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

Response functions and configurational averaging

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1. Outline of the talk

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

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

  (V_i random, site independent)
- ▷ charge transport — electrical conductivity
- ▷ character of electron eigenstates — density response
- ▷ Ward identities and the diffusion pole
- ▷ relaxation of density variations, electron diffusion

- ▷ contributions of elementary 2P diagrams
  - quasi-classical conductivity (ladder diagrams)
  - weak localization (maximally crossed diagrams)

2. Electrical conductivity

Linear response to external electric field (Kubo formula)

$$j_\alpha = \sum_\beta \sigma_{\alpha\beta} E_\beta$$

$$\sigma_{xx} = -\frac{e^2\hbar}{4\pi V}\,\mathrm{Tr}\left\{\left[\hat{\mathcal{G}}^R(E_F) - \hat{\mathcal{G}}^A(E_F)\right]\hat{v}_x\left[\hat{\mathcal{G}}^R(E_F) - \hat{\mathcal{G}}^A(E_F)\right]\hat{v}_x\right\}$$

noninteracting electrons, too many parameters (V_i), no apparent symmetry	conf. averaging $\longrightarrow$	translational symmetry, $e-e$ correlations, $\langle\mathcal{G}\mathcal{G}\rangle \neq \langle\mathcal{G}\rangle\langle\mathcal{G}\rangle$

Nontrivial two-particle Green function

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

Conductivity contributions

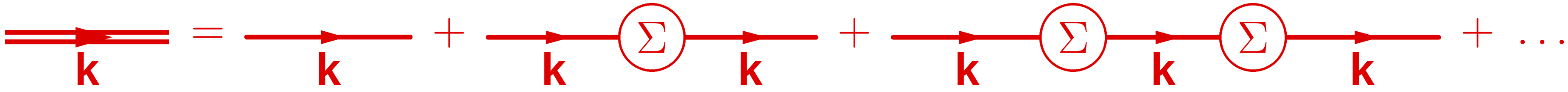
$$GG \;\sim\; \sigma_0 = \frac{ne^2}{m^*}\tau \qquad \text{and} \qquad \Gamma \;\sim\; \text{“vertex corrections”}\;\; \delta\sigma < 0$$

3. Many-body diagrammatics

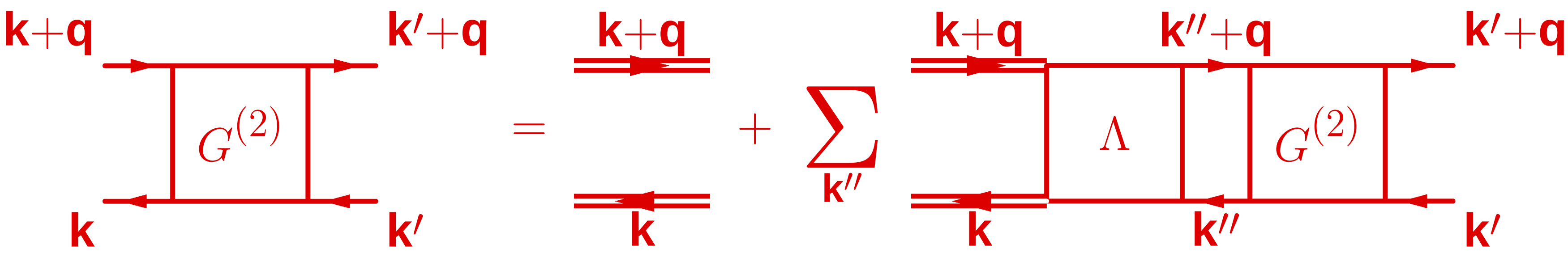
Perturbation expansion before configurational averaging (noninteracting)

$$\mathcal{G}_{ij}(z) = G^{(0)}_{ij}(z) + \sum_{i'} G^{(0)}_{ii'}(z)\, V_{i'}\, G^{(0)}_{i'j}(z) + \sum_{i'j'} G^{(0)}_{ii'}(z)\, V_{i'}\, G^{(0)}_{i'j'}(z)\, V_{j'}\, G^{(0)}_{j'j}(z) + \ldots$$

Averaging term by term ($\longrightarrow$ many-body) — *Dyson equation* . . .



. . . and *Bethe-Salpeter equation*



4. Density response

Linear response to a spatially and time dependent electric field $\varphi(t, \mathbf{r})$

$$\delta n(t, \mathbf{r}) = \int_{-\infty}^{\infty} dt' \int d^3r' \chi(t - t'; \mathbf{r}, \mathbf{r}')\, e\varphi(t, \mathbf{r}')$$

Response function

$$\chi(\omega + i0, \mathbf{q}) = \int_{-\infty}^{\infty} \frac{dE}{2\pi i} \Big\{ [f(E+\omega) - f(E)] \Phi^{AR}(E, E+\omega; \mathbf{q}) \\ + f(E) \Phi^{RR}(E, E+\omega; \mathbf{q}) - f(E+\omega) \Phi^{AA}(E, E+\omega; \mathbf{q}) \Big\}$$

Correlation function

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

5. Ward identity (Velický)

G and $G^{(2)}$ not independent $\longleftrightarrow$ gauge invariance, particle number conservation

Gauge transformation $V = e\varphi_g = z_1 - z_2$ (shift of the zero level of energy)

$$\hat{\mathcal{G}}(z_2) = \frac{1}{z_2 - \hat{H}} = \frac{1}{z_1 - (\hat{H} + z_1 - z_2)} = \hat{\mathcal{G}}(z_1) + \hat{\mathcal{G}}(z_1)\underbrace{(z_1 - z_2)}_{V}\hat{\mathcal{G}}(z_2)$$

$$\Downarrow$$

$$\sum_{i'} G^{(2)}_{ii',i'j}(z_1, z_2) = \frac{1}{z_2 - z_1}\left[G_{ij}(z_1) - G_{ij}(z_2)\right]$$

$$\Downarrow$$

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

Note that $\mathbf{q} = \mathbf{0}$.

6. Velický identity for irreducible functions

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

$\frac{1}{N}\sum_{\mathbf{k}'}$ and $G_{\mathbf{k}}(z_1)G_{\mathbf{k}}(z_2) = \dfrac{G_{\mathbf{k}}(z_1) - G_{\mathbf{k}}(z_2)}{\dfrac{1}{G_{\mathbf{k}}(z_2)} - \dfrac{1}{G_{\mathbf{k}}(z_1)}}$ and Velický identity

$$\frac{G_{\mathbf{k}}(z_1) - G_{\mathbf{k}}(z_2)}{z_2 - z_1} = \frac{G_{\mathbf{k}}(z_1) - G_{\mathbf{k}}(z_2)}{z_2 - z_1 + \Sigma_{\mathbf{k}}(z_1) - \Sigma_{\mathbf{k}}(z_2)} \times \left[1 + \frac{1}{N}\sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}(z_1, z_2; \mathbf{0}) \frac{G_{\mathbf{k}''}(z_1) - G_{\mathbf{k}''}(z_2)}{z_2 - z_1} \right]$$

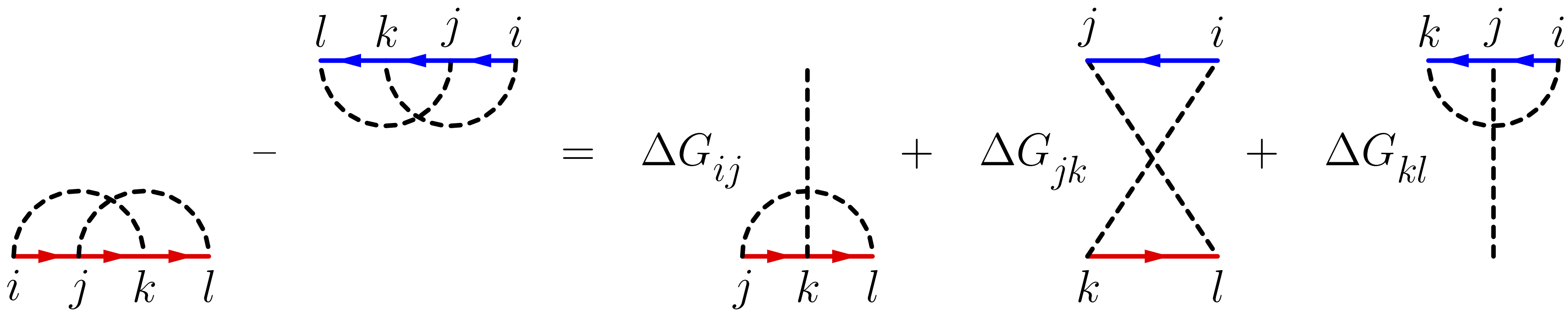
$$\Sigma_{\mathbf{k}}(z_1) - \Sigma_{\mathbf{k}}(z_2) = \frac{1}{N}\sum_{\mathbf{k}''} \Lambda_{\mathbf{k}\mathbf{k}''}(z_1, z_2; \mathbf{0}) \left[G_{\mathbf{k}''}(z_1) - G_{\mathbf{k}''}(z_2) \right]$$

7. Ward identity (Vollhardt & Wölfle)

Closely related to continuity equation; proof — diagrammatic, order by order.

$$G^R_{ij}G^R_{jk}G^R_{kl} - G^A_{ij}G^A_{jk}G^A_{kl} = \overbrace{\left(G^R_{ij} - G^A_{ij}\right)}^{\Delta G_{ij}} G^R_{jk}G^R_{kl} + G^A_{ij}G^R_{jk}G^R_{kl} - G^A_{ij}G^A_{jk}G^A_{kl}$$

$$= \ldots = \Delta G_{ij}\, G^R_{jk}G^R_{kl} + G^A_{ij}\,\Delta G_{jk}\, G^R_{kl} + G^A_{ij}G^A_{jk}\,\Delta G_{kl}$$



$$\Sigma_{\mathbf{k}+\mathbf{q}}(z_1) - \Sigma_{\mathbf{k}}(z_2) = \frac{1}{N}\sum_{\mathbf{k}'} \Lambda_{\mathbf{k}\mathbf{k}'}(z_1, z_2; \mathbf{q}) \left[G_{\mathbf{k}'+\mathbf{q}}(z_1) - G_{\mathbf{k}'}(z_2)\right]$$

8. Relation between conductivity and density response

Continuity equation for Heisenberg operators ...

$$-e\frac{\partial \hat{n}(t,\mathbf{r})}{\partial t} + \mathrm{div}\,\hat{\boldsymbol{j}}(t,\mathbf{r}) = 0$$

... and for expectation values

$$i\omega e\delta n(\omega,\mathbf{q}) + i\,\mathbf{q}\cdot\mathbf{j}(\omega,\mathbf{q}) = 0$$

Linear response formulae for density and current

$$\delta n(\omega,\mathbf{q}) = e\chi(\omega,\mathbf{q})\varphi(\omega,\mathbf{q})$$

$$\mathbf{j}(\omega,\mathbf{q}) = \boldsymbol{\sigma}(\omega,\mathbf{q})\cdot\mathbf{E}(\omega,\mathbf{q}) = -i\boldsymbol{\sigma}(\omega,\mathbf{q})\cdot\mathbf{q}\;\varphi(\omega,\mathbf{q})$$

All together

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

9. Slow variations in space and time

$$\lim_{\mathbf{q}\to\mathbf{0}} \lim_{\omega\to 0} \chi(\omega + i0, \mathbf{q}) = \left(\frac{\partial n}{\partial \mu}\right)$$ (Velický id.)

$$\lim_{\omega\to 0} \lim_{\mathbf{q}\to\mathbf{0}} \chi(\omega + i0, \mathbf{q}) = \lim_{\omega\to 0} \lim_{\mathbf{q}\to\mathbf{0}} \frac{q^2}{-ie^2\omega}\sigma = 0$$ (Vollhardt & Wölfle id.)

Non-analyticity at $\omega = 0$ and $\mathbf{q} = \mathbf{0}$, helps with selection of relevant diagrams

$$\chi(\omega + i0, \mathbf{q}) \sim \frac{\frac{\sigma}{e^2} q^2}{-i\omega + \frac{\sigma}{e^2} q^2 \left(\frac{\partial n}{\partial \mu}\right)^{-1}} = \frac{\left(\frac{\partial n}{\partial \mu}\right) D q^2}{-i\omega + D q^2}$$

Einstein relation, D is the diffusion constant

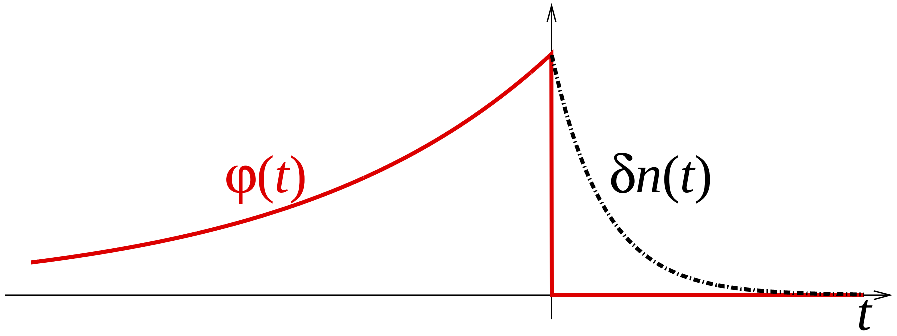
$$\sigma = e^2 D \left(\frac{\partial n}{\partial \mu}\right)$$

10. Diffusive relaxation

Non-equilibrium $n(t, \mathbf{r})$ — not a Hamiltonian perturbation

Trick: external field — adiabatic switch on, sudden switch off

$$\varphi(t, \mathbf{q}) = \theta(-t) \exp(\varepsilon t) \varphi(\mathbf{q})$$



Relaxation of induced density variation ($t > 0$)

$$\delta n(t, \mathbf{q}) = \underbrace{e\varphi(\mathbf{q})}_{-\delta\mu(t=0)} \underbrace{\theta(t) \int_{-\infty}^{0} dt' e^{\varepsilon t'} \chi(t - t', \mathbf{q})}_{\phi(t, \mathbf{q})} = e\varphi(\mathbf{q}) \phi(t, \mathbf{q})$$

Relaxation function

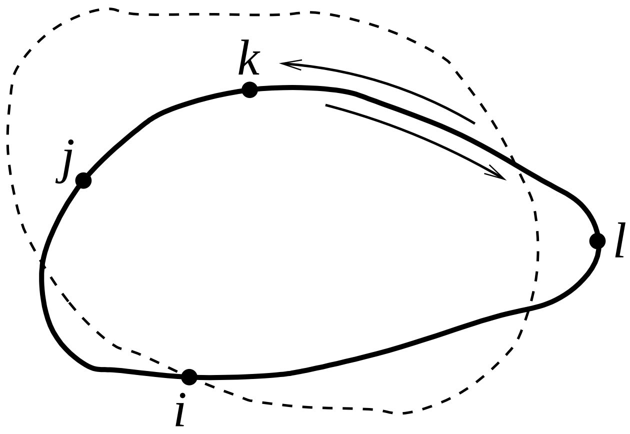
$$\phi(\omega + i0, \mathbf{q}) = \frac{1}{i} \frac{\chi(\omega + i0, \mathbf{q}) - \chi(i0, \mathbf{q})}{\omega - i0} = \frac{(\partial n / \partial \mu)}{-i\omega + Dq^2}$$

$$\boxed{\delta n(t, \mathbf{q}) = \frac{(\partial n / \partial \mu) e\varphi(\mathbf{q})}{-i\omega + Dq^2} = \frac{\delta n(0, \mathbf{q})}{i\omega - Dq^2}} \quad \longleftrightarrow \quad \boxed{\left(\frac{\partial}{\partial t} - D\Delta \right) \delta n(t, \mathbf{r}) = 0}$$

11. Quantum interference

Does the diffusing particle return back?

$$P_{i\to i}(t\to\infty) \overset{?}{>} 0$$



Probability amplitude . . .

$$A_{i\to i} = A_{ijkli} + A_{ilkji}$$

. . . and probability itself

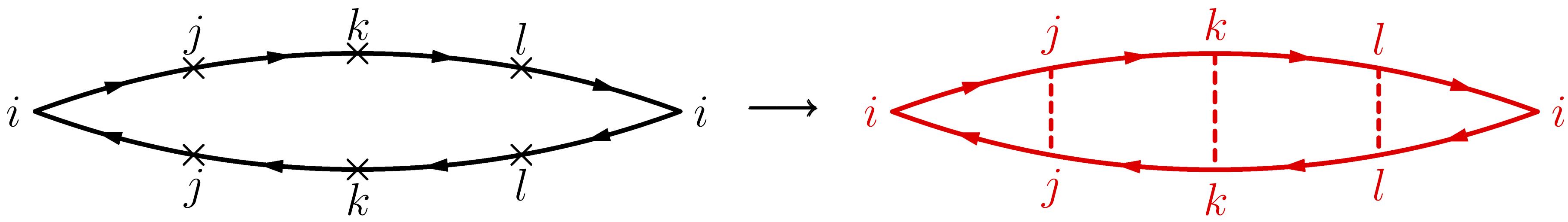
$$P_{i\to i} = |A_{i\to i}|^2 = \underbrace{|A_{ijkli}|^2 + |A_{ilkji}|^2}_{\text{classical part}} + \underbrace{A^*_{ijkli}A_{ilkji} + A_{ijkli}A^*_{ilkji}}_{\text{quantum contribution}}$$

No magnetic field

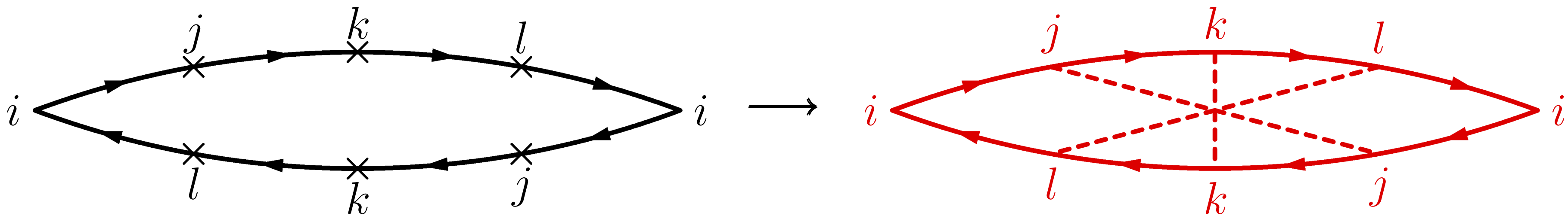
$$A_{ijkli} = A_{ilkji} \quad \Longrightarrow \quad P_{i\to i} = 2P^{\text{class.}}_{i\to i}$$

Quantum coherence enhances backscattering.

12. Quasi-classical contribution and weak localization



$$|A_{ijkli}|^2 \quad \sim \quad \sigma_0 = \frac{ne^2}{m^*}\tau = e^2 D_0 \left(\frac{\partial n}{\partial \mu}\right), \quad \text{respectively} \quad \tau \longrightarrow \tau_{\text{tr}}$$



$$A^*_{ijkli} A_{ilkji} \quad \sim \quad \delta\sigma_{\text{sing.}}(\omega) = -e^2 K_d \, D_0^{1-d/2} \times \begin{cases} \omega^{d/2-1} & \text{if } d \text{ is odd} \\ \omega^{d/2-1} \ln \dfrac{1}{\omega\tau} & \text{if } d \text{ is even} \end{cases}$$

13. Conclusions

▷ transport properties and/or character of electron eigenstates } two-particle Green functions essential

▷ selfenergy renormalizations insufficient

▷ diffusion technically more convenient than conductivity

▷ importance of diffusion pole (and Ward identities)

▷ simple perturbation theory not appropriate

$$\delta\sigma_{2\mathrm{D}}(\omega) \approx -\frac{e^2}{4\pi^2}\ln\frac{1}{\omega\tau} \xrightarrow[\omega\to 0]{} -\infty$$

$\longrightarrow$ better method for diagram summation inevitable — 2P selfconsistency

14. Next seminar

- ▷ CPA / electron-hole symmetry / parquet scheme } Anderson localization
- ▷ mean-field approximation via the asymptotic limit $d \to \infty$ (but <u>*not*</u> strict $d = \infty$)
- ▷ conservation laws in conflict with causality

Asymmetric binary alloy

E . . . position in the band

Δ . . . disorder strength

w . . . half band-width