Quantum diffusion in a random potential: A consistent perturbation theory

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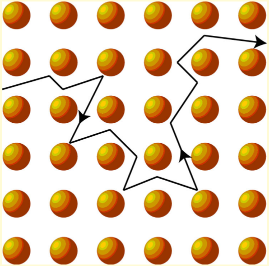
Outline

Classical (charge) diffusion – Drude theory

Scattering of electrons on ions



- Probability of scattering events: τ^{-1}
- Electric current:
  $j = -en\bar{v} = \frac{e^2 n\tau}{m} E = \sigma E$
- Ohm's behavior – dissipative forces (heat generation)
- Probability distribution of charge density

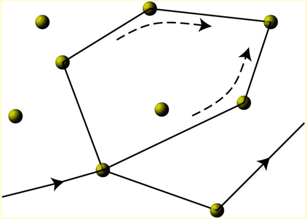
Classical transport - Boltzmann equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_r + \frac{1}{m}\mathbf{F}\cdot\nabla_v\right) f(\mathbf{r},\mathbf{v},t) = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

Collision term: many-body contribution

Quantum diffusion – coherence & wave interference

Quantum coherence and backscatterings on impurities



- Only imperfections in the crystal matter
- Nonlocal character of quantum particles (waves)
- Quantum coherence of admissible classical trajectories

$$P_{quant} = |A_+ + A_-|^2 = \underbrace{|A_+|^2 + |A_-|^2}_{P_{class}} + (A_+ A_-^* + A_+^* A_-) > P_{class}$$

Quantum coherence increases probability of scatterings on impurities – decrease of mobility and reduction of diffusion

Macroscopic vs. microscopic in (quantum) diffusion

Macroscopic - observables

- Long-distance and long-time particle propagation in inhomogeneous media
- Relevant parameters: diffusion constant/conductivity
- Classical or quantum origin not distinguishable – diffusion equation

Microscopic - origin & theory

- Quantum dynamics of random systems - 2P functions relevant
- Not exactly solvable - approximate treatments
- Macroscopic relations (conservation laws) not easily implementable in microscopic theory
- Anderson localization - what causes vanishing of diffusion?

Diagrammatic approaches to quantum diffusion

Vollhardt-Wölfle

- Ward identity assumed - conserving theory
- Expansion for current kernel - maximally crossed diagrams
- Ad hoc 2P self-consistency for the diffusion constant (not microscopic)
- No systematic extensions possible (No BS equations)

Janiš-Kolorenč

- Systematic classification of 2P diagrams (BS equations)
- 2P self-consistency in Green functions
- A bifurcation point in 2P functions – eh symmetry broken (Anderson localization?)
- Dynamical WI not implemented - not conserving

Model description of scatterings on impurities

Noninteracting lattice electrons in a random lattice (impurities) in tight-binding representation:

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

Disorder distribution (site independent):

$$\langle X(V_i) \rangle_{av} = \int_{-\infty}^{\infty} dV \rho(V) X(V)$$

binary alloy: $\rho(V) = c_A \delta(v - V_A) + c_B \delta(V - V_B)$

Quenched disorder: Averaged free energy (thermodynamics)

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

Good for thermodynamics and averaged one-electron functions, no information on transport and dynamical quantities

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One-particle Green function

Averaged quantities (thermodynamic limit) – restore translational invariance

One-electron resolvent (z - complex energy to cover dissipation)

$$G(\mathbf{k}, z) = \frac{1}{z - \epsilon(\mathbf{k}) - \Sigma(\mathbf{k}, z)} = \frac{1}{N}\sum_{i,j} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} \left\langle \left[z\widehat{1} - \widehat{t} - \widehat{V}\right]^{-1}_{ij} \right\rangle_{av}$$

$\mathbf{k}$ – quasimomenta, label the complete set of extended states (Bloch waves)

Density of states: $\rho(E) = -\frac{1}{\pi N}\sum_{\mathbf{k}} \Im G(\mathbf{k}, E + i0^+)$

determines the energy spectrum: $\rho(E) > 0, \quad \Im G \propto \Im\Sigma$
no information about spatial extension of wave function

Elastic scatterings on impurities only - energy conserved (not a dynamical variable)

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Two-particle Green function

Averaged two-particle resolvent (direct lattice space)

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

Fourier transform to momenta

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

Two-particle Green function $G^{RA} = G^{(2)}_{\mathbf{k}\mathbf{k}'}(E + i0, E - i0)$ carries information about the spatial extension of the wave function

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Diffusion: Electron-hole correlation function

- Electron-hole correlation function

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

- Diffusion pole – low-energy asymptotics ($q \to 0, \omega/q \to 0$):

$$\Phi^{RA}_{E_F}(\mathbf{q},\omega) \approx \frac{2\pi n_F}{-i\omega + D(\omega)q^2}$$

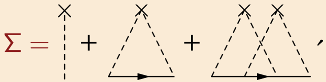
- Dynamical diffusion constant $D(\omega)$ – center of interest

Diffusion constant is not a primary object of the perturbation theory

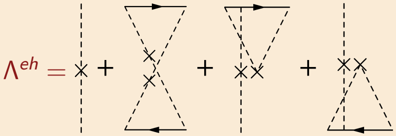
Diagrammatic representation

Perturbation expansion in the random potential V_i (inhomogeneous) – diagrammatic representation

Self-energy (one-particle irreducible vertex)



Irreducible electron-hole vertex (2P self-energy)



Ward identities

- 1P & 2P (Green) functions not independent – charge conservation (Ward identities) & gauge invariance
- Velický identity – probability conservation (no restriction)

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

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

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

$G^{(2)} = GG + GG\Lambda \star G^{(2)}$ – Bethe-Salpeter equation

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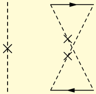
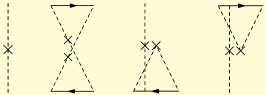
Inability to obey Ward identity in PT

Conflict between causality and WI (beyond mean field)

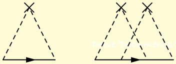
- Causal vertex $\Lambda_{\mathbf{kk}'}(E + i0^+, E - i0^+; \mathbf{0}) \geq 0$ (second order)



- Conserving vertex (second order)



- Self-energy (second order) – not causal ($\Im\Sigma_{\mathbf{k}}(z) \propto -Imz$)



Exactly solvable model (mean field): $d = \infty$

- Limit to high spatial dimensions – scaled hopping $t \to t/\sqrt{2d}$
  Power counting: $G_{\mathbf{ij}} \propto d^{-|\mathbf{i}-\mathbf{j}|/2}$, $\Sigma_{\mathbf{ij}} \propto d^{-\frac{3}{2}|\mathbf{i}-\mathbf{j}|}$
- Mean-field $d = \infty$ limit (Coherent Potential Approximation)
  – separation of local and non-local elements of 1P functions
- Local self-energy: $\Sigma(z)$ $(G(z) \equiv G_0(z - \Sigma(z)))$

$$G(z) = \left\langle \frac{1}{G^{-1}(z) + \Sigma(z) - V_i} \right\rangle_{av}$$

- Local irreducible and full 2P vertices $\lambda(z_1, z_2)$ and $\gamma(z_1, z_2)$

$$\lambda(z_1, z_2) = \frac{\Sigma(z_1) - \Sigma(z_2)}{G(z_1) - G(z_2)}, \quad \gamma(z_1, z_2) = \frac{\lambda(z_1, z_2)}{1 - \lambda(z_1, z_2) G(z_1) G(z_2)}$$

Only single-site scatterings & 1P functions consistent
No backscatterings and Anderson localization

Beyond mean field – nonlocal scatterings

- Mean-field diffusion constant - Drude ($\pi n_F D = \left\langle (\hat{\mathbf{q}} \cdot \mathbf{v}_\mathbf{k})^2 \Im G^2_\mathbf{k} \right\rangle_\mathbf{k}$)
- Expansion beyond MFT needed: non-local (off-diagonal) 1PGF

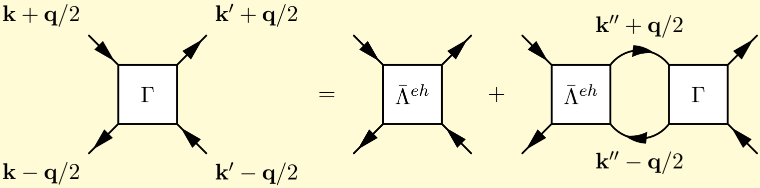
$$\overline{G}(E_\pm, \mathbf{k}) = \frac{1}{N} \sum_{\mathbf{k}'} \frac{N\delta_{\mathbf{k},\mathbf{k}'} - 1}{E \pm \omega/2 \pm i0^+ - \epsilon(\mathbf{k}') - \Sigma(E \pm \omega/2 \pm i0^+, \mathbf{k})}$$

- Distinguishing two-particle propagation
  - Electron-hole simultaneous propagation: $\overline{G}(E_+, \mathbf{k})\overline{G}(E_-, \mathbf{q} + \mathbf{k})$
  - Electron-electron simultaneous propagation: $\overline{G}(E_+, \mathbf{k})\overline{G}(E_-, \mathbf{q} - \mathbf{k})$
- Static theory – only non-local scatterings can distinguish electron form hole
- Local diagrams – fully 2P irreducible

Bethe-Salpeter equations I

- BS equation with multiple nonlocal *eh* scatterings

$$\widetilde{\Gamma}_{\mathbf{k}\mathbf{k}'}(E_+, E_-; \mathbf{q}) = \overline{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}'}(E_+, E_-; \mathbf{q}) + \frac{1}{N}\sum_{\mathbf{k}''} \overline{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}''}(E_+, E_-; \mathbf{q}) \times \overline{G}(E_+, \mathbf{k}'')\overline{G}(E_-, \mathbf{k}'' + \mathbf{q})\widetilde{\Gamma}_{\mathbf{k}''\mathbf{k}'}(E_+, E_-; \mathbf{q})$$

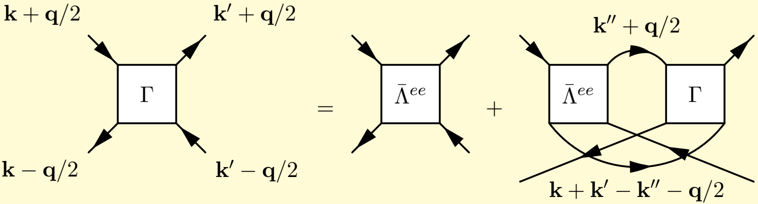


Bethe-Salpeter equations II

- BS equation with multiple nonlocal *ee* scatterings

$$\widetilde{\Gamma}_{\mathbf{k}\mathbf{k}'}(E_+,E_-;\mathbf{q}) = \overline{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(E_+,E_-;\mathbf{q}) + \frac{1}{N}\sum_{\mathbf{k}''}\overline{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}''}(E_+,E_-;\mathbf{q}+\mathbf{k}'-\mathbf{k}'')$$
$$\times\, \overline{G}(E_+,\mathbf{k}'')\overline{G}(E_-,\mathbf{Q}-\mathbf{k}'')\widetilde{\Gamma}_{\mathbf{k}''\mathbf{k}'}(E_+,E_-;\mathbf{q}+\mathbf{k}-\mathbf{k}'')$$

$\mathbf{Q} = \mathbf{q}+\mathbf{k}+\mathbf{k}'$



Parquet equation

- Sets of *eh* and *ee* reducible diagrams do not overlap (nonequivalent representations)
- Reducible diagrams in one channel – irreducible in the other
- Parquet equation

$$\Gamma_{\mathbf{kk}'}(E_+, E_-; \mathbf{q}) = \overline{\Lambda}^{eh}_{\mathbf{kk}'}(E_+, E_-; \mathbf{q}) + \overline{\Lambda}^{ee}_{\mathbf{kk}'}(E_+, E_-; \mathbf{q}) - \mathcal{I}_{\mathbf{kk}'}(E_+, E_-; \mathbf{q})$$

Fully irreducible vertex $\mathcal{I}$ - contains all local and multiply crossed diagrams

- Simplest approximation (CPA full local vertex)

$$\mathcal{I}_{\mathbf{kk}'}(E_+, E_-; \mathbf{q}) = \gamma(E_+, E_-) = \frac{\lambda(E_+, E_-)}{1 - \lambda(E_+, E_-)G(E_+)G(E_-)}$$

Electron-hole symmetry - single 2PIR vertex

- Charge & time reflection (bipartite lattice)

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

- Two-particle symmetry (missing in CPA): Full vertex

$$\Gamma_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) = \Gamma_{\mathbf{k}\mathbf{k}'}(z_+, z_-; -\mathbf{Q}) = \Gamma_{-\mathbf{k}'-\mathbf{k}}(z_+, z_-; \mathbf{Q})$$

- Irreducible vertices: Symmetry transformation

$$\bar{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) = \bar{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; -\mathbf{Q}) = \bar{\Lambda}^{eh}_{-\mathbf{k}'-\mathbf{k}}(z_+, z_-; \mathbf{Q})$$

- Single parquet (nonlinear) equation in the ee channel

$$\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \frac{1}{N}\sum_{\mathbf{k}''} \bar{\Lambda}_{\mathbf{k}\mathbf{k}''}(-\mathbf{q}-\mathbf{k}-\mathbf{k}')\bar{G}_+(\mathbf{k}'')\bar{G}_-(\mathbf{q}+\mathbf{k}+\mathbf{k}'-\mathbf{k}'')$$
$$\times \left[\bar{\Lambda}_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}+\mathbf{k}-\mathbf{k}'') + \bar{\Lambda}_{\mathbf{k}''\mathbf{k}'}(-\mathbf{q}-\mathbf{k}-\mathbf{k}') - \gamma\right]$$

Vertex for the Ward identity & self-energy

- Self-energy in the 1P propagator of the parquet equations
  ($E_\pm = E \pm \omega/2$, $\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E;\omega,\mathbf{q}) = \Lambda_{\mathbf{k}\mathbf{k}'}(E_+ + i0^+, E_- - i0^+;\mathbf{q})$)

$$\Im\Sigma^R(E,\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{k}'} \Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E;0,\mathbf{0})\Im G^R(E,\mathbf{k}')$$

$$\Re\Sigma^R(E,\mathbf{k}) = \Sigma_\infty + P\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\Im\Sigma^R(\omega,\mathbf{k})}{\omega - E}$$

- Vertex Λ – irreducible also locally
  (eh and ee processes indistinguishable)
- Irreducible vertex for the Ward identity from the vertex of the parquet equations $\bar\Lambda$

$$\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \bar\Lambda^{RA}_{\mathbf{k}\mathbf{k}''}(\mathbf{q}) + \frac{1}{N}\sum_{\mathbf{k}''}\bar\Lambda^{RA}_{\mathbf{k}\mathbf{k}''}(\mathbf{q})\left[G^R_+(\mathbf{k}'')\left\langle G^A_-\right\rangle + \left\langle G^R_+\right\rangle G^A_-(\mathbf{k}_-)\right.$$
$$\left. - \left\langle G^R_+\right\rangle\left\langle G^A_-\right\rangle\right]\Lambda^{RA}_{\mathbf{k}''\mathbf{k}'}(\mathbf{q})$$

$\langle G_\pm\rangle = N^{-1}\sum_{\mathbf{k}} G(E_\pm, k)$

Parquet equation for vertex Λ

- Parquet equation ($E_\pm = E \pm \omega/2$)

$$\frac{1}{N}\sum_{\mathbf{k}''}\left[\delta_{\mathbf{k}\mathbf{k}''} - \Lambda^{RA}_{\mathbf{k}_+\mathbf{k}''_+}(E;\omega,\mathbf{k}+\mathbf{k}'')G^R_{\mathbf{k}''_+}(E_+)G^A_{\mathbf{k}''_-}(E_-)\right]$$
$$\times\left[\sum_{\mathbf{k}'''}\left(\delta_{\mathbf{k}'''\mathbf{k}''} + \mathcal{I}^{RA}_{\mathbf{k}''_+\mathbf{k}'''_+}(E;\omega,\mathbf{q})S^{RA}_{\mathbf{k}'''}(E;\omega,\mathbf{q})\right)\right.$$
$$\left.\times\Lambda^{RA}_{\mathbf{k}''_+\mathbf{k}'_+}(E;\omega,\mathbf{q}) - \mathcal{I}^{RA}_{\mathbf{k}''_+\mathbf{k}'_+}(E;\omega,\mathbf{q})\right]$$
$$= \frac{1}{N}\sum_{\mathbf{k}''}\Lambda^{RA}_{\mathbf{k}_+\mathbf{k}''_+}(E;\omega,\mathbf{k}+\mathbf{k}'')\left[G^R_{\mathbf{k}''_+}(E_+)G^A_{\mathbf{k}''_-}(E_-)\right.$$
$$\left.-S^{RA}_{\mathbf{k}''}(E;\omega,\mathbf{q})\right]\Lambda^{RA}_{\mathbf{k}''_+\mathbf{k}'_+}(E;\omega,\mathbf{k}+\mathbf{k}'')$$

with

$$S^{RA}_{\mathbf{k}}(E;\omega,\mathbf{q}) = G^R_{\mathbf{k}_+}(E_+)G^A(E_-) + G^R(E_+)G^A_{\mathbf{k}_-}(E_-) - G^R(E_+)G^A(E_-)$$

- Singular integral kernel for $\omega = 0, \mathbf{k}+\mathbf{k}' = 0$

Restoring WI – making the theory conserving I

- New quantities to define a vertex compatible with WI

$$\Delta G_{\mathbf{k}}(\omega,\mathbf{q}) = G^R(E_+,\mathbf{k}_+) - G^A(E_-,\mathbf{k}_-)$$
$$\Delta\Sigma_{\mathbf{k}}(\omega,\mathbf{q}) = \Sigma^R_{\mathbf{k}_+}(E_+,\mathbf{k}_+) - \Sigma^A(E_-,\mathbf{k}_-)$$
$$R_{\mathbf{k}}(\omega,\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}'}\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(\omega,\mathbf{q})\Delta G_{\mathbf{k}'}(\omega,\mathbf{q}) - \Delta\Sigma_{\mathbf{k}}(\omega,\mathbf{q})$$
$$\left\langle \Delta G(\omega,\mathbf{q})^2\right\rangle = \frac{1}{N}\sum_{\mathbf{k}}\Delta G_{\mathbf{k}}(\omega,\mathbf{q})^2$$

$E_\pm = E \pm \omega/2$, $\mathbf{k}_\pm = \mathbf{k} \pm \mathbf{q}/2$

- New integral kernel of fundamental BS equation

$$L^{RA}_{\mathbf{k}\mathbf{k}'} = \Lambda^{RA}_{\mathbf{k}\mathbf{k}'} - \frac{1}{\langle\Delta G^2\rangle}\left[\Delta G_{\mathbf{k}} R_{\mathbf{k}'} + R_{\mathbf{k}}\Delta G_{\mathbf{k}'} - \frac{\Delta G_{\mathbf{k}}\Delta G_{\mathbf{k}'}}{\langle\Delta G^2\rangle}\langle R\Delta G\rangle\right]$$

Restoring WI – making the theory conserving II

- Fundamental BS equation for a thermodynamically consistent (physical) 2P vertex Γ

$$\frac{1}{N}\sum_{\mathbf{k}''}\left\{\delta_{\mathbf{k},\mathbf{k}''} - \left[\Lambda_{\mathbf{k}\mathbf{k}''} - \frac{\Delta G_{\mathbf{k}} R_{\mathbf{k}''}}{\langle \Delta G^2\rangle} - \frac{R_{\mathbf{k}}\Delta G_{\mathbf{k}''}}{\langle \Delta G^2\rangle} + \langle R\Delta G\rangle \frac{\Delta G_{\mathbf{k}}\Delta G_{\mathbf{k}''}}{\langle \Delta G^2\rangle^2}\right] \times G_{\mathbf{k}'_+} G_{\mathbf{k}'_-}\right\}\Gamma_{\mathbf{k}''\mathbf{k}'} = \Lambda_{\mathbf{k}\mathbf{k}'} - \frac{\Delta G_{\mathbf{k}} R_{\mathbf{k}'}}{\langle \Delta G^2\rangle} - \frac{R_{\mathbf{k}}\Delta G_{\mathbf{k}'}}{\langle \Delta G^2\rangle} + \langle R\Delta G\rangle \frac{\Delta G_{\mathbf{k}}\Delta G_{\mathbf{k}'}}{\langle \Delta G^2\rangle^2}$$

- Relation to the vertex from the perturbation theory

$$\widetilde{\Gamma}^{RA}_{\mathbf{k}\mathbf{k}'}(E;0,\mathbf{0}) = \Gamma^{RA}_{\mathbf{k}\mathbf{k}'}(E;0,\mathbf{0})$$

All macroscopic quantities derived from vertex $\Gamma^{RA}_{\mathbf{k}\mathbf{k}'}(E;\omega,\mathbf{q})$

Singularity in the two-particle vertex

- New function

$$\mathcal{G}_{\mathbf{k}_+}(E;\omega,\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}'}\Gamma^{RA}_{\mathbf{k}_+\mathbf{k}'_+}(E;\omega,\mathbf{q})\frac{\Delta G_{\mathbf{k}}(E;\omega,\mathbf{q})}{\Delta\Sigma_{\mathbf{k}}(E;\omega,\mathbf{q})}$$

- Left eigenvector (WI)

$$\langle \Im G|\widehat{L} = \frac{1}{N^2\sqrt{\langle \Im G^2\rangle}}\sum_{\mathbf{k}\mathbf{k}'}\Im G_{\mathbf{k}'}L^{RA}_{\mathbf{k}'\mathbf{k}}\langle \mathbf{k}| = \frac{1}{N\sqrt{\langle \Im G^2\rangle}}\sum_{\mathbf{k}}\Im G_{\mathbf{k}}\langle \mathbf{k}| = \langle \Im G|$$

where $\langle \Im G^2\rangle = \langle \Im G^2_{\mathbf{k}}\rangle_{\mathbf{k}}$

- Low-frequency singularity

$$\langle \Im G_{\mathbf{k}}\mathcal{G}_{\mathbf{k}}(\omega)\rangle_{\mathbf{k}} = \frac{2\left\langle \Im G^2_{\mathbf{k}}\right\rangle_{\mathbf{k}}\left\langle \Im \Sigma^2_{\mathbf{k}}\right\rangle_{\mathbf{k}}}{i\omega\left\langle \Im \Sigma_{\mathbf{k}}\Im G_{\mathbf{k}}\right\rangle_{\mathbf{k}}}$$

with $\langle f_{\mathbf{k}}\rangle_{\mathbf{k}} = N^{-1}\sum_{\mathbf{k}} f_{\mathbf{k}}$

- Singularity of the homogeneous vertex depends only on 1P functions (Velický WI)

Diffusion pole and diffusion constant

- Low-energy asymptotics of the electron-hole correlation function

$$\Phi^{RA}(E;\omega,\mathbf{q}) \doteq \frac{2\pi n_F}{-i\omega + \dfrac{iq\left\langle(\hat{\mathbf{q}}\cdot\mathbf{v_k})|G^R_{\mathbf{k}}|^2\mathcal{G}^-_{\mathbf{k}}(E;0,\mathbf{q})\right\rangle_{\mathbf{k}} + q^2\left\langle\mathcal{D}_{\mathbf{k}}\mathcal{G}_{\mathbf{k}}(E;\omega,\mathbf{0})\right\rangle_{\mathbf{k}}}{\left\langle|G^R_{\mathbf{k}}|^2\mathcal{G}_{\mathbf{k}}(E;\omega,\mathbf{0})\right\rangle_{\mathbf{k}}}}$$

with $\mathcal{D}_{\mathbf{k}} = -(\hat{\mathbf{q}}\cdot\mathbf{v_k})|G^R_{\mathbf{k}}|^2\left[(\hat{\mathbf{q}}\cdot\mathbf{v_k})\Im G^R_{\mathbf{k}} + \Im\left(G^R_{\mathbf{k}}(\hat{\mathbf{q}}\cdot\nabla_{\mathbf{k}})\Sigma^R_{\mathbf{k}}\right)\right]$

- Static diffusion constant (exact expression) via Kubo-like formula

$$\pi n_F D = \left\langle(\hat{\mathbf{q}}\cdot\mathbf{v_k})|G_{\mathbf{k}}|^2\left[N\delta_{\mathbf{k},\mathbf{k}'} + \Gamma_{\mathbf{kk}'}|G_{\mathbf{k}'}|^2\right] \times \left[\Im G_{\mathbf{k}'}\hat{\mathbf{q}}\cdot\mathbf{v}_{\mathbf{k}'} + \Im\left(G_{\mathbf{k}'}\hat{\mathbf{q}}\cdot\nabla_{\mathbf{k}'}\Sigma_{\mathbf{k}'}\right)\right]\Im\Sigma_{\mathbf{k}'}\right\rangle_{\mathbf{kk}'}$$

all functions on r.h.s are static ($\omega = 0$) from perturbation theory

Simple approximations

- Local (mean-field) approximation – Drude formula

$$\pi n_F D = \left\langle (\hat{\mathbf{q}} \cdot \mathbf{v_k})^2 \Im G_{\mathbf{k}}^2 \right\rangle_{\mathbf{k}}$$

- Maximally crossed diagrams – next step beyond mean-field

$$\pi n_F D = \left\langle \frac{(\hat{\mathbf{q}} \cdot \mathbf{v_k})^2 \Im G_{\mathbf{k}}^2}{1 + |G_{\mathbf{k}}|^2 \left\langle \delta\Lambda^{RA}(q) \right\rangle_{\mathbf{q}}} \right\rangle_{\mathbf{k}}$$

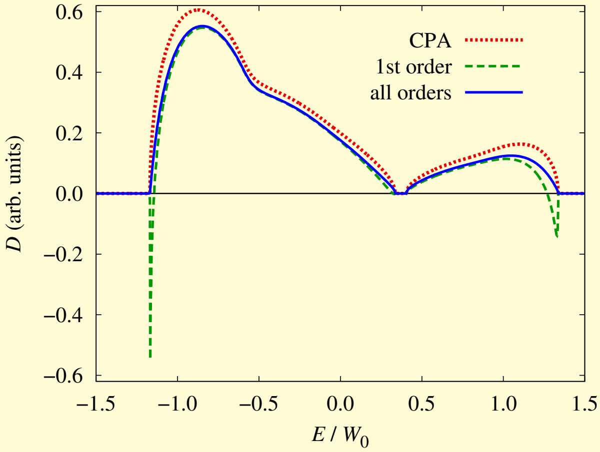
with

$$\left\langle \delta\Lambda^{RA}(q) \right\rangle_{\mathbf{q}} = \frac{1}{\chi_+^{RA}(0)} \left[\left\langle \frac{\chi_+^{RA}(0) - |G|^2}{\chi_+^{RA}(0) - \chi_+^{RA}(\mathbf{q})} \right\rangle_{\mathbf{q}} - 1 \right] .$$

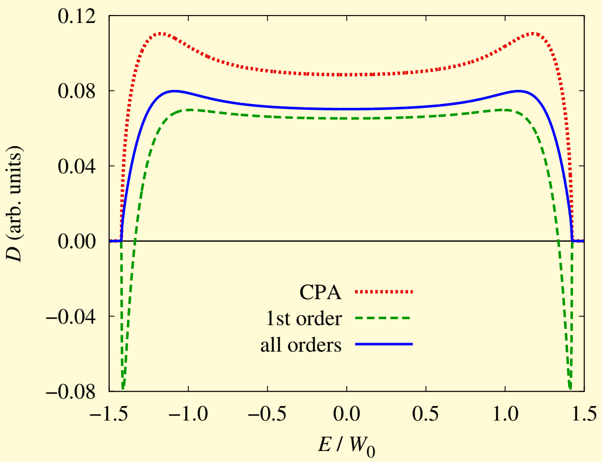
and

$$\chi_+^{RA}(E;\omega,\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} G^R_{\mathbf{k}_+}(E_+) G^A_{-\mathbf{k}_-}(E_-)$$

Maximally crossed diagrams – binary alloy



Maximally crossed diagrams – box disorder



Conclusions

Perturbation theory

1. Inability to satisfy WI in perturbation theory
2. 2P functions from PT - auxiliary
3. 2P self-consistency - only with non-local approximations
4. Low-energy singularities - integrable

Quantum diffusion

1. WI introduced via a redefinition of 2PIR vertex
2. Canonical form of the diffusion pole restored
3. Diffusion constant - composite (not primary) quantity, exact microscopic representation via GF's
4. Local approximations trivial (irrelevant)
5. What is a microscopic (PT) criterion for AL?

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