

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

Parquet scheme and the asymptotic limit to high spatial dimensions

Jindřich Kolorenč and Václav Janiš

1. Outline of the talk

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

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

- ▷ 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)

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

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

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

Averaging over disorder configurations \Rightarrow electron-electron correlations

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

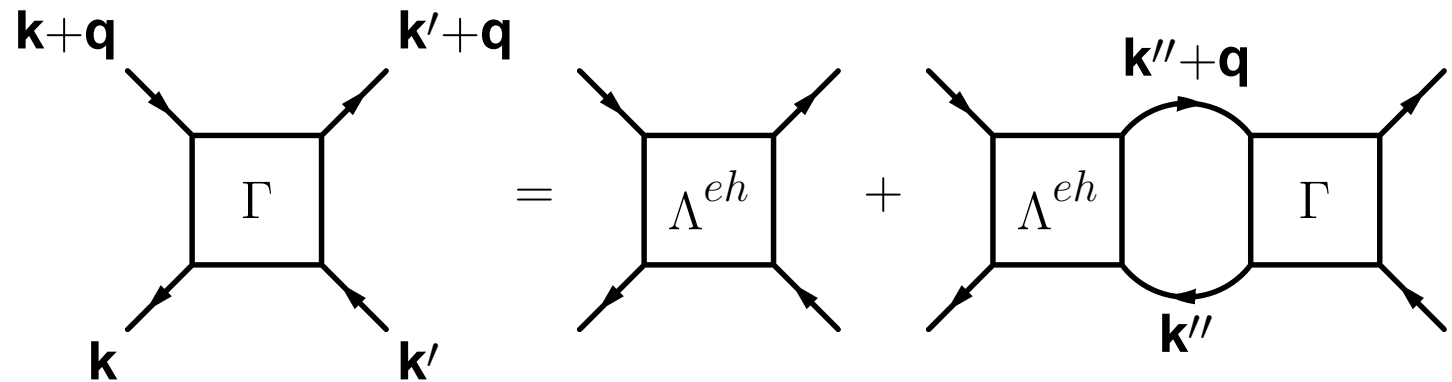
3. Bethe-Salpeter equations

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

electron-hole

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

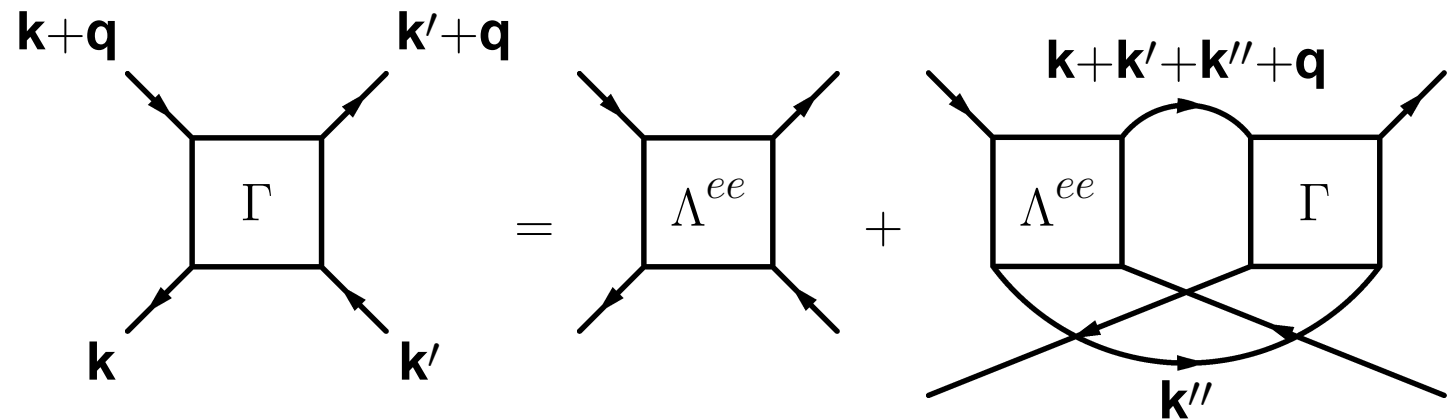
(quasi)classical
terms



electron-electron

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

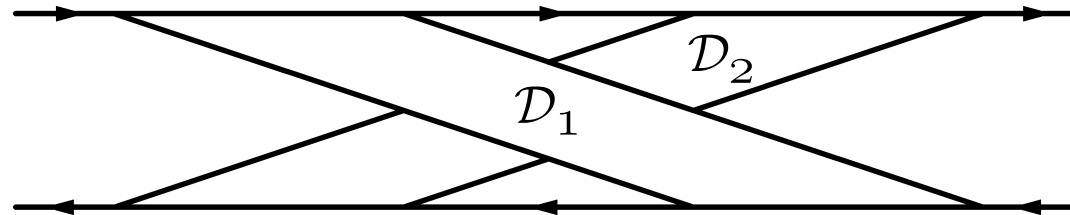
coherent
backscattering



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

4. Parquet equation

ee-reducible diagram



cannot result from *eh*-multiplication

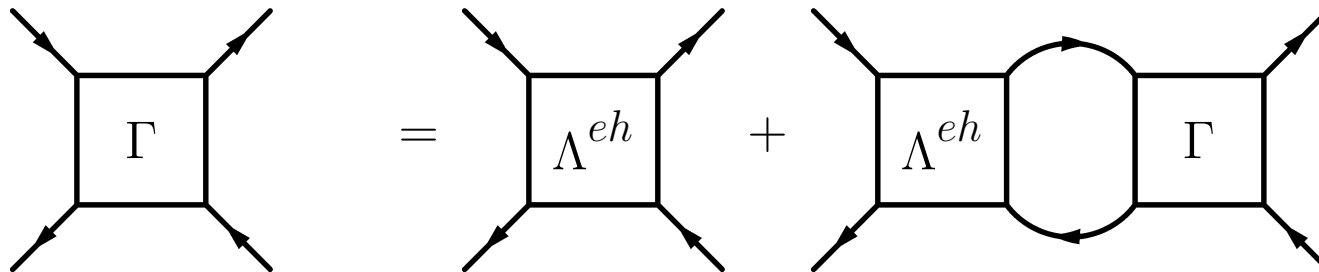


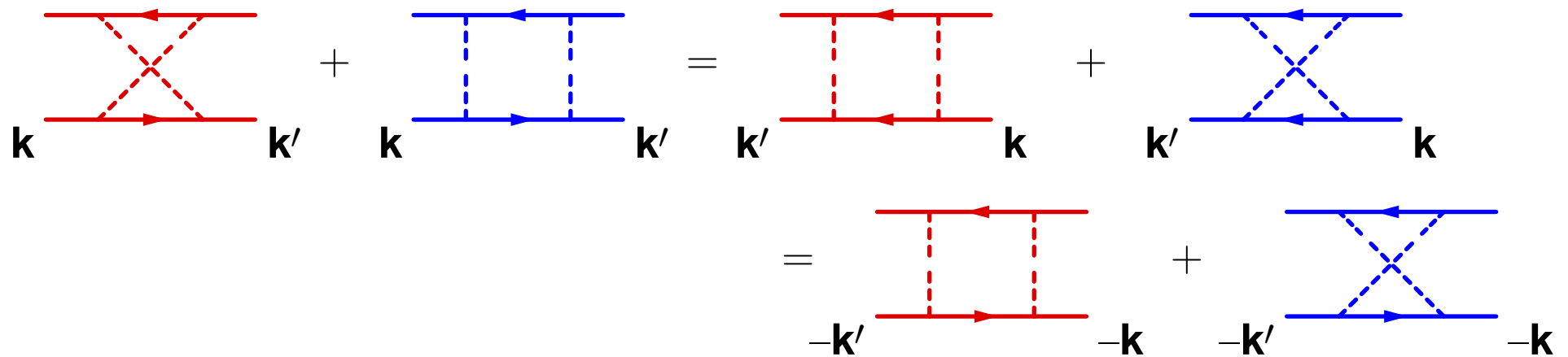
Diagram reducible in one channel is irreducible in other scattering channels.

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

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)

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

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

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

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

6. Parquet scheme

Selfconsistent equations for (irreducible) two-particle vertices

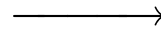
Input: completely irreducible vertex I

General system

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

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

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



Time-reversal invariant case

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

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

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

How to find selfenergy?

No diagrammatic representation, Ward identity + Kramers-Kronig relation

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

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

7. Limit to high spatial dimensions

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

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

Reduction of momentum dependencies — limit to high spatial dimensions

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

Off-diagonal elements loose their weight with increasing d

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

Different treatment of diagonal and off-diagonal elements.

→

- ▷ 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 $d \rightarrow \infty$

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

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

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

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

“Wick theorem” (Gaussian random variables)

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

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, $\bar{\chi} \bar{G} \bar{G} \bar{\chi}$)

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

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

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

CPA & WL

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

$1/d$ perturbation expansion (adding 1, 2, ... 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)

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

\Downarrow

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

- 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

$$1 - \bar{\gamma} \bar{\chi}(\mathbf{0})|_{\omega=0} = 0 \quad \Leftrightarrow \quad \Im \Sigma^A(E) = \frac{\bar{\gamma}}{1 + \bar{\gamma} G^A(E) G^R(E)} \Big|_{\omega=0} \Im G^A(E)$$

11. Mean-field approximation

First step: Gaussian $\bar{\chi}$ from $d \rightarrow \infty$ \rightarrow 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)

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

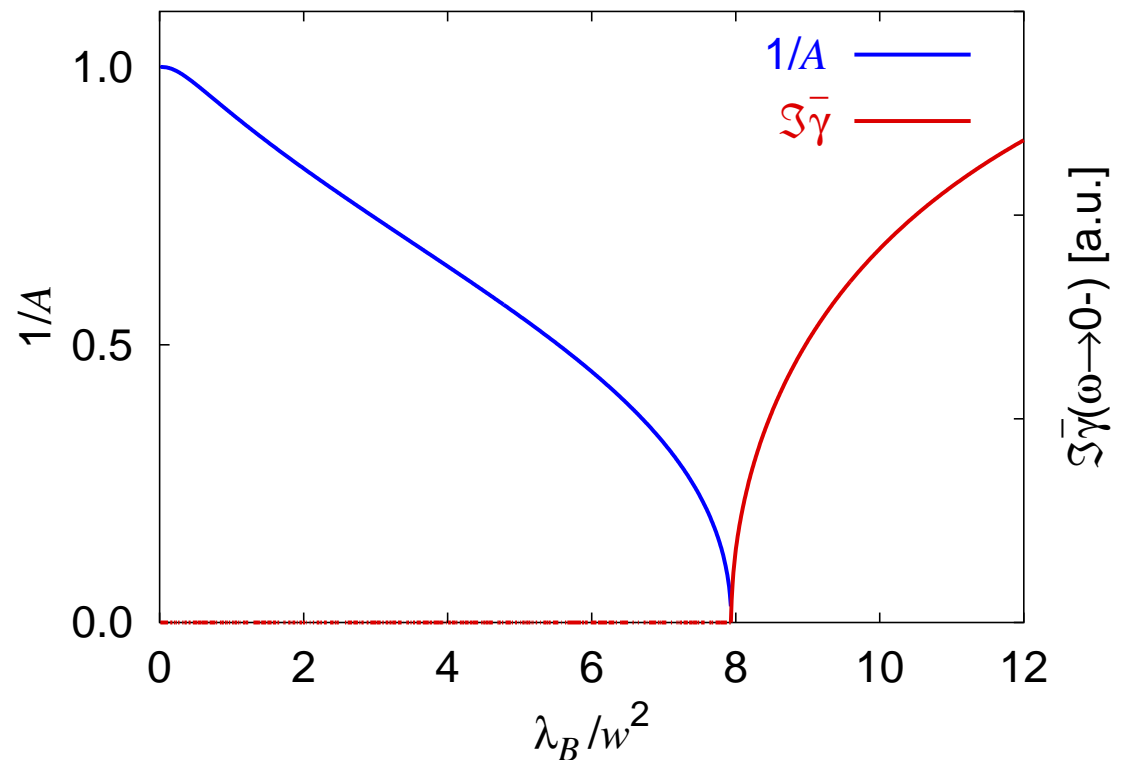
- ▷ $\Im \bar{\gamma}$ behaves as Landau-like order parameter, $\Im \bar{\gamma} > 0$ — no diffusion pole

**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

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

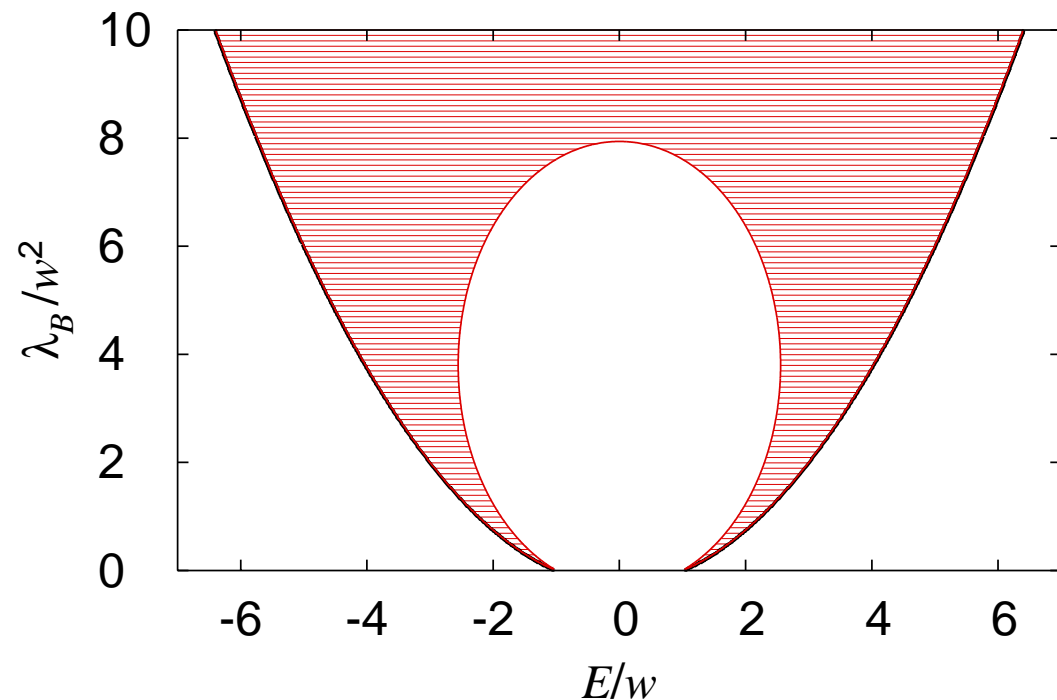
Only g_F/A states are diffusive, others do not contribute to diffusion.

Phase diagram (localized states hatched)

E ... position in the band

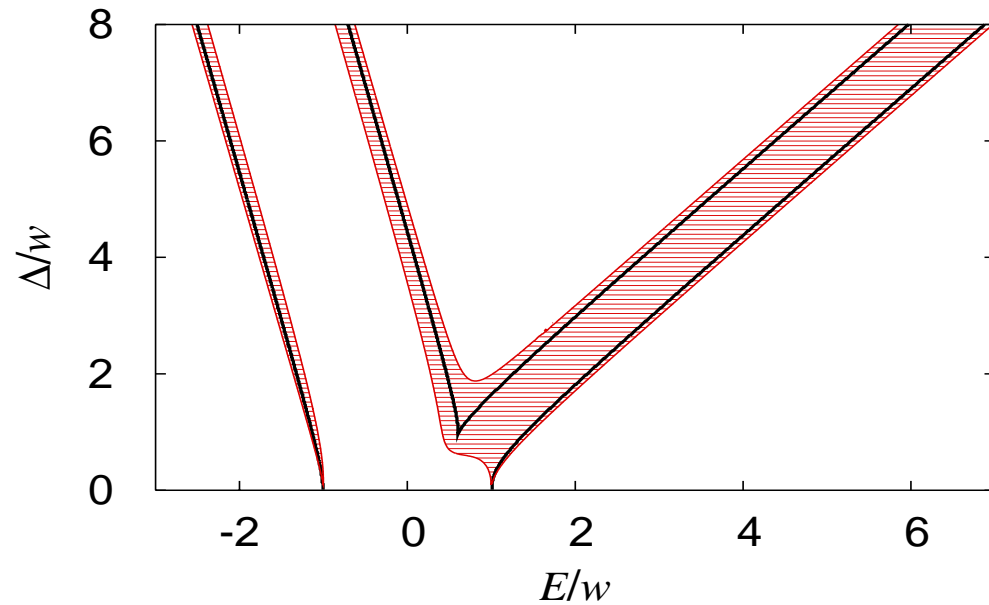
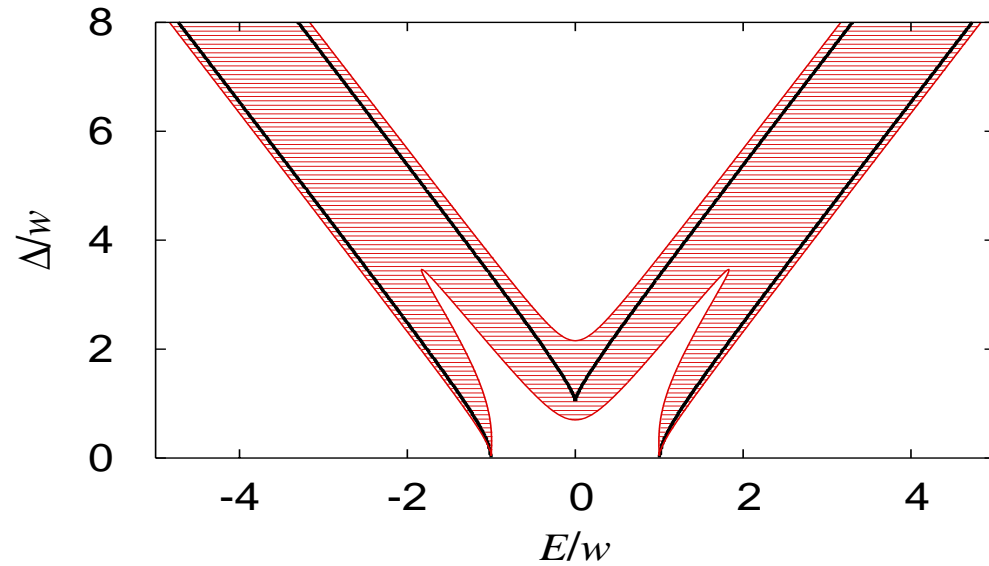
λ_B ... Born irreducible vertex

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
↔ Ward identities cannot be fulfilled in principle.

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

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

Diffusive regime

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

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

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

15. Conclusions

What we did?

- ▷ formulated parquet scheme for the use in high spatial dimensions
- ▷ solved these equations in the asymptotic limit $d \rightarrow \infty$
- ▷ 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

