Towards mean-field theory of the Anderson metal-insulator transition, part II

Parquet scheme and the asymptotic limit to high spatial dimensions

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1. Outline of the talk

- ▷ noninteracting electrons on an impure lattice at $T = 0\,$K (no phonons)

$$\hat{H} = t \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i \,, \qquad V_i \text{ random, site independent}$$

- ▷ self-consistent equations for two-particle vertices (parquet scheme)
  - ▷ systematics of 2P diagrams
  - ▷ time-reversal symmetry

- ▷ asymptotic limit to high spatial dimensions
  - ▷ leading order of $1/d$-expansion $\longrightarrow$ CPA $+$ weak localization
  - ▷ addition of $O(1/d)$ terms $+$ self-consistency

- ▷ return to finite dimensions $\longrightarrow$ mean-field
  - ▷ weak disorder $\sim$ diffusion
  - ▷ strong disorder $\sim$ localization
  - ▷ ?? Ward identities, particle number conservation ??

2. Diffusion

Relaxation of density inhomogeneities

$$\frac{\delta n(t,\mathbf{q})}{\delta n(0,\mathbf{q})} \sim \phi(t,\mathbf{q}) \sim \Phi^{AR}(t,\mathbf{q})$$

Relaxation function (electron-hole correlation function)

$$\Phi^{AR}(\omega,\mathbf{q}) = \frac{1}{N^2}\sum_{\mathbf{kk}'} G^{(2)}_{\mathbf{kk}'}(E_F - i0, E_F + \omega + i0; \mathbf{q})$$

Slow variations in space and time, $\mathbf{q} \to \mathbf{0}$ and $\omega \to 0$

$$\Phi^{AR}(\omega,\mathbf{q}) \approx \frac{2\pi g_F}{-i\omega + Dq^2}$$

Averaging over disorder configurations $\Rightarrow$ electron-electron correlations

$$\langle\mathcal{G}\mathcal{G}\rangle \neq \langle\mathcal{G}\rangle\langle\mathcal{G}\rangle \longrightarrow G^{(2)} = GG + GG\Gamma GG$$

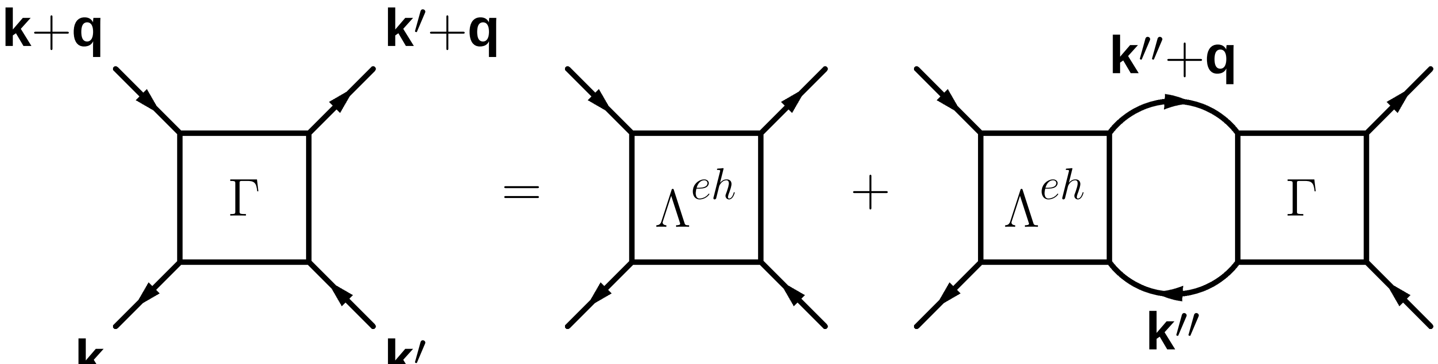
3. Bethe-Salpeter equations

2P irreducibility not uniquely defined — 3 *topologically nonequivalent* scattering channels:

electron-hole

$f^{eh}_{BS}(\Gamma, \Lambda^{eh}) = 0$

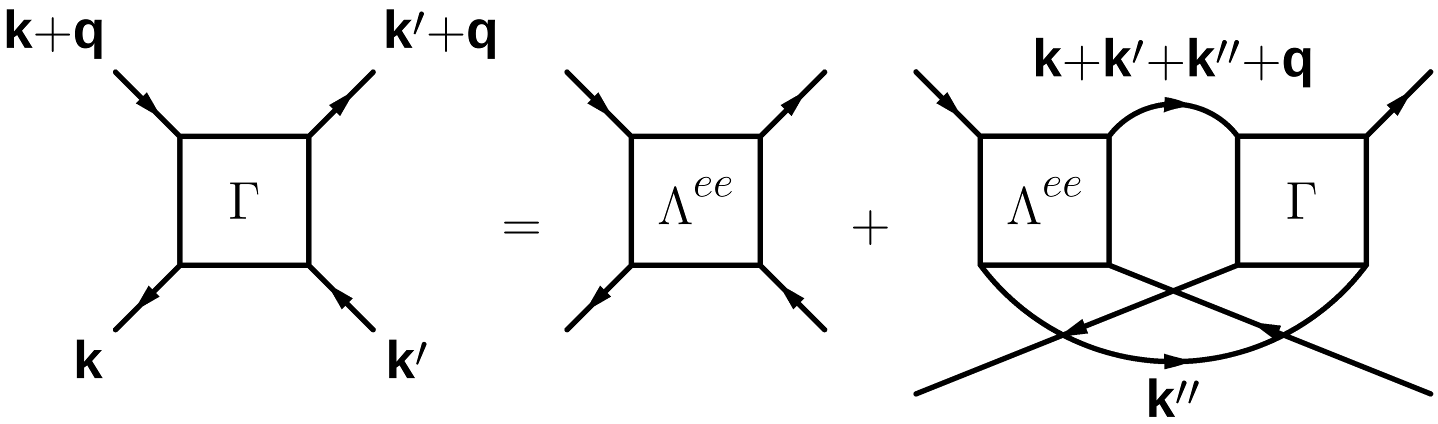
(quasi)classical terms



electron-electron

$f^{ee}_{BS}(\Gamma, \Lambda^{ee}) = 0$

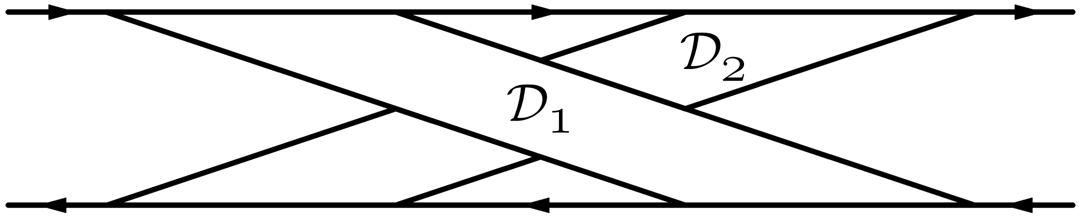
coherent backscattering



The last one, so-called *vertical channel*, is irrelevant.

4. Parquet equation

ee-reducible diagram



cannot result from eh-multiplication

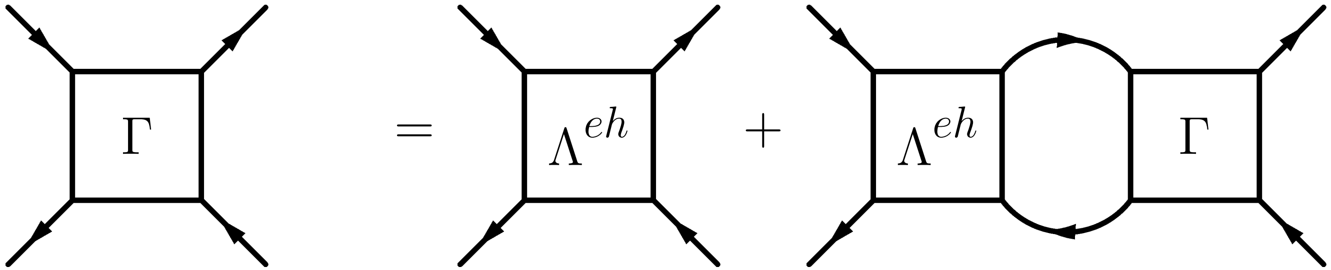
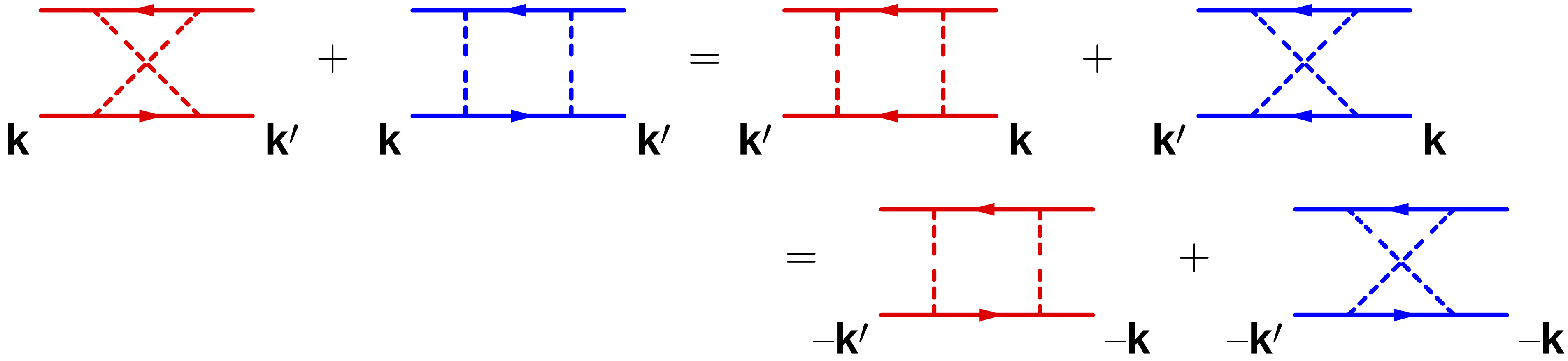


Diagram reducible in one channel is irreducible in other scattering channels.

$$I \overset{\text{def.}}{=} \Lambda^{eh} \cap \Lambda^{ee}, \qquad \left.\begin{array}{l} \Gamma - \Lambda^{ee} \subset \Lambda^{eh} \\ \Gamma - \Lambda^{ee} \supset \Lambda^{eh} - I \end{array}\right\} \quad \boxed{\Lambda^{eh} - I = \Gamma - \Lambda^{ee}}$$

5. Invariance w. r. t. time reversal

Electron states $|\mathbf{k}\rangle$ and $|-\mathbf{k}\rangle$ are equivalent. $\longleftrightarrow$ $G(z,\mathbf{k}) = G(z,-\mathbf{k})$



Time-reversal transformation $\mathcal{T}$ (electron-hole symmetry)

$$(\mathcal{T}F)_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) \stackrel{\text{def.}}{=} F_{-\mathbf{k}',-\mathbf{k}}(\mathbf{q}+\mathbf{k}+\mathbf{k}')$$

$$(\mathcal{T}\Gamma)_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) = \Gamma_{-\mathbf{k}',-\mathbf{k}}(\mathbf{q}+\mathbf{k}+\mathbf{k}') = \Gamma_{\mathbf{k},\mathbf{k}'}(\mathbf{q})$$

$$(\mathcal{T}\Lambda^{ee})_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) = \Lambda^{ee}_{-\mathbf{k}',-\mathbf{k}}(\mathbf{q}+\mathbf{k}+\mathbf{k}') = \Lambda^{eh}_{\mathbf{k},\mathbf{k}'}(\mathbf{q})$$

$$(\mathcal{T}\Lambda^{eh})_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) = \Lambda^{eh}_{-\mathbf{k}',-\mathbf{k}}(\mathbf{q}+\mathbf{k}+\mathbf{k}') = \Lambda^{ee}_{\mathbf{k},\mathbf{k}'}(\mathbf{q})$$

6. Parquet scheme

Selfconsistent equations for (irreducible) two-particle vertices

Input: completely irreducible vertex I

General system

$$f^{eh}_{BS}(\Gamma, \Lambda^{eh}) = 0$$

$$f^{ee}_{BS}(\Gamma, \Lambda^{ee}) = 0$$

$$\Lambda^{ee} + \Lambda^{eh} - I = \Gamma$$

$\longrightarrow$

Time-reversal invariant case

$$f^{eh}_{BS}(\Gamma, \Lambda^{eh}) = 0$$

$$\Lambda^{eh} = \mathcal{T}\Lambda^{ee}$$

$$\Lambda^{ee} + \Lambda^{eh} - I = \Gamma$$

How to find selfenergy?

No diagrammatic representation, *Ward identity + Kramers-Kronig relation*

$$\Im\Sigma_{\mathbf{k}}(z_1) = \frac{1}{N}\sum_{\mathbf{k}''} \Lambda^{eh}_{\mathbf{k}\mathbf{k}''}(z_1, \bar{z}_1; \mathbf{0})\, \Im G_{\mathbf{k}''}(z_1)$$

$$\Re\Sigma_{\mathbf{k}}(E - i0) = \Sigma_{\mathbf{k}}(\infty) + P\int_{-\infty}^{\infty} \frac{dE'}{\pi}\, \frac{\Im\Sigma_{\mathbf{k}}(E' - i0)}{E' - E}$$

7. Limit to high spatial dimensions

Single equation to be solved: $f^{eh}_{BS}(\underbrace{\Lambda^{ee} + \mathcal{T}\Lambda^{ee} - I}_{\Gamma}, \underbrace{\mathcal{T}\Lambda^{ee}}_{\Lambda^{eh}}) = 0$

$$\Lambda^{ee}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = I_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) + \frac{1}{N}\sum_{\mathbf{k}''} \Lambda^{ee}_{-\mathbf{k}'',-\mathbf{k}}(\mathbf{q}+\mathbf{k}+\mathbf{k}'')\, G(z_1,\mathbf{k}''+\mathbf{q})G(z_2,\mathbf{k}'')$$
$$\times \left[\Lambda^{ee}_{-\mathbf{k}',-\mathbf{k}''}(\mathbf{q}+\mathbf{k}'+\mathbf{k}'') + \Lambda^{ee}_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}) - I_{\mathbf{k}''\mathbf{k}'}(\mathbf{q})\right]$$

Reduction of momentum dependencies — limit to high spatial dimensions

$$\hat{H}_d = \frac{t}{\sqrt{d}}\sum_{\langle ij\rangle} \hat{c}^\dagger_i \hat{c}_j + \sum_i V_i \hat{c}^\dagger_i \hat{c}_i$$

Off-diagonal elements loose their weight with increasing d

$$G_{ii} \longleftrightarrow G(z) = \frac{1}{N}\sum_{\mathbf{k}} G(z,\mathbf{k}) \sim 1\,, \qquad \underset{i\neq j}{G_{ij}} \longleftrightarrow \bar{G}(z,\mathbf{k}) = G(z,\mathbf{k}) - G(z) \sim \frac{1}{\sqrt{d}}$$

Different treatment of diagonal and off-diagonal elements. $\longrightarrow$

- ▷ *all* local diagrams $\mathcal{D}[G_{ii}]$ inserted into I
- ▷ off-diagonal contributions included via parquet scheme
- ▷ $\Gamma,\ G,\ \Lambda^{eh},\ \Lambda^{ee},\ I \longrightarrow \Gamma,\ \bar{G},\ \bar{\Lambda}^{eh},\ \bar{\Lambda}^{ee},\ \bar{I} = \gamma$

8. Convolutions in the asymptotic limit $d \to \infty$

Elementary convolutions (“contractions”), $W_{ij} = t^2 \langle G^2(z_i) \rangle \langle G^2(z_j) \rangle$

$$\frac{1}{N} \sum_{\mathbf{k}} \bar{G}_1(\mathbf{k} + \mathbf{q}_1) \bar{G}_2(\mathbf{k} + \mathbf{q}_2) = \bar{G}_1(\mathbf{q}_1) \bar{G}_2(\mathbf{q}_2) \overset{\text{def.}}{=} \bar{\chi}_{12}(\mathbf{q}_1 - \mathbf{q}_2)$$

$$\frac{1}{N} \sum_{\mathbf{k}} \bar{G}_1(\mathbf{k} + \mathbf{q}_1) \bar{\chi}_{23}(\mathbf{k} + \mathbf{q}_2) = \bar{G}_1(\mathbf{q}_1) \bar{\chi}_{23}(\mathbf{q}_2) \doteq \frac{W_{23}}{4d} \bar{G}_1(\mathbf{q}_1 - \mathbf{q}_2)$$

$$\frac{1}{N} \sum_{\mathbf{k}} \bar{\chi}_{12}(\mathbf{k} + \mathbf{q}_1) \bar{\chi}_{34}(\mathbf{k} + \mathbf{q}_2) = \bar{\chi}_{12}(\mathbf{q}_1) \bar{\chi}_{34}(\mathbf{q}_2) \doteq \frac{W_{12}}{4d} \bar{\chi}_{34}(\mathbf{q}_1 - \mathbf{q}_2)$$

“Wick theorem” (Gaussian random variables)

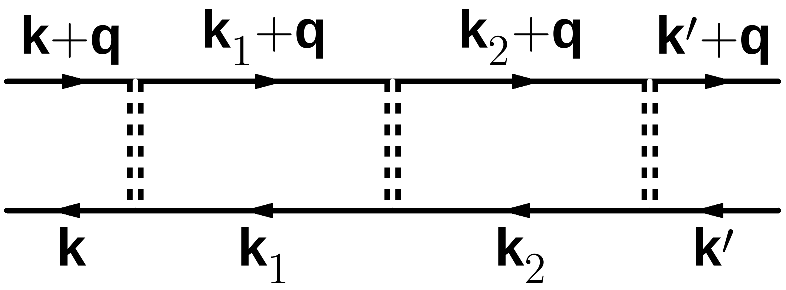
$$\frac{1}{N} \sum_{\mathbf{k}} \bar{G}_1(\mathbf{k} + \mathbf{q}_1) \bar{G}_2(\mathbf{k} + \mathbf{q}_2) \bar{G}_3(\mathbf{k} + \mathbf{q}_3) \bar{G}_4(\mathbf{k} + \mathbf{q}_4)$$

$$\doteq \bar{G}_1(\mathbf{q}_1) \bar{G}_2(\mathbf{q}_2) \bar{G}_3(\mathbf{q}_3) \bar{G}_4(\mathbf{q}_4) + \bar{G}_1(\mathbf{q}_1) \bar{G}_2(\mathbf{q}_2) \bar{G}_3(\mathbf{q}_3) \bar{G}_4(\mathbf{q}_4)$$

$$+ \bar{G}_1(\mathbf{q}_1) \bar{G}_2(\mathbf{q}_2) \bar{G}_3(\mathbf{q}_3) \bar{G}_4(\mathbf{q}_4)$$

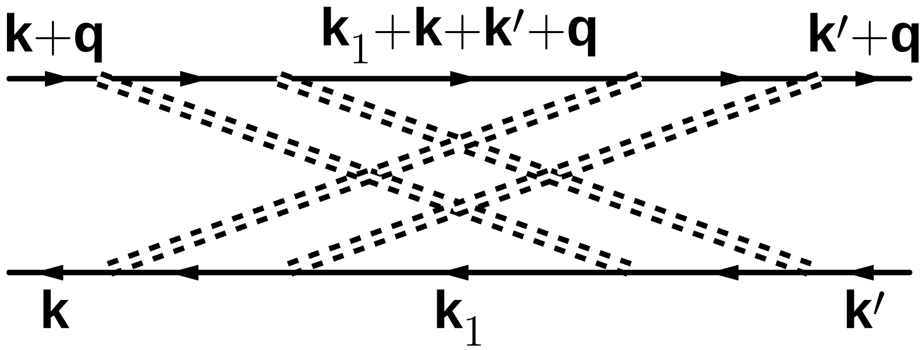
9. 2P vertices in strict $d = \infty$ (no parquet eq.)

Ladder diagrams



$$= \gamma^3 \bar{\chi}^2(\mathbf{q})$$

Channel mixing (ee-multiplication of two eh-ladders, $\bar{\chi}\,\bar{G}\bar{G}\,\bar{\chi}$)



$$= \frac{\gamma^4 W^2}{4d}\left[\bar{\chi}(\mathbf{k}')\bar{\chi}(\mathbf{k}'+\mathbf{q}) + \bar{\chi}(\mathbf{k})\bar{\chi}(\mathbf{k}+\mathbf{q}) + \bar{\chi}(\mathbf{k}-\mathbf{k}')\bar{\chi}(\mathbf{k}+\mathbf{k}'+\mathbf{q})\right]$$

Channel crossing costs a factor $1/d \quad \Rightarrow \quad$ only ladders survive to $d = \infty$.

$$\Gamma^{(\infty)}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \underbrace{\frac{\gamma}{1-\gamma\,\bar{\chi}(\mathbf{q})}}_{\bar{\Lambda}^{ee}} + \underbrace{\frac{\gamma}{1-\gamma\,\bar{\chi}(\mathbf{k}+\mathbf{k}'+\mathbf{q})}}_{\bar{\Lambda}^{eh}} - \gamma$$

CPA & WL

10. 2P vertices in the asymptotics $d \to \infty$

$1/d$ perturbation expansion (adding 1, 2, $\ldots$ channel crossings) — no new quality, we seek *non-linear* equations for 2P vertices

"ansatz" similar to strict $d = \infty$ case (other diagrams do not renormalize the poles)

$$\bar{\Lambda}^{ee}_{\mathbf{kk}'}(\mathbf{q}) = \sum_{n=0}^{\infty} \Lambda_n \, \bar{\chi}^n(\mathbf{q}) \qquad \longrightarrow \qquad f^{eh}_{BS}(\Lambda^{ee} + \mathcal{T}\Lambda^{ee} - I, \mathcal{T}\Lambda^{ee}) = 0$$

$$\Downarrow$$

$$\bar{\Lambda}^{ee}_{\mathbf{kk}'}(\mathbf{q}) = \gamma + \bar{\gamma}\,\frac{\bar{\gamma}\,\bar{\chi}(\mathbf{q})}{1 - \bar{\gamma}\,\bar{\chi}(\mathbf{q})} \qquad \text{where} \qquad \bar{\gamma} = \gamma + \bar{\gamma}\frac{1}{N}\sum_{\mathbf{q}} \frac{\bar{\gamma}^2\,\bar{\chi}^2(\mathbf{q})}{1 - \bar{\gamma}\,\bar{\chi}(\mathbf{q})}$$

Selfenergy:

- ▷ no Λ^{eh} to generate our $\Gamma = \bar{\Lambda}^{eh} + \bar{\Lambda}^{ee} - \gamma$ from Bethe-Salpeter equation $\Rightarrow$ no Vollhardt-Wölfle identity
- ▷ diffusion pole needed to match the weak scattering limit

$$1 - \bar{\gamma}\,\bar{\chi}(\mathbf{0})\big|_{\omega=0} = 0 \qquad \Leftrightarrow \qquad \Im\Sigma^A(E) = \left.\frac{\bar{\gamma}}{1 + \bar{\gamma}\,G^A(E)G^R(E)}\right|_{\omega=0} \Im G^A(E)$$

11. Mean-field approximation

First step: Gaussian $\bar{\chi}$ from $d \to \infty$ $\longrightarrow$ realistic $\bar{\chi}$ from d dimensions

Second step: pole suppression

- ▷ the higher the dimension the better (in $d = 1$ and $d = 2$ the pole is crucial)

$$\bar{\gamma} = \gamma + \bar{\gamma}\frac{1}{N}\sum_{\mathbf{q}} \frac{\bar{\gamma}^2\,\bar{\chi}^2(\mathbf{q})}{1 - \bar{\gamma}\,\bar{\chi}(\mathbf{q})} \qquad \longrightarrow \qquad \bar{\gamma} = \gamma + \frac{W^2}{8d}\bar{\gamma}^3 = \gamma + C_d W^2 \bar{\gamma}^3$$

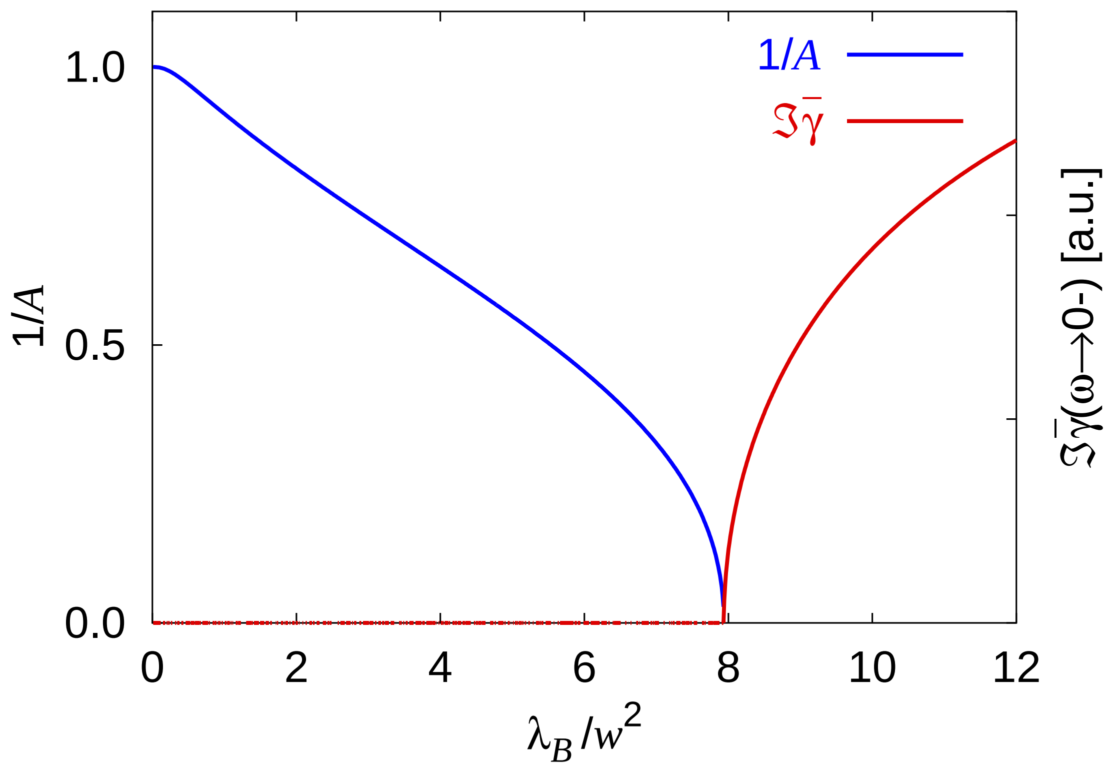
- ▷ $\Im\bar{\gamma}$ behaves as Landau-like order parameter, $\Im\bar{\gamma} > 0$ — no diffusion pole

Model calculation based on Born approximation (not CPA)

$1/A$ . . . diffusion pole weight

λ_B . . . Born irreducible vertex

w . . . half band-width



12. Diffusion pole

Ward identity holds only for $\omega = 0$

$$\Sigma^A(E) - \Sigma^R(E+\omega) \neq \frac{\bar{\gamma}(\omega)}{1 + \bar{\gamma}(\omega)\, G^A(E) G^R(E+\omega)} \left[G^A(E) - G^R(E+\omega) \right]$$

$\Rightarrow$ *weighted pole* in the correlation function

$$\Phi^{AR}(\omega, \mathbf{q}) = \frac{2\pi g_F / A}{-i\omega + Dq^2} \quad \longleftrightarrow$$

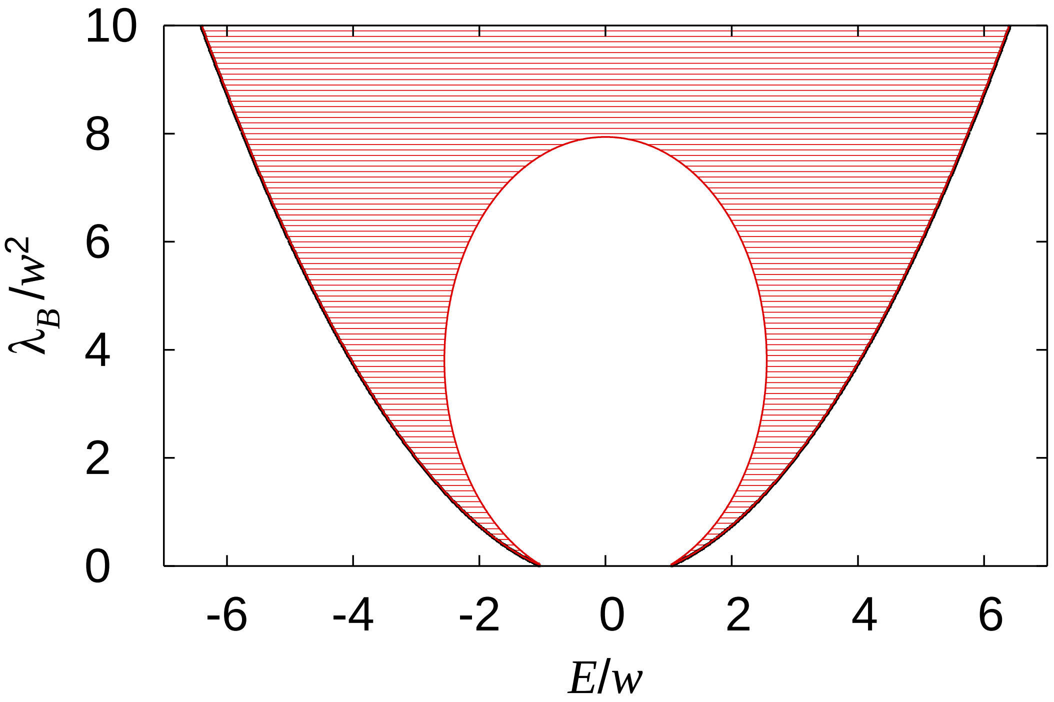
Only g_F/A states are diffusive, others do not contribute to diffusion.

Phase diagram (localized states hatched)

E . . . position in the band

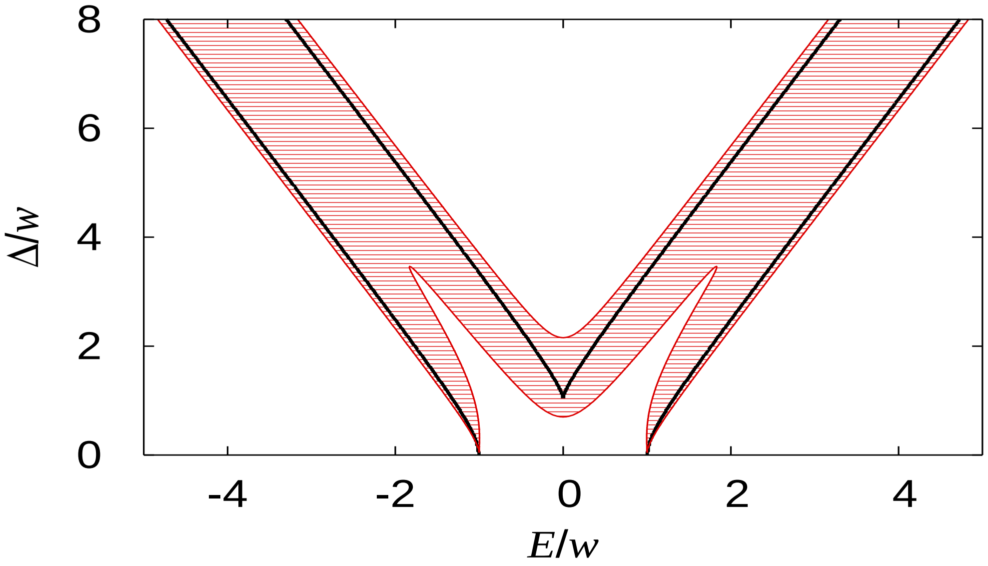
λ_B . . . Born irreducible vertex

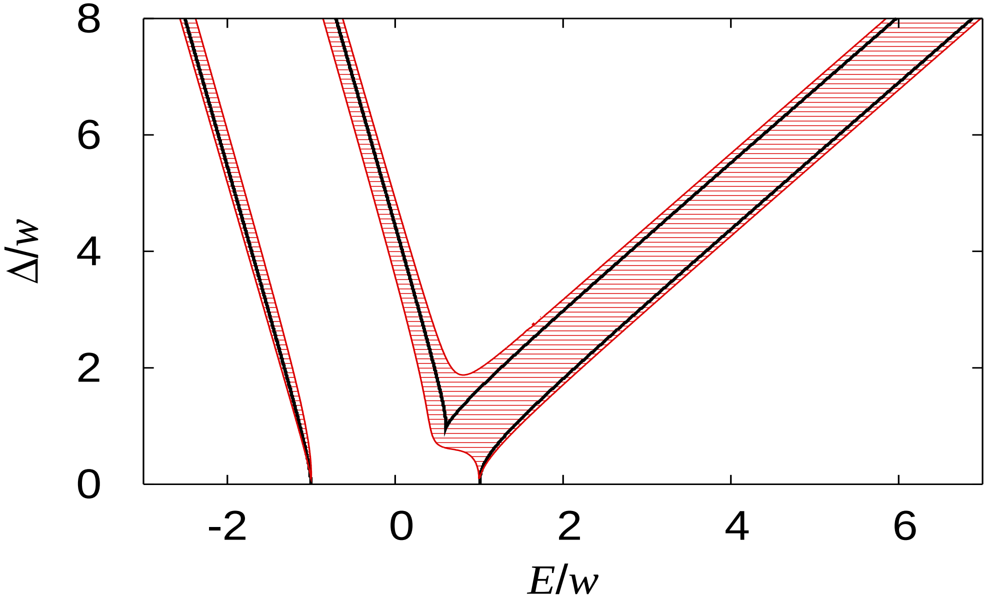
w . . . half band-width



13. (A)symmetric binary alloy

Localization tendencies most pronounced at the *band edges* . . .





. . . and in the *impurity band*.

14. Ward identity vs. analyticity

The weight $1/A < 1$ *is not* an artifact of our approximations
$\longleftrightarrow$ Ward identities cannot be fulfilled in principle.

Ward identity: $$\Sigma_{\mathbf{k}}(z_1) - \Sigma_{\mathbf{k}}(z_2) = \frac{1}{N}\sum_{\mathbf{k}''} \Lambda^{eh}_{\mathbf{k}\mathbf{k}''}(z_1, z_2; \mathbf{0})\,[G_{\mathbf{k}''}(z_1) - G_{\mathbf{k}''}(z_2)]$$

- left-hand side — analytic (selfenergy)
- right-hand side — diffusion/Cooper pole in Λ^{eh}

Diffusive regime

$$\Lambda^{eh} \sim \frac{1}{-i\omega + D(\mathbf{k}+\mathbf{k}'+\mathbf{q})^2} \quad \to \quad \left\langle \frac{\partial \Sigma^R}{\partial E} \right\rangle \sim \lim_{\omega\to 0} |\omega|^{d/2-2} \begin{cases} 1\,, & d \neq 4l \\ \ln \frac{Dk_F^2}{|\omega|}\,, & d = 4l \end{cases}$$

Localized regime ($D(\omega) = -i\omega\xi^2$, Vollhardt & Wölfle)

$$\Lambda^{eh} \sim \frac{1}{-i\omega}\frac{1}{1+\xi^2(\mathbf{k}+\mathbf{k}'+\mathbf{q})^2} \quad \to \quad \Im\Sigma(E) \sim \lim_{\omega\to 0} \frac{1}{\omega}$$

15. Conclusions

What we did?

- ▷ formulated parquet scheme for the use in high spatial dimensions
- ▷ solved these equations in the asymptotic limit $d \to \infty$
- ▷ applied this solution as a mean-field approximation

What such an approximation indicates?

- ▷ disorder-driven metal-insulator transition
- ▷ inability to comply with particle number conservation

How to understand the surprising inconsistency?

- ▷ formulation using configurationally averaged (translationally invariant) Green functions does not fully cover the physical Hilbert space
- ▷ extended and localized eigenstates co-exist in the diffusive phase