Towards mean-field theory of the Anderson metal-insulator transition, part II
Parquet scheme and the asymptotic limit to high spatial dimensions

Jindřich Kolorenc and Václav Janiš
1. Outline of the talk

- noninteracting electrons on an impure lattice at $T = 0\, \text{K}$ (no phonons)
  \[
  \hat{H} = t \sum_{\langle i,j \rangle} \hat{c}^\dagger_i \hat{c}_j + \sum_i V_i \hat{c}^\dagger_i \hat{c}_i, \quad V_i \text{ random, site independent}
  \]

- 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)

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

Slow variations in space and time, \( \mathbf{q} \to 0 \) 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

\[
\langle \mathcal{G} \mathcal{G} \rangle \neq \langle \mathcal{G} \rangle \langle \mathcal{G} \rangle \quad \rightarrow \quad G^{(2)} = GG + GG \Gamma GG
\]
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**

\[ \begin{array}{c}
\text{cannot result from } eh\text{-multiplication}
\end{array} \]

\[ \Gamma = \Lambda^{eh} + \Lambda^{eh} \]

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

\[ I \overset{\text{def.}}{=} \Lambda^{eh} \cap \Lambda^{ee}, \quad \Gamma - \Lambda^{ee} \subseteq \Lambda^{eh} \]

\[
\left\{ \begin{array}{l}
\Lambda^{eh} - I = \Gamma - \Lambda^{ee}
\end{array} \right. \]
5. Invariance w. r. t. time reversal

Electron states $|k\rangle$ and $|-k\rangle$ are equivalent.  

\[ G(z, k) = G(z, -k) \]

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

\[ (\mathcal{T} F)_{k,k'}(q) \overset{\text{def.}}{=} F_{-k',-k}(q + k + k') \]

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

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

\[ (\mathcal{T} \Lambda^{eh})_{k,k'}(q) = \Lambda^{eh}_{-k',-k}(q + k + k') = \Lambda^{ee}_{k,k'}(q) \]
6. Parquet scheme

Selfconsistent equations for (irreducible) two-particle vertices

*Input: completely irreducible vertex $I$*

**General system**

\[
\begin{align*}
    f^{eh}_{BS}(\Gamma, \Lambda^{eh}) &= 0 \\
    f^{ee}_{BS}(\Gamma, \Lambda^{ee}) &= 0 \\
    \Lambda^{ee} + \Lambda^{eh} - I &= \Gamma
\end{align*}
\]

**Time-reversal invariant case**

\[
\begin{align*}
    f^{eh}_{BS}(\Gamma, \Lambda^{eh}) &= 0 \\
    \Lambda^{eh} &= T \Lambda^{ee} \\
    \Lambda^{ee} + \Lambda^{eh} - I &= \Gamma
\end{align*}
\]

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How to find selfenergy?

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

\[
\begin{align*}
    \Im \Sigma_k(z_1) &= \frac{1}{N} \sum_{k''} \Lambda^{eh}_{kk''}(z_1, \bar{z}_1; 0) \Im G_{k''}(z_1) \\
    \Re \Sigma_k(E - i0) &= \Sigma_k(\infty) + P \int_{-\infty}^{\infty} \frac{dE'}{\pi} \frac{\Im \Sigma_k(E' - i0)}{E' - E}
\end{align*}
\]
7. Limit to high spatial dimensions

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

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

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 \( d \)

\[
G_{ii} \longleftrightarrow G(z) = \frac{1}{N} \sum_k G(z, k) \sim 1, \quad G_{ij} \leftrightarrow \tilde{G}(z, k) = G(z, k) - G(z) \sim \frac{1}{\sqrt{d}}
\]

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
- \( \Gamma, G, \Lambda^{eh}, \Lambda^{ee}, I \longrightarrow \Gamma, \tilde{G}, \Lambda^{eh}, \Lambda^{ee}, \bar{I} = \gamma \)
8. Convolutions in the asymptotic limit $d \to \infty$

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

$$
\frac{1}{N} \sum_k \bar{G}_1(k + q_1) \bar{G}_2(k + q_2) = \bar{G}_1(q_1) \bar{G}_2(q_2) \overset{\text{def.}}{=} \bar{\chi}_{12}(q_1 - q_2)
$$

$$
\frac{1}{N} \sum_k \bar{G}_1(k + q_1) \bar{\chi}_{23}(k + q_2) = \bar{G}_1(q_1) \bar{\chi}_{23}(q_2) \overset{\text{def.}}{=} \frac{W_{23}}{4d} \bar{G}_1(q_1 - q_2)
$$

$$
\frac{1}{N} \sum_k \bar{\chi}_{12}(k + q_1) \bar{\chi}_{34}(k + q_2) = \bar{\chi}_{12}(q_1) \bar{\chi}_{34}(q_2) \overset{\text{def.}}{=} \frac{W_{12}}{4d} \bar{\chi}_{34}(q_1 - q_2)
$$

“Wick theorem” (Gaussian random variables)

$$
\frac{1}{N} \sum_k \bar{G}_1(k + q_1) \bar{G}_2(k + q_2) \bar{G}_3(k + q_3) \bar{G}_4(k + q_4)
\overset{\text{def.}}{=} \bar{G}_1(q_1) \bar{G}_2(q_2) \bar{G}_3(q_3) \bar{G}_4(q_4) + \bar{G}_1(q_1) \bar{G}_2(q_2) \bar{G}_3(q_3) \bar{G}_4(q_4)
\overset{\text{def.}}{=} \bar{G}_1(q_1) \bar{G}_2(q_2) \bar{G}_3(q_3) \bar{G}_4(q_4) + \bar{G}_1(q_1) \bar{G}_2(q_2) \bar{G}_3(q_3) \bar{G}_4(q_4)
$$
9. 2P vertices in strict $d = \infty$ (no parquet eq.)

**Ladder diagrams**

\[
\begin{align*}
&k + q & k_1 + q & k_2 + q & k' + q \\
&\vdots & \vdots & \vdots & \vdots \\
&k & k_1 & k_2 & k'
\end{align*}
\]

\[= \gamma^3 \bar{\chi}^2(q)\]

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

\[
\begin{align*}
&k + q & k_1 + k + k' + q & k' + q \\
&\vdots & \vdots & \vdots \\
&k & k_1 & k'
\end{align*}
\]

\[= \gamma^4 W^2 \frac{1}{4d} \left[ \bar{\chi}(k')\bar{\chi}(k' + q) + \bar{\chi}(k)\bar{\chi}(k + q) + \bar{\chi}(k - k')\bar{\chi}(k + k' + q) \right] \]

*Channel crossing costs a factor \(1/d\) ⇒ only ladders survive to \(d = \infty\).*

\[
\Gamma_{kk'}^{(\infty)}(q) = \frac{\gamma}{1 - \gamma \bar{\chi}(q)} + \frac{\gamma}{1 - \gamma \bar{\chi}(k + k' + q)} - \gamma
\]

\(\Lambda_{ee}, \Lambda_{eh}\)

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 \textit{non-linear} equations for 2P vertices

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

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

\[ \downarrow \]

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

Selfenergy:

- no $\Lambda^{eh}$ 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

$$
1 - \bar{\gamma} \bar{\chi}(0) \bigg|_{\omega=0} = 0 \quad \Leftrightarrow \quad \Im \Sigma^{A}(E) = \frac{\bar{\gamma}}{1 + \bar{\gamma} G^{A}(E) G^{R}(E)} \bigg|_{\omega=0} \Im G^{A}(E)
$$
11. Mean-field approximation

**First step:** Gaussian $\bar{\chi}$ from $d \to \infty \quad \rightarrow \quad$ 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)
  
  \[
  \tilde{\gamma} = \gamma + \tilde{\gamma} \frac{1}{N} \sum_q \frac{\tilde{\gamma}^2 \bar{\chi}^2(q)}{1 - \tilde{\gamma} \bar{\chi}(q)} \quad \rightarrow \quad \tilde{\gamma} = \gamma + \frac{W^2}{8d} \tilde{\gamma}^3 = \gamma + C_d W^2 \tilde{\gamma}^3
  \]

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

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**Model calculation based on Born approximation (not CPA)**

1/A . . . diffusion pole weight

$\lambda_B$ . . . 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

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

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

Phase diagram (localized states hatched)

$E \ldots$ position in the band

$\lambda_B \ldots$ Born irreducible vertex

$w \ldots$ half band-width
Localization tendencies most pronounced at the 
band edges ...
14. Ward identity vs. analyticity

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

Ward identity:

$$\Sigma_k(z_1) - \Sigma_k(z_2) = \frac{1}{N} \sum_{k''} \Lambda^{eh}_{kk''}(z_1, z_2; 0) \left[ G_{k''}(z_1) - G_{k''}(z_2) \right]$$

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

Diffusive regime

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

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

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