Diffusion, probability conservation and Anderson localisation in disordered electron systems

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Layout

- Many-body perturbation theory in the Anderson disordered model – beyond the mean-field description

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- Parquet approach - self-consistent 2P approximations

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- Symmetry breaking & order parameters

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- Parquet approach - self-consistent 2P approximations
- Ward identities and 1P self-energy from the vertex function
- New solution at the 2P (vertex) level
- Symmetry breaking & order parameters
- Consequences for the density response, diffusion, conductivity, normalization of the wave function & Anderson localisation

Model

Anderson model of disordered electrons:

$$\hat{H}_{AD} = \sum_{<ij>} t_{ij} c_i^{\dagger} c_j + \sum_i V_i c_i^{\dagger} c_i$$

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Averaged free energy:

$$F_{av} = -k_B T \left\langle \ln \mathrm{Tr} \exp \left\{ -\beta \widehat{H}_{AD}(t_{ij,} V_i) \right\} \right\rangle_{av}$$

good for averaged one-electron functions

Two-particle functions

Averaged two-particle resolvent needed for the electrical conductivity

$$G^{(2)}_{ij,kl}(z_1, z_2) = \left\langle \left[z_1 \hat{1} - \hat{t} - \hat{V} \right]^{-1}_{ij} \left[z_2 \hat{1} - \hat{t} - \hat{V} \right]^{-1}_{kl} \right\rangle_{av}$$

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Fourier transform

$$G^{(2)}_{\mathbf{k}\mathbf{k}'}(z_1, z_2; \mathbf{q}) = \frac{1}{N} \sum_{ijkl} e^{-i(\mathbf{k}+\mathbf{q}/2)\mathbf{R}_i} e^{i(\mathbf{k}'+\mathbf{q}/2)\mathbf{R}_j} \times e^{-i(\mathbf{k}'-\mathbf{q}/2)\mathbf{R}_k} e^{i(\mathbf{k}-\mathbf{q}/2)\mathbf{R}_l} G^{(2)}_{ij,kl}(z_1, z_2)$$

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$$\times\, e^{-i(\mathbf{k}'-\mathbf{q}/2)\mathbf{R}_k} e^{i(\mathbf{k}-\mathbf{q}/2)\mathbf{R}_l} G^{(2)}_{ij,kl}(z_1, z_2)$$

In noninteracting systems – energies z_1, z_2 are not dynamical variables (externally fixed)

N-energy averaged grand potential

Independent replica for each energy with small enforced external coupling

$$\Omega^\nu(E_1, E_2, \ldots, E_\nu; U) =$$

$$- k_B T \left\langle \ln \mathrm{Tr} \exp \left\{ -\beta \sum_{i,j=1}^{\nu} \left(\widehat{H}^{(i)}_{AD} \delta_{ij} - E_i \widehat{N}^{(i)} \delta_{ij} + \Delta \widehat{H}^{(ij)} \right) \right\} \right\rangle_{av}$$

External perturbation: $\Delta \widehat{H}^{(ij)} = \sum_{kl} U^{(ij)}_{kl} c^{(i)\dagger}_k c^{(j)}_l$

Potential $\Omega^\nu(E_1, E_2, \ldots, E_\nu; U)$ expanded up to U^2 for the conductivity

Mean-field solution ($d = \infty$)

Perturbation expansion for one-particle functions – decoupling of diagonal and off-diagonal contributions
$\Rightarrow$ asymptotc limit to infinite lattice dimensions (mean-field, i. e., CPA)

$$G = G^{diag}[d^0] + G^{off}[d^{-1/2}], \qquad \Sigma = \Sigma^{diag}[d^0] + \Sigma^{off}[d^{-3/2}]$$

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Two-particle functions – generalised Soven equation (2 × 2 matrix)

$$\widehat{G}(z_1, z_2; U) \;=\; \left\langle \left[\widehat{G}^{-1}(z_1, z_2; U) + \widehat{\Sigma}(z_1, z_2; U) - \widehat{V}_i \right]^{-1} \right\rangle_{av}$$

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Single local two-particle irreducible vertex function

Nonlocal vertex functions

Bethe-Salpeter equations for 2P vertex functions

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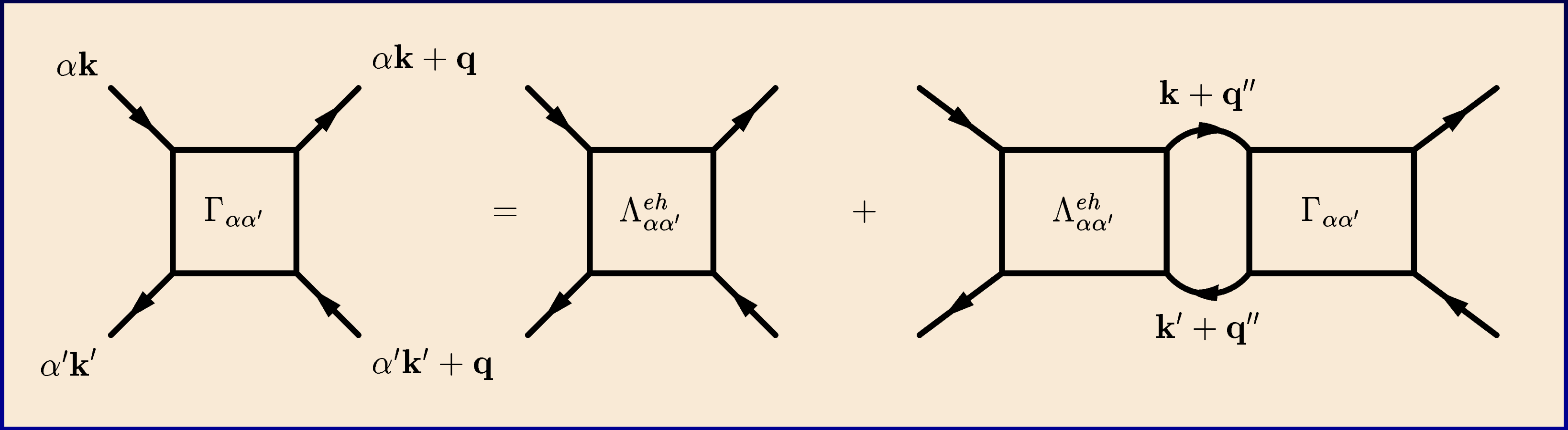
Electron-hole channel



One-particle propagator beyond CPA

$$\widetilde{G}(\mathbf{k},z) = G(\mathbf{k},z) - G^{CPA}(z)$$

weak scattering: bare vertex $\lambda = \langle V_i^2 \rangle_{av}$

strong disorder: the local CPA vertex $\gamma(z_+, z_-)$

Nonlocal vertex functions

Bethe-Salpeter equations for 2P vertex functions

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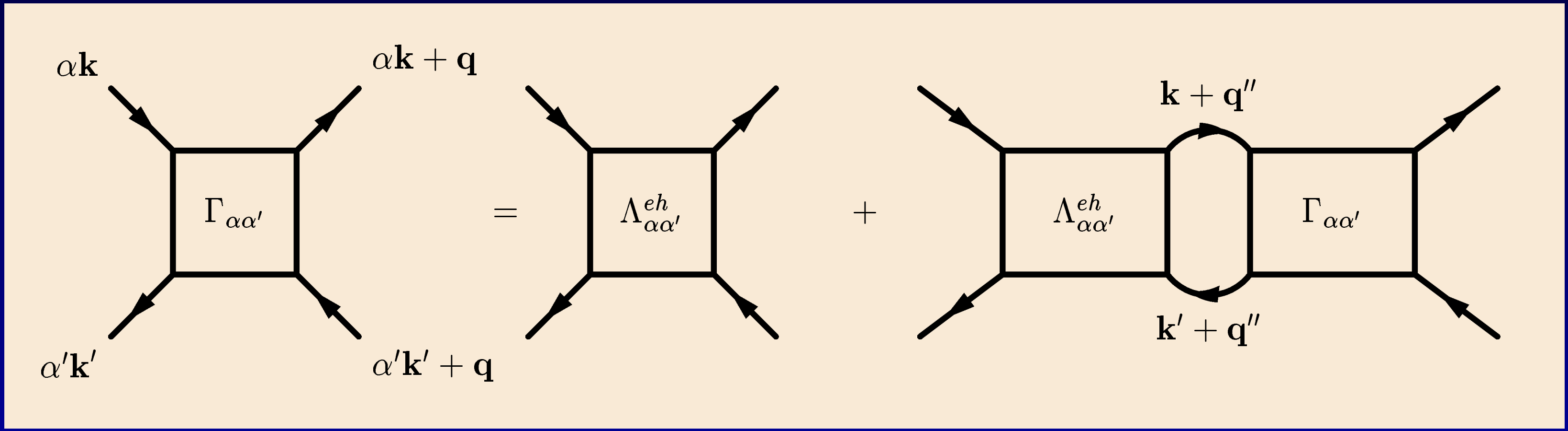

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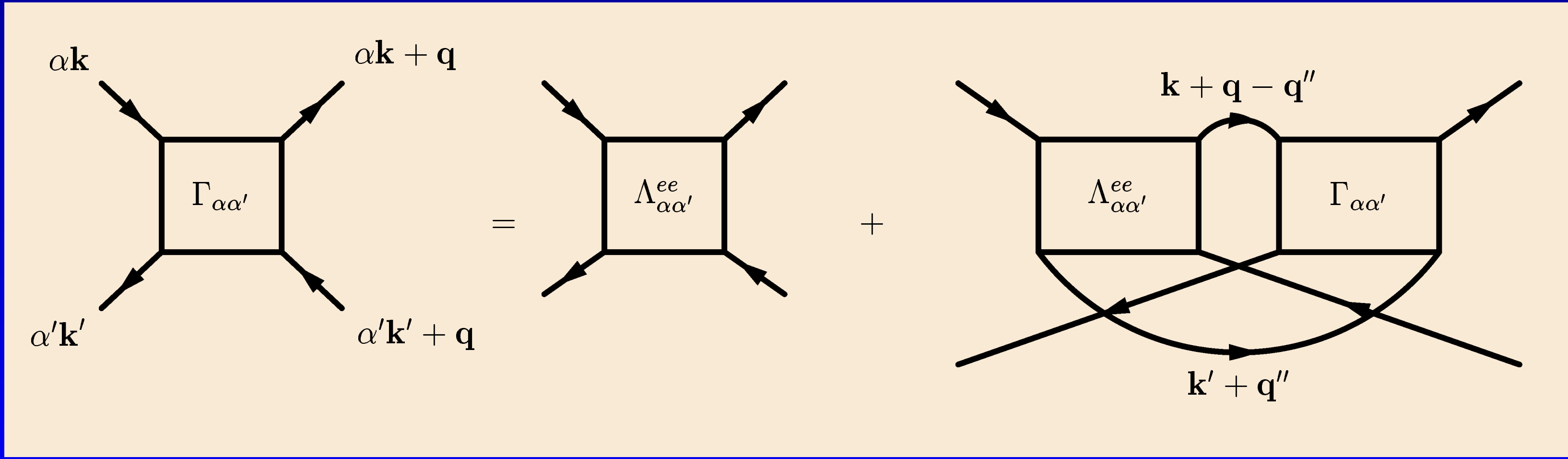

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- Γ excluded from the r.h.s. by Bethe-Salpeter equations in the respective channel

Simplified parquet equations

Formal solution to the parquet equations for the vertex functions

$$\Lambda^{eh}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) = \lambda + \left[\Lambda^{ee} G_+ G_- \left\{1 - \Lambda^{ee} G_+ G_-\right\}^{-1} \Lambda^{ee}\right]_{ee} (\mathbf{k}, \mathbf{k}', \mathbf{q})$$

$$\Lambda^{ee}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) = \lambda + \left[\Lambda^{eh} G_+ G_- \left\{1 - \Lambda^{eh} G_+ G_-\right\}^{-1} \Lambda^{eh}\right]_{eh} (\mathbf{k}, \mathbf{k}', \mathbf{q})$$

with one-particle averaged resolvent

$$G_\pm(\mathbf{k}) = [z_\pm - \epsilon(\mathbf{k} \pm \mathbf{q}/2) - \Sigma_\pm(\mathbf{k} \pm \mathbf{q}/2)]^{-1}$$

Simplified parquet equations

Approximate diagonalization – quasi-algebraic equations:

$$\Lambda^{eh}_{\eta}(E,\omega;\mathbf{q}) = \frac{\lambda}{1 - \left\langle \Lambda^{ee}_{\eta}(E,\omega) G^{+}_{\eta}(E+\omega) G^{-}_{-\eta}(E-\omega) \right\rangle_{ee}(\mathbf{q})}$$

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Principal quality of the full parquet equations – nonlinearity in 2P functions & integrability of singularities

Simplified parquet equations

On-particle propagator:

$$G_\eta^\pm(\mathbf{k}, E) = \left[E + i\eta - \epsilon(\mathbf{k} \pm \mathbf{q}/2) - \Sigma_\pm(\mathbf{k}, E)\right]^{-1}$$

Bubble integrals:

$$\left\langle \Lambda_\eta^{ee}(E,\omega) G_\eta^+(E+\omega) G_\eta^-(E-\omega) \right\rangle_{ee}(\mathbf{q})$$
$$= \frac{1}{N} \sum_{\mathbf{k}} \Lambda_\eta^{ee}(E,\omega;\mathbf{k}) G_\eta^+(\mathbf{k}, E+\omega) G_{-\eta}^-(-\mathbf{k}, E-\omega)$$

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- 1P & 2P (Green) functions not independent – conservation laws – Ward identities
- Velický identity – conservation of probability

$$\frac{1}{N}\sum_{\mathbf{k}'} G^{(2)}_{\mathbf{k}\mathbf{k}'}(z_1, z_2; \mathbf{0}) = \frac{1}{z_2 - z_1}\left[G(\mathbf{k}, z_1) - G(\mathbf{k}, z_2)\right]$$

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- Vollhardt-Wölfle identity ($\mathbf{k}_\pm = \mathbf{k} \pm \mathbf{q}/2$)

$$\Sigma(\mathbf{k}_+, z_+) - \Sigma(\mathbf{k}_-, z_-) = \frac{1}{N}\sum_{\mathbf{k}'} \Lambda_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) \times \left[G(\mathbf{k}'_+, z_+) - G(\mathbf{k}'_-, z_-)\right]$$

1P self-energy

Self-energy from the 2P IR via a Ward identity, simplified parquet equations ⇒ momentum-indipendent self-energy ($\mathbf{q} = 0, z_+ - z_- = 2i\eta$)

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Kramers-Kronig relation (causality)

$$\Re\Sigma_\eta(E) = P\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\Im\Sigma_\eta(\omega + i\eta)}{\omega - E}$$

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Closed set of self-consistent equations for 1P & 2P irreducible functions

2P vertex functions

$$\Lambda_\eta^{eh}(E,\omega;\mathbf{q})$$

$$= \frac{\lambda}{1 - \left\langle \Lambda_\eta^{ee}(E,\omega) G_\eta^{+}(E+\omega) G_{-\eta}^{-}(E-\omega) \right\rangle_{ee}(\mathbf{q})}$$

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- Three different energy derivatives

$$\Lambda'_\eta(E+\omega, E-\omega) = \frac{\partial}{\partial\omega}\Lambda_\eta(E+\omega, E-\omega)$$

$$\dot{\Lambda}_\eta(E+\omega, E-\omega) = \frac{\partial}{\partial\eta}\Lambda_\eta(E+\omega, E-\omega)$$

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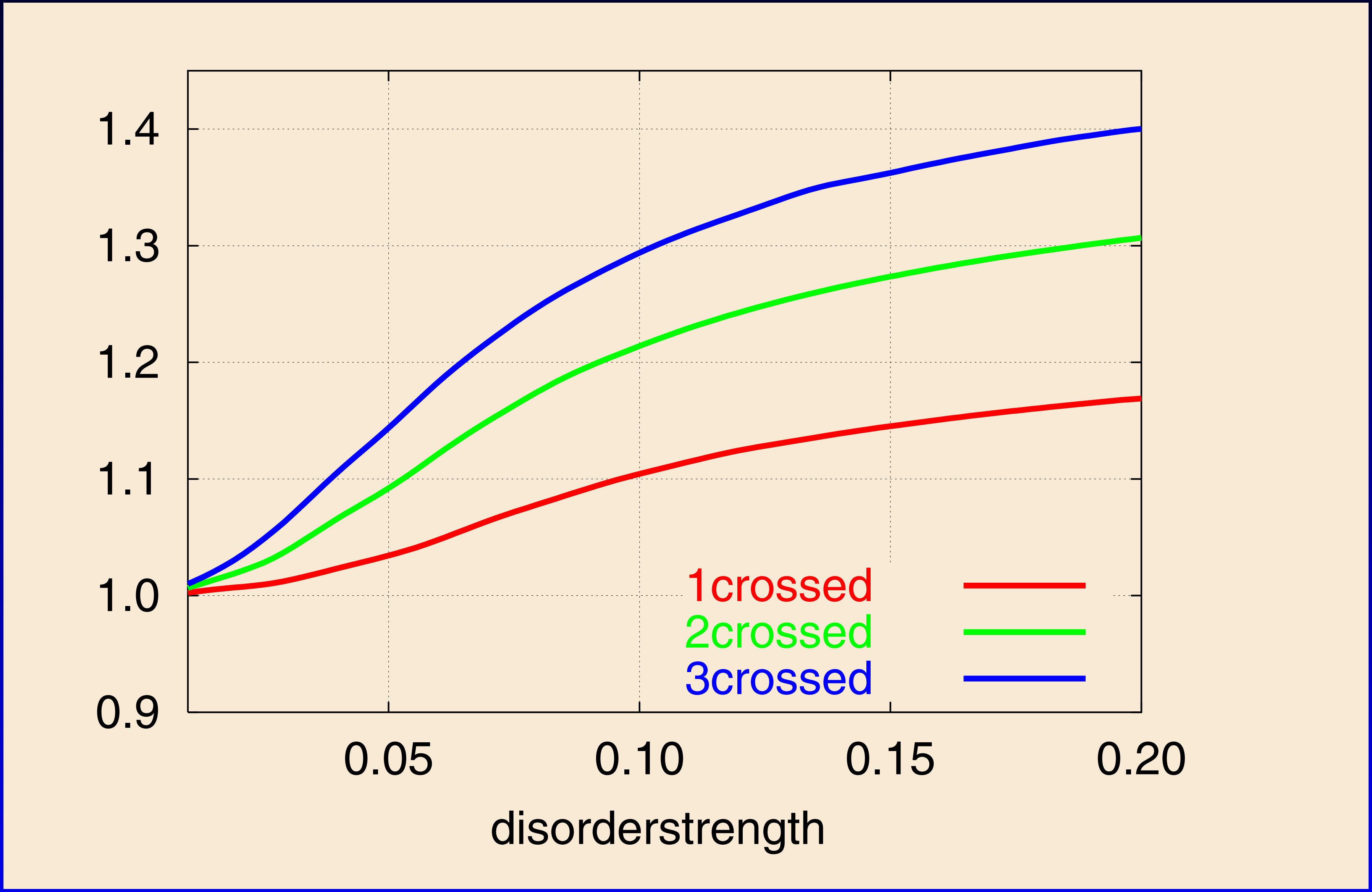
- Real frequency difference ω relevant:

$$\Lambda'_\eta(E, E) \xrightarrow[\lambda\nearrow\lambda_c]{} \infty$$

Derivative of the vertex function



Symmetry breaking in the new solution

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- Mirror symmetry in complex energies broken

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- Order parameters (simplified solution):

$$\Im\Lambda_{\eta}(E,E;\mathbf{0})$$

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- Symmetry-breakig field – real-frequency difference ω

Consequences: density response

- Electron-hole correlation function

$$\Phi^{AR}(\mathbf{q},\omega) = $$

$$\frac{\langle G^{+}_{\eta}(E+\omega) G^{-}_{-\eta}(E-\omega)\rangle_{eh}}{1 - \langle \Lambda^{eh}_{\eta}(E+\omega, E-\omega) G^{+}_{\eta}(E+\omega) G^{-}_{-\eta}(E-\omega)\rangle_{eh}}$$

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- Low energy and momentum limit ($T = 0$)

$$\Phi^{AR}(\mathbf{q},\omega) = \frac{1}{\Lambda'}\frac{2\pi n_F}{-i\omega + D'/\Lambda' q^2}$$

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$$\Phi^{AR}(\mathbf{q},\omega) = \frac{1}{\Lambda'}\frac{2\pi n_F}{-i\omega + D'/\Lambda' q^2}$$

- Density response ($\omega/q \ll 1$)

$$\chi(\mathbf{q},\omega) = \chi(\mathbf{q},0) + \frac{i\omega}{2\pi}\left(\Phi^{AR}(\mathbf{q},0) + O(q^0)\right) + O(\omega^2)$$

Consequences: conductivity

- From Ward identities with real energy difference

$$\sigma(\mathbf{q},\omega) = \frac{-ie^2\omega}{q^2}\chi(\mathbf{q},\omega)$$

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- Low-energy representation with electron-hole correlation function

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- New solution indicates electron localisation,

however, for the nonlocal 2P IR vertex Λ Ward identities seem to be in conflict with the Kramers-Kronig relations for $\omega \neq 0$

Consequences: diffusion

- Quantum diffusion from quantum Fick's law

$$\langle \mathbf{j}(\mathbf{q},\omega)\rangle_{av} = -ie\mathbf{q}D(\mathbf{q},\omega)\left\langle \delta\widetilde{n}(\mathbf{q},\omega)\right\rangle_{av}$$

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- Ward identities – Einstein relation & electron-hole correlation function

$$\sigma(\omega) = e^2 D(\omega)\left(\frac{\partial n}{\partial \mu}\right)_T, \qquad \left(\sigma = \frac{e^2 n_F D'}{\Lambda'(E,E)^2}\right)$$

$$\Phi^{AR}(\mathbf{q},\omega) = \frac{2\pi n_F}{-i\omega + Dq^2}, \qquad \left(\Phi^{AR}(\mathbf{q},\omega) = \frac{1}{\Lambda'}\,\frac{2\pi n_F}{-i\omega + D'/\Lambda' q^2}\right)$$

Consequences: probability

Probability conservation (Ward identity)

$$\Sigma(\mathbf{k}_+, z_+) - \Sigma(\mathbf{k}_-, z_-) = \frac{1}{N} \sum_{\mathbf{k}'} \Lambda_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) \times \left[G(\mathbf{k}'_+, z_+) - G(\mathbf{k}'_-, z_-) \right]$$

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in conflict with causality (Kramers-Krong relation) for $\Re(z_+ - z_-) \neq 0$

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Probability not conserved when approaching the localisation transition – Bloch wave, normalised to volume, goes over to a localised state, normalised to unity

Conclusions

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- Weight of the diffusion pole decreases to zero as $1/\Lambda' \to 0$ and the effective static diffusion ($D = D'/\Lambda'$) vanishes in the new phase
- MFT for Anderson localisation?