Dynamical Mean-Field Theory of Disordered Electrons: Coherent Potential Approximation and Beyond

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The Physics of Correlated Insulators, Metals, and Superconductors

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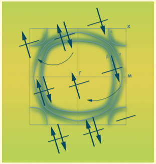

Collaborator: Jindřich Kolorenč (IoP CAS)

Outline

1. Introduction – Resistivity of metals
2. Electron gas in random lattices
   - Electron scatterings on impurities
   - Many-body theory of disordered electrons
3. Dynamical Mean Field Theory
   - Renormalization of perturbation expansion
   - Limit to infinite dimensions
4. Diffusion and transport properties (non-equilibrium)
   - Transport properties within CPA
   - Beyond CPA – Backscatterings
5. Conclusions

Electrons in crystalline solids

Most of properties of solids are determined by the behavior of electrons

Important influencing factors

- Temperature & structure
- Correlations
- Disorder

Low-temperature behavior

- Quantum dynamics & fluctuations
- Noncommuting of operators in Hamiltonian
- Indistinguishable particles – Fermi statistics

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Resistivity of metals

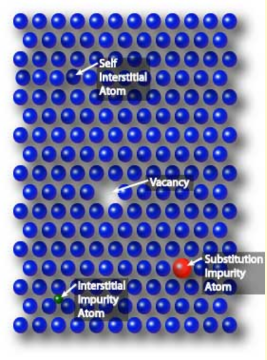
Two types of problems in disordered systems:

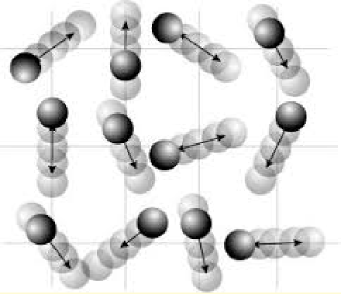
1. Thermodynamic equilibrium – spectral function
2. Weak non-equilibrium – Linear Response Theory (Kubo formalism for electrical conductivity)

Resistivity of metals

Electrons in perfect crystals are Bloch waves
do not scatter on ions (no resistivity)

Resistivity of metals





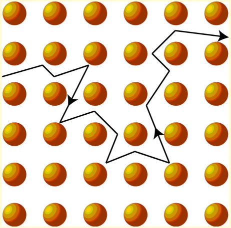
Thermal fluctuations

Imperfections in crystals

Perfect translational symmetry must be broken

Classical electron motion in crystals – Drude theory

Scattering of electrons on ions



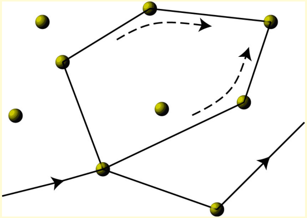
- Probability of scattering events: τ^{-1}
- Electric current:
  $j = -en\bar{v} = \frac{e^2 n\tau}{m} E = \sigma E$
- Ohm's behavior – dissipative forces (heat generation)
- Probability distribution of charge density

Classical transport - Boltzmann equation

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

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 decreases mobility and reduces diffusion

Electron gas in a random alloy

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

$$\widehat{H} = \sum_{nm} |m\rangle \, W_{mn} \, \langle n| + \sum_{n} |n\rangle \, V_n \, \langle n| = \widehat{W} + \widehat{V}$$

$W_{mn} = W(\vec{R}_m - \vec{R}_n)$ with $W_{nn} = 0$

- Disorder distribution (site independent):

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

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

- Quantum fluctuations: $[\widehat{W}, \widehat{V}] \neq 0$

Averaged T-matrix and coherent potential I

- Basic object: Resolvent operator

$$G_{mn}(z) = \left\langle m \left| \left[z\hat{1} - \widehat{W} - \widehat{V} \right]^{-1} \right| n \right\rangle$$

- Density of states (averaged)

$$\rho(E) = -\frac{1}{\pi V} \sum_n \Im G_{nn}(E + i0^+) = \langle \rho_{nn}(E) \rangle_{av}$$

- Only averaged quantities are reproducible

Averaged T-matrix and coherent potential II

- Perturbation expansion in the random potential

$$\langle G_{mn}(z)\rangle_{av} = G^{(0)}_{m-n}(z) + \sum_i G^{(0)}_{m-i}(z)\,\langle V_i\rangle_{av}\, G^{(0)}_{i-n}(z) + \sum_{i,j} G^{(0)}_{m-i}(z)\left\langle V_i G^{(0)}_{i-j}(z) V_j\right\rangle_{av} G^{(0)}_{j-n}(z) + \ldots$$

- T-matrix operator

$$\mathbb{G}(z) = \left\langle \widehat{G}(z)\right\rangle_{av} + \left\langle \widehat{G}(z)\right\rangle_{av} \mathbb{T}(z) \left\langle \widehat{G}(z)\right\rangle_{av}$$

- Coherent potential: absorbs multiple onsite scatterings

$$\widehat{\sigma}(z) = \sum_n |n\rangle\, \sigma_n(z)\, \langle n|$$

Averaged T-matrix and coherent potential III

- Local T-matrix with the coherent potential

$$\mathbb{T}_n(z) = \frac{V_n - \sigma_n(z)}{1 - \left(V_n - \sigma_n(z)\right) G_{nn}(z)}$$

- Random potential replaced by the local T-matrix

$$\mathbb{T}(z) = \sum_n \mathbb{T}_n(z) \left[\widehat{1} + \langle \mathbb{G}(z) \rangle_{av} \sum_{m \neq n} \mathbb{Q}_m(z)\right]$$

$$\mathbb{Q}_n(z) = \mathbb{T}_n(z) + \left[\widehat{1} + \langle \mathbb{G}(z) \rangle_{av} \sum_{m \neq n} \mathbb{Q}_m(z)\right]$$

Averaged T-matrix and coherent potential IV

- Coherent Potential Approximation (CPA) : vanishing of the local T-matrix

$$\langle \mathbb{T}_n(z)\rangle_{av} = \left\langle \frac{V_n - \sigma(z)}{1 - (V_n - \sigma(z))\,\langle G_{nn}(z)\rangle_{av}} \right\rangle_{av} = 0$$

- Multiple scattering on distinct lattice sites neglected

Response functions not uniquely defined.
Many-body approach meeded.

Many-body approach (Statistical mechanics)

- Second quantization – indistinguishable particles (fermions)
- Fock space with creation & annihilation operators
- Thermodynamic limit – restoring translational invariance
- Averaged Green functions – the only ingredients
- Spectral and response functions simultaneously
- Equilibrium thermodynamics in natural way

Many-body model and grand potential

- Hamiltonian for Anderson disordered model

$$\widehat{H} = \sum_{<ij>} t_{ij} \widehat{c}_i^\dagger \widehat{c}_j + \sum_i V_i \widehat{c}_i^\dagger \widehat{c}_i$$

- Averaged grand potential

$$\Omega(\mu) = -\frac{1}{\beta} \left\langle \ln \mathrm{Tr} \exp\left\{ -\beta \widehat{H} + \beta\mu\widehat{N} \right\} \right\rangle_{av}$$

- Ergodic hypothesis:
  Configurational averaging = Spatial averaging
- Perturbation (diagrammatic) expansion in the random potential: averaging term by term

One-particle Green function

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: $\rho(E) > 0, \quad \Im G \propto \Im \Sigma \propto -\Im z$

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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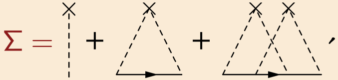
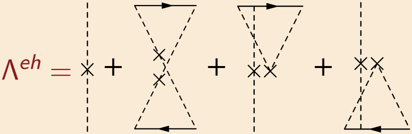
Diagrammatic representation

Perturbation expansion in the random potential V_i – 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)
  ($\mathbf{k}_\pm = \mathbf{k} \pm \mathbf{q}/2$)

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

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

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 for Anderson localization

Diffusion pole only if WI obeyed!

Functional-integral representation

Unifying formalism for finding a generating (thermodynamic) functional

Functional-integral representation of the grand potential

$$\Omega\left\{G^{(0)-1}\right\} = -\beta^{-1}\ln\left[\int \mathcal{D}\varphi\mathcal{D}\varphi^* \exp\left\{-\varphi^*\eta G^{(0)-1}\varphi + h^*\varphi + \varphi^* h + U[\varphi,\varphi^*]\right\}\right]$$

- Complex (Grassmann) fluctuating fields φ (depend on all degrees of freedom)
- (nonlocal) kinetic energy $G^{(0)-1} = H_0 - \mu N$
- (auxiliary) external field h, $\eta = \pm 1$ for bosons/fermions
- Particle interaction (local, random): U

Baym-Kadanoff formalism of renormalizations I

Replacing bare one-particle quantities by renormalized ones (mass renormalization)

- Introducing the full propagator G and self-energy Σ

$$G^{(0)-1} = G^{-1} + \Sigma$$

to be determined self-consistently from a generating functional $\Psi[G, \Sigma]$

Baym-Kadanoff formalism of renormalizations II

- Legendre transformation of the grand potential

$$\Omega[G,\Sigma] = \Omega_\Sigma + \Omega_G + \Omega\left\{G^{(0)-1}\right\}$$

with stationarity condictions

$$\frac{\delta\beta\Omega_\Sigma}{\delta\Sigma} = \frac{\delta\beta\Omega_G}{\delta G^{-1}} = -\frac{\delta\beta\Omega}{\delta G^{(0)-1}}$$

Explicit solution

$$\beta\Omega_\Sigma = \eta\left\{\operatorname{tr}\ln\left[G^{(0)-1} - \Sigma\right] + m^*\left[G^{(0)-1} - \Sigma\right]m\right\},$$
$$\beta\Omega_G = -\eta\left[\operatorname{tr}\ln G^{-1} + m^* G^{-1} m\right] .$$

Baym-Kadanoff formalism of renormalizations III

- New grand potential

$$-\beta\Omega\left[m, H; G, \Sigma\right] = -\eta \mathrm{tr}\ln\left[G^{(0)-1} - \Sigma\right] + \eta \mathrm{tr}\ln G^{-1}$$
$$- m^{*}\eta G^{(0)-1} m + H^{*} m + m^{*} H - \beta F\left[m, H; G^{-1} + \Sigma\right]$$

- Renormalized thermodynamic potential (perturbation theory)

$$-\beta F\left[m, H; G^{-1} + \Sigma\right] = \ln \int \mathcal{D}\phi\mathcal{D}\phi^{*}$$
$$\exp\left\{-\phi^{*}\eta\left[G^{-1} + \Sigma\right]\phi + H^{*}\phi + \phi^{*}H + U\left[\phi + m, \phi^{*} + m^{*}\right]\right\}$$

- Stationarity equations

$$\frac{\delta\Omega}{\delta\Sigma} = \frac{\delta\Omega}{\delta G} = 0$$

Limit to infinite lattice dimensions

Exact solution in a specific (mean-field) limit

- Energy must be linearly proportional to volume

$$E_{kin} = -t \sum_{<ij>\sigma} \left\langle c^\dagger_{i\sigma} c_{j\sigma} \right\rangle_{av} = -it \sum_{<ij>\sigma} G_{ij,\sigma}(0^+) \propto 2d\mathcal{N}t^2$$

- Correct scaling of the hopping parameter $t = \frac{t^*}{\sqrt{2d}}$
- Behavior of renormalized quantities

$$G = G^{diag}\left[d^0\right] + G^{off}\left[d^{-1/2}\right],$$

$$\Sigma = \Sigma^{diag}\left[d^0\right] + \Sigma^{off}\left[d^{-3/2}\right]$$

Disordered Anderson model (CPA) I

- Anderson Hamiltonian with random atomic potential

$$\widehat{H} = -t \sum_{<ij>} c_i^\dagger c_j + \sum_i V_i c^\dagger c_i = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) c^\dagger(\mathbf{k}) c(\mathbf{k}) + \sum_i V_i c_i^\dagger c_i$$

- Grand potential in the mean-field limit

$$\mathcal{N}^{-1}\Omega\left[G_n, \Sigma_n\right] = -\beta^{-1} \sum_{n=-\infty}^{\infty} e^{i\omega_n 0^+} \left\{ \int_{-\infty}^{\infty} d\epsilon \rho_\infty(\epsilon) \ln\left[i\omega_n + \mu - \Sigma_n - \epsilon\right] + \left\langle \ln\left[1 + G_n\left(\Sigma_n - V_i\right)\right]\right\rangle_{av} \right\}$$

Disordered Anderson model (CPA) II

- Density of states for hypercubic lattie

$$\rho_\infty(\epsilon) = \frac{1}{\sqrt{2\pi}t^*} \exp\left\{-\epsilon^2/2t^{*2}\right\}$$

- Stationarity equations
  - Soven equation

$$\frac{\delta\beta\Omega}{\delta G_n} = 0 = \left\langle \frac{\Sigma_n - V_i}{1 + G_n(\Sigma_n - V_i)} \right\rangle_{av}$$

  - Dyson equation

$$\frac{\delta\beta\Omega}{\delta\Sigma_n} = 0 = -\int_{-\infty}^{\infty} \frac{d\epsilon\rho_\infty(\epsilon)}{i\omega_n + \mu - \Sigma_n - \epsilon} + G_n$$

Response to external perturbation I

How to desribe the response functions?
Higher-oder Green functions.

- Replication of the system for each energy (conserved)

$$\Omega^{\nu}(\mu_1, \mu_2, \ldots \mu_\nu; \Delta)$$
$$= -\frac{1}{\beta}\left\langle \ln \mathrm{Tr} \exp\left\{ -\beta \sum_{i,j=1}^{\nu} \left(\widehat{H}^{(i)}\delta_{ij} - \mu_i \widehat{N}^{(i)}\delta_{ij} + \Delta\widehat{H}^{(ij)} \right) \right\} \right\rangle_{av}$$

- Replica-mixing term: $\Delta\widehat{H}^{(ij)} = \sum_{kl} \Delta_{kl}^{(ij)} \widehat{c}_k^{(i)\dagger} \widehat{c}_l^{(j)}$

Response to external perturbation II

- Matrix propagator with two energies (response funtion)

$$\widehat{G}^{-1}(\mathbf{k}_1, z_1, \mathbf{k}_2, z_2; \Delta) = \begin{pmatrix} z_1 - \epsilon(\mathbf{k}_1) - \Sigma_{11}(\Delta) & \Delta - \Sigma_{12}(\Delta) \\ \Delta - \Sigma_{21}(\Delta) & z_2 - \epsilon(\mathbf{k}_2) - \Sigma_{22}(\Delta) \end{pmatrix}$$

- Two-particle irreducible vertex (unique)

$$\lambda(z_1, z_2) = \left.\frac{\delta \Sigma_U(z_1, z_2)}{\delta G_U(z_1, z_2)}\right|_{U=0} = \frac{1}{G(z_1)G(z_2)}\left[1- \left\langle \frac{1}{1 + [\Sigma(z_1) - V_i]\, G(z_1)} \frac{1}{1 + [\Sigma(z_2) - V_i]\, G(z_2)} \right\rangle_{av}^{-1}\right]$$

- DMFT generates only local irreducible higher-order vertices

CPA conductivity and vertex corrections I

- Full nonlocal two-particle vertex

$$\Gamma^{\pm}_{\mathbf{kk}'}(z_1, z_2; \mathbf{q}^{\pm}) = \frac{\lambda(z_1, z_2)}{1 - \lambda(z_1, z_2)\chi^{\pm}(z_1, z_2; \mathbf{q}^{\pm})}$$

with a two-particle bubble

$\chi^{\pm}(z_1, z_2; \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} G(\mathbf{k}, z_1) G(\mathbf{q} \pm \mathbf{k}, z_2)$

- CPA conductivity at zero temperature

$$\sigma_{\alpha\alpha} = \frac{e^2}{2\pi N^2} \sum_{\mathbf{kk}'} v_\alpha(\mathbf{k}) v_\alpha(\mathbf{k}') \left[G^{AR}_{\mathbf{kk}'} - \Re G^{RR}_{\mathbf{kk}'} \right]$$

with
$$G^{AR}_{\mathbf{kk}'}(\omega, \omega'; \mathbf{q}) = G^{\{2\}}_{\mathbf{kk}'}(\omega - i0^+, \omega' + i0^+; \mathbf{q})$$
$$G^{RR}_{\mathbf{kk}'}(\omega, \omega'; \mathbf{q}) = G^{\{2\}}_{\mathbf{kk}'}(\omega + i0^+, \omega' + i0^+; \mathbf{q})$$

CPA conductivity and vertex corrections II

- Full electrical conductivity

$$\sigma_{\alpha\alpha} = \frac{e^2}{\pi N} \sum_{\mathbf{k}} |v_\alpha(\mathbf{k})|^2 \left| \Im G^R(\mathbf{k}) \right|^2 + \Delta\sigma_{\alpha\alpha}$$

- Vertex corrections (beyond CPA)

$$\Delta\sigma_{\alpha\alpha} = \frac{e^2}{2\pi N^2} \sum_{\mathbf{k}\mathbf{k}'} v_\alpha(\mathbf{k}) v_\alpha(\mathbf{k}') \left\{ \left| G^R_{\mathbf{k}} \right|^2 \Delta\Gamma^{AR}_{\mathbf{k}\mathbf{k}'} \left| G^R_{\mathbf{k}'} \right|^2 - \Re \left[\left(G^R_{\mathbf{k}} \right)^2 \Delta\Gamma^{RR}_{\mathbf{k}\mathbf{k}'} \left(G^R_{\mathbf{k}'} \right)^2 \right] \right\}$$

Vertex corrections only beyond local mean field

Electron-hole (time reversal) symmetry

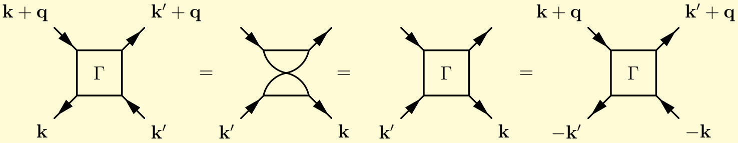
- Electron-hole symmetry: reflection in momentum space

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

- Two-particle vertex

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

- Graphical representation



Nonlocal CPA vertex breaks electron-hole symmetry

Electron-hole (time reversal) symmetry

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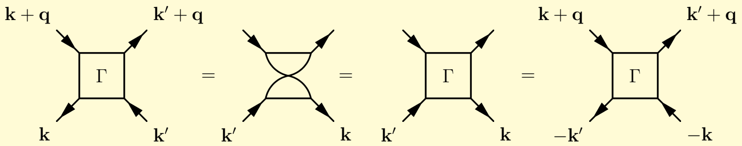

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Expansion around mean field

- Expansion parameter – off-diagonal propagator

$$\bar{G}(\mathbf{k},\zeta) = \frac{1}{\zeta - \epsilon(\mathbf{k})} - \int \frac{d\epsilon\rho(\epsilon)}{\zeta - \epsilon}$$

- Off-diagonal two-particle bubble

$$\bar{\chi}(\zeta,\zeta';\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} \bar{G}(\mathbf{k},\zeta)\bar{G}(\mathbf{k}+\mathbf{q},\zeta') = \chi(\zeta,\zeta';\mathbf{q}) - G(\zeta)G(\zeta')$$

- Conductivity with vertex corrections

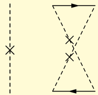
$$\sigma_{\alpha\beta} = \frac{e^2}{2\pi N^2}\sum_{\mathbf{k}\mathbf{k}'} v_\alpha(\mathbf{k}) \left\{ G^A_{\mathbf{k}} \left[1 - \widehat{\bar{\Lambda}}^{RA}\star\right]^{-1}_{\mathbf{k}\mathbf{k}'} G^R_{\mathbf{k}'} - \Re\left(G^R_{\mathbf{k}} \left[1 - \widehat{\bar{\Lambda}}^{RR}\star\right]^{-1}_{\mathbf{k}\mathbf{k}'} G^R_{\mathbf{k}'} \right) \right\} v_\beta(\mathbf{k}')$$

- Perturbation expansion for the irreducible vertices Λ

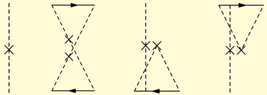
Inability to obey Ward identity in PT beyond DMFT

Conflict between causality and WI (beyond mean field)

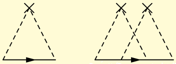
- Causal vertex $\Lambda_{\mathbf{k}\mathbf{k}'}(E+i0^+, E-i0^+; \mathbf{0}) \geq 0$ (second order)



- Conserving vertex (second order)



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



Restoring WI – making the theory conserving I

- VW-WI with the conserving irreducible vertex L^{RA}

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

- New quantities to define a vertex compatible with WI

$$\Delta G_{\mathbf{k}}(\omega,\mathbf{q}) = G^R(E_+,\mathbf{k}_+) - G^A(E_-,\mathbf{k}_-)$$
$$\Delta\Sigma_{\mathbf{k}}(\omega,\mathbf{q}) = \Sigma^R_{\mathbf{k}_+}(E_+,\mathbf{k}_+) - \Sigma^A(E_-,\mathbf{k}_-)$$

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

- Irreducible vertex from perturbation theory Λ^{RA}
- Reduced WI: Imaginary part of the self-energy

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

Restoring WI – making the theory conserving II

- Real part from Kramers-Kronig

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

- Correction function

$$R_{\mathbf{k}}(\omega,\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}'}\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(\omega,\mathbf{q})\Delta G_{\mathbf{k}'}(\omega,\mathbf{q}) - \Delta\Sigma_{\mathbf{k}}(\omega,\mathbf{q})$$

vanishes if WI is obeyed

- New integral kernel of fundamental BS equation

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

- Notation: $\langle\Delta G(\omega,\mathbf{q})^2\rangle = \frac{1}{N}\sum_{\mathbf{k}}\Delta G_{\mathbf{k}}(\omega,\mathbf{q})^2$

Restoring WI – making the theory conserving III

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

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

- Relation to the vertex from the perturbation theory

$$\Gamma^{RA}_{\mathbf{k}\mathbf{k}'}[\Lambda](E;0,\mathbf{0}) = \Gamma^{RA}_{\mathbf{k}\mathbf{k}'}[L](E;0,\mathbf{0})$$

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

Conclusions - CPA

Equilibrium

1. Best local approximation – all single-site contributions
2. Generating (conserving) functional for equilibrium thermodynamics
3. Ward identity obeyed
4. Only local irreducible vertices directly

Non-equilibrium – Linear Response

1. Diffusive behavior – no backscatterings
2. Nonlocal response functions ambiguous
3. Electron-hole symmetry not obeyed in response functions

Expansion beyond DMFT

Beyond CPA

1. Scattering on spatially distinct sites – distinguishes electrons from holes
2. Backscatterings emerge due to restored electron-hole symmetry
3. PT beyond mean-field unable to satisfy WI
4. WI restored by correcting the perturbative vertex
5. Diffusion behavior restored – towards Anderson localization
6. New two-particle self-consistency (missing in CPA) – parquet equations
7. What is a microscopic (PT) criterion for AL?