) — flat band. Dashed line represents similar dependence for semi – elliptic band for $\Delta = 0$.

Disorder Effects: Local Pairs Number



 $n=<n_{\uparrow}>=0.25$ $<n_{\uparrow}n_{\downarrow}> \rightarrow n^2$ при U/2D<<1 $<n_{\uparrow}n_{\downarrow}> \rightarrow n$ при U/2D>>1

Chemical potential



$$\frac{1}{U_B} = \int_{-D}^D d\xi \frac{N_0(\xi)}{2\xi + D}$$

 $U_B/2D = 1$

 $\Delta \neq 0 \qquad D \to D_{eff}$