Parquet approach in interacting and disordered quantum itinerant systems

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Outline

1. Parquet approach in many-body systems
   - Model & fundamental relations
   - Bethe-Salpeter & parquet equations
   - Simplified parquet equations

2. Vertex functions for disordered systems
   - Mean-field theory - limit to high lattice dimensions
   - Beyond MFT - parquet theory for non-local vertices
   - Ward identities -- relevance & applicability
   - Asymptotic solution for $d \to \infty$
   - Results

3. Conclusions

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Equilibrium Hamiltonian & general perturbation

Equilibrium hamiltonian: Tight-binding description

$$\widehat{H} = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{i}\sigma} V_i \widehat{n}_{\mathbf{i}\sigma} + U \sum_{\mathbf{i}} \widehat{n}_{\mathbf{i}\uparrow} \widehat{n}_{\mathbf{i}\downarrow}$$

General perturbation: Normal & anomalous terms

$$\widehat{H}_{ext} = \int d1d2 \left\{ \sum_\sigma \eta^{||}_\sigma(1,2) c^\dagger_\sigma(1) c_\sigma(2) \right. \quad \ldots \text{conserves charge \& spin}$$

$$+ \sum_\sigma \left[\bar{\xi}^{||}_\sigma(1,2) c_\sigma(1) c_\sigma(2) + \xi^{||}_\sigma(1,2) c^\dagger_\sigma(1) c^\dagger_\sigma(2) \right] \quad \ldots \text{changes charge \& spin}$$

$$+ \left[\eta^{\perp}(1,2) c^\dagger_\uparrow(1) c_\downarrow(2) + \bar{\eta}^{\perp}(1,2) c^\dagger_\downarrow(2) c_\uparrow(1) \right] \quad \ldots \text{conserves charge}$$

$$\left. + \left[\bar{\xi}^{\perp}(1,2) c_\uparrow(1) c_\downarrow(2) + \xi^{\perp}(1,2) c^\dagger_\downarrow(2) c^\dagger_\uparrow(1) \right] \quad \ldots \text{conserves spin} \right\}$$

Thermodynamics & Green functions

- Thermodynamic potential with external sources (weak non-equilibrium)

$$\Omega[G^{(0)-1}, H] = -\beta^{-1} \log \mathrm{Tr}\left[\exp\left\{-\beta\left(\widehat{H} + \widehat{H}_{ext} - \mu\widehat{N}\right)\right\}\right]$$

unperturbed 1P Green function $G^{(0)-1} = [i\omega_n - \epsilon(\mathbf{k}) - \mu]$

- 1P Green function

$$G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\tau,\tau') = -\frac{1}{\hbar}\mathrm{Tr}\left\{\widehat{\rho}_H \mathcal{T}\left[c^\dagger_{\mathbf{k}\sigma}(\tau)c_{\mathbf{k}'\sigma'}(\tau')\right]\right\} = \frac{\delta\Omega[G^{(0)-1}, H]}{\delta G^{(0)-1}(\mathbf{k},\tau;\mathbf{k}',\tau')}$$

- 2P Green function

$$G_2(12,34) = -\frac{1}{\hbar^2}\mathrm{Tr}\left\{\widehat{\rho}_H \mathcal{T}\left[\widehat{\psi}(1)\widehat{\psi}(3)\widehat{\psi}(4)^\dagger\widehat{\psi}(2)^\dagger\right]\right\}$$

$1 = (\mathbf{R}_1, \tau_1)$ ...

Green functions from a renormalized functional

- Renormalized generating functional -- "Legendre transform" of the thermodynamic potential

$$\Phi[G,H] = \Omega[G^{(0)-1},H] - \int d\,\bar{1}\left(G^{(0)-1}(1,\bar{1}) - G^{-1}(1,\bar{1})\right) G(\bar{1},1')$$

- 1P Green function (equilibrium)

$$G^{\alpha}(12) = \left.\frac{\delta\Phi[G,H]}{\delta H_{\bar{\alpha}}(2,1)}\right|_{H=0}$$

- 2P Green function (equilibrium)

$$G^{(2)\alpha}(13,24) = \left.\frac{\delta^2\Phi[G,H]}{\delta H_{\alpha}(4,3)\delta H_{\bar{\alpha}}(2,1)}\right|_{H=0}$$

Fundamental relations between 1P & 2P GF

- Dyson equation

$$G^{(0)-1}(1,2) - G^{-1}(1,2) = \Sigma^{\alpha}(12) = \left.\frac{\delta\Phi[G,H]}{\delta G_{\alpha}(2,1)}\right|_{H=0}$$

- Schwinger-Dyson equation -- projection of Schrödinger equation

$$\Sigma_{\sigma}(k) = \frac{U}{\beta N}\sum_{k'} G_{-\sigma}(k')\left[1 - \frac{1}{\beta N}\sum_{q}\Gamma_{\sigma-\sigma}(k,k';q)G_{\sigma}(k+q)G_{-\sigma}(k'+q)\right]$$

- Bethe-Salpeter equations

$$\Gamma(k,k';q) = \Lambda^{\alpha}(k,k';q) - \left[\Lambda^{\alpha}GG\odot\Gamma\right](k,k';q)$$

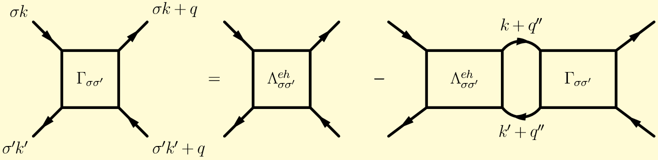
- Generalized Ward identity (thermodynamic consistency)

$$\Lambda^{\alpha}(13,24) = \frac{\delta\Sigma^{\alpha}(1,2)}{\delta G^{\alpha}(4,3)}$$

- SD & WI hold simultaneously in full exact but none approximate (even asymptotically exact) theory

Bethe- Salpeter equation - electron-hole channel

- Multiple simultaneous scatterings -- electron-hole ladder



- Conserving (bosonic) transfer (four)momentum: $k - k'$

$$\Gamma_{\sigma\sigma'}(k, k'; q) = \Lambda^{eh}_{\sigma\sigma'}(k, k'; q) - \frac{1}{\beta\mathcal{N}} \sum_{q''} \Lambda^{eh}_{\sigma\sigma'}(k, k'; q'')$$

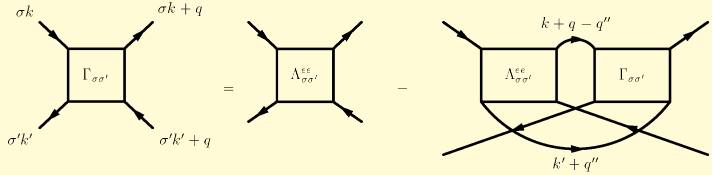
$$\times\, G_{\sigma}(k + q'') G_{\sigma'}(k' + q'') \Gamma_{\sigma\sigma'}(k + q'', k' + q''; q - q'')$$

- Decomposition of the full vertex: All $=$ irreducible $\cup$ reducible (diagrams)

$$\Gamma_{\sigma\sigma'} = \Lambda^{eh}_{\sigma\sigma'} + \mathcal{K}^{eh}_{\sigma\sigma'}$$

Bethe- Salpeter equation - electron-electron channel

- Multiple simultaneous scatterings -- electron-electron ladder



- Conserving (bosonic) transfer (four)momentum: $k + k' + q$

$$\Gamma_{\sigma\sigma'}(k, k'; q) = \Lambda^{ee}_{\sigma\sigma'}(k, k'; q) - \frac{1}{\beta\mathcal{N}} \sum_{q''} \Lambda^{ee}_{\sigma\sigma'}(k, k' + q''; q - q'')$$

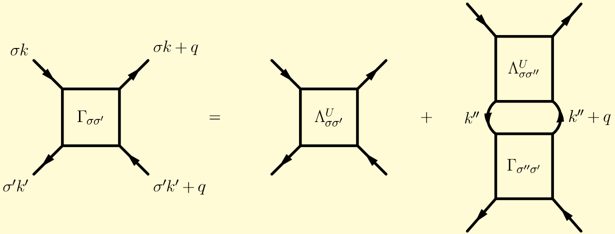
$$\times G_{\sigma}(k + q - q'') G_{\sigma'}(k' + q'') \Gamma_{\sigma\sigma'}(k + q - q'', k'; q'')$$

- Decomposition of the full vertex: All $=$ irreducible $\cup$ reducible (diagrams)

$$\Gamma_{\sigma\sigma'} = \Lambda^{ee}_{\sigma\sigma'} + \mathcal{K}^{ee}_{\sigma\sigma'}$$

Bethe- Salpeter equation - vertical channel

- Multiple simultaneous scatterings -- vacuum electron-hole bubbles (triplet)



- Conserving (bosonic) transfer (four)momentum: q

$$\Gamma_{\sigma\sigma'}(k,k';q) = \Lambda^{U}_{\sigma\sigma'}(k,k';q) + \frac{1}{\beta\mathcal{N}}\sum_{\sigma''k''}\Lambda^{U}_{\sigma\sigma'}(k,k'';q)$$
$$\times\, G_{\sigma''}(k'')G_{\sigma''}(k''+q)\Gamma_{\sigma\sigma'}(k'',k';q)$$

Vertex functions – Parquet approach (two channels)

- BS singlet decompositions: $\Gamma_{\sigma\sigma'} = \Lambda^{ee}_{\sigma\sigma'} + \mathcal{K}^{ee}_{\sigma\sigma'} = \Lambda^{eh}_{\sigma\sigma'} + \mathcal{K}^{eh}_{\sigma\sigma'}$
- Fully irreducible vertex: $\mathcal{I} = \Lambda^{eh} \cap \Lambda^{ee}$
- Existence (applicability) of the parquet decomposition:

$$\mathcal{K}^{ee} \cap \mathcal{K}^{eh} = \emptyset$$

- Parquet reasoning: α-channel: $\Lambda^{\alpha} \cap \mathcal{K}^{\alpha} = \emptyset$
  $\Lambda^{eh} = \Lambda^{eh} \cap \Gamma = (\Lambda^{eh} \cap \Lambda^{ee}) \cup (\Lambda^{eh} \cap \mathcal{K}^{ee}) \subset \mathcal{I} \cup \mathcal{K}^{ee}$
  $\mathcal{K}^{ee} = \mathcal{K}^{ee} \cap \Gamma = (\mathcal{K}^{ee} \cap \Lambda^{eh}) \cup (\mathcal{K}^{ee} \cap \mathcal{K}^{eh}) = \mathcal{K}^{ee} \cap \Lambda^{eh}$
  $\Rightarrow \mathcal{K}^{ee} \subset \Lambda^{eh}$ & $\Lambda^{eh} = \mathcal{I} \cup \mathcal{K}^{ee}$
- Fundamental parquet decomposition:

$$\Gamma = \mathcal{I} \cup \mathcal{K}^{ee} \cup \mathcal{K}^{eh} = \Lambda^{eh} \cup \Lambda^{ee} \setminus \mathcal{I}$$

$$= \mathcal{I} + \mathcal{K}^{eh} + \mathcal{K}^{ee} = \Lambda^{ee} + \Lambda^{eh} - \mathcal{I}$$

- Parquet equations: Bethe-Salpeter equations with Γ replaced by the fundamental parquet decomposition

Parquet equations -- intermediate & strong coupling

- Bethe-Salpeter equations

$$\Gamma(k,k';q) = \Lambda^\alpha(k,k';q) - [\Lambda^\alpha GG \odot \Gamma][q](k,k')$$

- Stability of solutions of BS equations (α channel)

$$min_{\mathbf{q}} [\Lambda^\alpha GG]^\alpha [\mathbf{q}, 0](\mathbf{Q}^\alpha, 0) \geq -1$$

$\mathbf{q}$ - conserving momentum, $\mathbf{Q}^\alpha$ - eigenvector in α-channel

- Singularity in BS equations of solutions of BS equations (α channel)

$$[\Lambda^\alpha GG]^\alpha [\mathbf{q}^\alpha, 0](\mathbf{Q}^\alpha, 0) = -1$$

- Symmetry breaking in the strong-coupling regime (beyond the singularity)

Approximate diagonalization of BS equations (based on the RPA pole)

Simplified parquet equations I

- Generalization of singlet *ee* and *eh* bubbles ($U \to \Lambda$)

$$\psi(q) = \frac{1}{\beta N} \sum_k G_\uparrow(k) G_\downarrow(q-k) \Lambda^{ee}_{\uparrow\downarrow}(q-k)$$

$$\phi(q) = \frac{1}{\beta N} \sum_k G_\uparrow(k) G_\downarrow(q+k) \Lambda^{eh}_{\uparrow\downarrow}(q+k)$$

- Decoupling of parquet equations (*eh* symmetric)

$$\psi(q) = \frac{U}{\beta N} \sum_k \frac{G_\uparrow(k) G_\downarrow(q-k)}{1 + \frac{U}{\beta N} \sum_{k'} \frac{G_\uparrow(k') G_\downarrow(q+k+k')}{1+\psi(q+k+k')}}$$

$$\phi(q) = \frac{U}{\beta N} \sum_k \frac{G_\uparrow(k) G_\downarrow(q+k)}{1 + \frac{U}{\beta N} \sum_{k'} \frac{G_\uparrow(k') G_\downarrow(q+k-k')}{1+\phi(q+k-k')}}$$

- Equations prepared to cover possible symmetry breakings in the strong-coupling regime

Simplified parquet equations II

Nonlinear equations with analytic structure simulating behavior of the full parquet equations

Full 2P vertex

$$\begin{aligned}\Gamma_{\uparrow\downarrow}(k,k';q) &= \Lambda^{eh}_{\uparrow\downarrow}(q+k+k') + \Lambda^{ee}_{\uparrow\downarrow}(q) - U \\ &= \frac{U}{1+\psi(q+k+k')} + \frac{U}{1+\phi(q)} - U\end{aligned}$$

Only integrable singularities admissible (due to the parquet 2P self-consistency)

Generalized RPA pole: $\phi(\mathbf{q},0) = -1$

Self-energies & 1P self-consistency

Which 1P Green functions to use in parquet equations?
How to renormalize 1P propagators in parquet equations?

- Spectral self-energy from the Schwinger-Dyson equation

$$\Delta\Sigma^{sp}_{\uparrow}(k) = -\frac{U^2}{(\beta N)^2}\sum_{q,k'} G_{\uparrow}(k+q)\left[\frac{U\phi(q)}{1+\phi(q)} + \frac{U}{1+\psi(q+k+k')}\right] \times G_{\downarrow}(k')G_{\downarrow}(q+k')$$

Not good in the parquet equations
-- does not reproduce singularities in BS equations

- Thermodynamic self-energy (from Ward identity - linearly)

$$\Sigma^{th}_{\uparrow}(k) = \frac{1}{\beta N}\sum_{k'}\Lambda_{\uparrow\downarrow}(k,k';0)G_{\downarrow}(k') = \frac{U}{\beta N}\sum_{k'}\frac{G_{\downarrow}(k')}{1+\psi(k+k')}$$

To be used in the parquet equations
-- reproduces the singularity of the generalized RPA pole

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: $\rho(V) = c\delta(V - \Delta) + (1 - c)\delta(V + \Delta)$

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

Exactly solvable model (thermodynamics) $d = \infty$

- Limit $d = \infty$ -- scaled hopping $t \to t/\sqrt{2d}$

  Power counting: $G_{\mathbf{ij}} \propto d^{-|\mathbf{i}-\mathbf{j}|/2}$, $\Sigma_{\mathbf{ij}} \propto d^{-\frac{3}{2}|\mathbf{i}-\mathbf{j}|}$
- Thermodynamic mean-field (Coherent Potential Approximation)
- Local self-energy:

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

- 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

Higher-order Green functions I

- Higher-order Green functions
  -- not derivable from thermodynamics
- One energy (mode) for each order

$$\Omega^{\nu}(E_1, E_2, \ldots, E_\nu; U)$$
$$= -\frac{1}{\beta}\left\langle \ln \mathrm{Tr} \exp\left\{-\beta \sum_{i,j=1}^{\nu}\left(\widehat{H}_{AD}^{(i)}\delta_{ij} - E_i \widehat{N}^{(i)}\delta_{ij} + \Delta\widehat{H}^{(ij)}\right)\right\}\right\rangle_{av}$$

mode-coupling (local) term: $\Delta\widehat{H}^{(ij)} = \sum_{kl} U_{kl}^{(ij)} \widehat{c}_k^{(i)\dagger} \widehat{c}_l^{(j)}$

- Matrix propagator (two energies)

$$\widehat{G}^{-1}(\mathbf{k}_1, z_1, \mathbf{k}_2, z_2; U) = \widehat{G}^{(0)-1} + \widehat{U} - \widehat{\Sigma}$$
$$= \begin{pmatrix} z_1 - \epsilon(\mathbf{k}_1) - \Sigma_{11}(U) & U - \Sigma_{12}(U) \\ U - \Sigma_{21}(U) & z_2 - \epsilon(\mathbf{k}_2) - \Sigma_{22}(U) \end{pmatrix}$$

Higher-order Green functions II

- Off-diagonal term – U proportional response is 2P GF $G^{(2)}$
- Local irreducible vertex from Ward identity

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

- Possible extension to non-local mode-coupling – new vertices (beyond mean field)

Nonolocal CPA vertex

- CPA 2P vertex -- *eh* channel with Ward identity for 2PIR vertex

$$\Gamma(z_1, \mathbf{k}_1; z_2, \mathbf{k}_2; \mathbf{q}) = \frac{\lambda(z_1, z_2)}{1 - \lambda(z_1, z_2)\chi^+(z_1, z_2; \mathbf{k}_2 - \mathbf{k}_1)}$$

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

- Local static scatterings do not distinguish between electrons & holes

$$\mathcal{K}^{eh}(z_1, z_2) = \mathcal{K}^{ee}(z_1, z_2)$$

Parquet approach does not apply within CPA

- CPA vertex does not cover all leading $d \to \infty$ contributions

Nonolocal vertex – high-dimensional asymptotics

- Asymptotic vertex in high dimensions: contributions from three channels

$$\Gamma(\mathbf{k}_1, z_1, \mathbf{k}_2, z_2; \mathbf{q}) = \lambda(z_1, z_2)$$
$$\times \left\{ \frac{1}{1 - \lambda(z_1, z_2)\chi^+(\mathbf{k}_2 - \mathbf{k}_1; z_1, z_2)} + \frac{1}{1 - \lambda(z_1, z_2)\chi^-(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{q}; z_1, z_2)} \right.$$
$$\left. + \frac{\prod_{i=1}^{2} \frac{1 - \lambda(z_i, z_i)G(z_i)G(z_i)}{[1 - \lambda(z_i, z_i)\chi^+(\mathbf{q}; z_i, z_i)]}}{1 - \lambda(z_1, z_2)G(z_1)G(z_2)} - \frac{2}{1 - \lambda(z_1, z_2)G(z_1)G(z_2)} \right\}$$

- Electron-hole & electron-electron vertex contributions (distinguishable non-local parts)
- Green terms unimportant – 1P self-correction & local vertex

Correct 2P vertex in $d \to \infty$ limit:
Expansion beyond local approximation (CPA)

2P electron-hole symmetry - missing in CPA

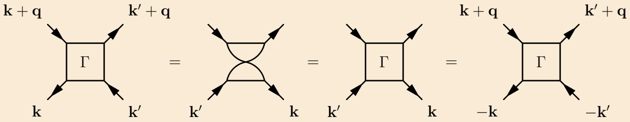
- Charge & time reflection (bipartite lattice)

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

- Two-particle symmetry: Full vertex

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

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



- Irreducible vertices: Symmetry transformation

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

Beyond CPA – parquet decomposition

- PT beyond CPA – relative propagator $\overline{G} = G - G_0^{CPA}$ w.r.t. CPA
- Bethe-Salpeter equation (*eh* channel)

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

- Parquet decomposition of 2P vertex

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

- New vertex functions irreducible only on distant sites

$$\overline{\Lambda}^{\alpha}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Lambda^{\alpha}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) + \frac{\mathcal{J}^0 G_+ G_-}{1 - \mathcal{J}^0 G_+ G_-}\mathcal{J}^0$$

- Fully irreducible vertex non-locally

$$\mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \mathcal{J}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) + \frac{\mathcal{J}^0 G_+ G_-}{1 - \mathcal{J}^0 G_+ G_-}\mathcal{J}^0$$

Parquet equations with electron-hole symmetry

- Irreducible vertices: Electron-hole symmetry transformation

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

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

- Bethe-Salpeter equations into a single non-linear integral equation:

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

- Input -- local full vertex from CPA

$$\mathcal{I} \equiv \gamma(z_1, z_2) = \frac{\lambda(z_1, z_2)}{1 - \lambda(z_1, z_2)G(z_1)G(z_2)}$$

High-dimensional off-diagonal 1P & 2P functions

- Off-diagonal CPA propagator

$$\overline{G}^{(0)}(\mathbf{k},z) = \frac{1}{z-\epsilon(\mathbf{k})} - \int \frac{d\epsilon\rho(\epsilon)}{z-\epsilon} = -i\int_0^\infty du\, e^{\pm iu\zeta_\pm} \prod_{\nu=1}^{d} \exp\{\pm\frac{itu}{\sqrt{d}}\cos k_\nu\}$$

- Off-diagonal two-particle bubble

$$\overline{\chi}^{\pm}(z_1,z_2;\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} \overline{G}(\mathbf{k},z_1)\overline{G}(\mathbf{q}\pm\mathbf{k},z_2) = -\int_0^\infty du \int_0^\infty dv\, e^{iu\zeta}\, e^{iv\zeta'}$$

$$\times \exp\{\frac{t^2(u^2+v^2)}{4}\} \prod_{\nu=1}^{d} \exp\{-\frac{uvt^2}{2d}\cos q_\nu\}$$

High-dimensional algebra of momentum convolutions

- High-dimensional simplification of momentum convolutions (leading order)

$$\frac{1}{N}\sum_{\mathbf{q}'} \overline{\chi}(\mathbf{q}' + \mathbf{q})\overline{G}_{\pm}(\mathbf{q}' + \mathbf{k}) \doteq \frac{Z}{4d}\,\overline{G}_{\pm}(\mathbf{q} - \mathbf{k}) \,,$$

$$\frac{1}{N}\sum_{\mathbf{q}} \overline{\chi}(\mathbf{q} + \mathbf{q}_1)\overline{\chi}(\mathbf{q} + \mathbf{q}_2) \doteq \frac{Z}{4d}\,\overline{\chi}(\mathbf{q}_1 - \mathbf{q}_2)$$

$Z = t^2\langle G_+^2\rangle\langle G_-^2\rangle$, $\langle G_\pm^2\rangle = N^{-1}\sum_{\mathbf{k}} G_\pm(\mathbf{k})^2$

Asymptotic form of vertex Λ in high dimensions available in leading order

Asymptotic vertex in high dimensions

- New reduced vertex

$$\overline{\Lambda}(\mathbf{q}) = \frac{1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}\overline{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$$

with

$$\frac{1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}\overline{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}+\mathbf{k}+\mathbf{k}') = \frac{1}{N}\sum_{\mathbf{q}}\overline{\Lambda}(\mathbf{q}) = \overline{\Lambda}_0$$

- Asymptotic parquet equation

$$\overline{\Lambda}(\mathbf{q}) = \gamma + \overline{\Lambda}_0 \frac{\overline{\Lambda}_0\overline{\chi}_0(\mathbf{q})}{1-\overline{\Lambda}_0\overline{\chi}_0(\mathbf{q})}$$

- Mean-field equation for the local 2P irreducible vertex

$$\overline{\Lambda}_0 = \gamma + \overline{\Lambda}_0^2\frac{1}{N}\sum_{\mathbf{q}}\frac{\overline{\chi}_0(\mathbf{q})}{1-\overline{\Lambda}_0\overline{\chi}_0(\mathbf{q})}$$

1P propagators in the parquet approach

- Off-diagonal 1P (averaged) propagator

$$\overline{G}(\mathbf{k},\omega_+) = [\omega_+ - \epsilon(\mathbf{k}) - \Sigma(\mathbf{k},\omega_+)]^{-1} - G_0^{CPA}(\omega_+)$$

$\omega_\pm = \omega + \pm i0^+$

- Self energy (imaginary part)- from (static) Ward identity (thermodynamic consistency)

$$\Im\Sigma(\mathbf{k},\omega_+) = \frac{1}{N}\sum_{\mathbf{k}'}\Lambda^{eh}(\mathbf{k},\omega_+,\mathbf{k},\omega_-;\mathbf{k}-\mathbf{k}')\Im G(\mathbf{k}',\omega_+)$$

- Full self-energy -- from analyticity

$$\Sigma(\mathbf{k},z) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi i}\,\frac{\Im\Sigma(\mathbf{k},\omega'_+)}{\omega'-z}$$

- Stability condition

$$\Lambda^{eh}(\mathbf{k},\omega_+,\mathbf{k},\omega_-;\mathbf{q}) \geq 0$$

Ward identities

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

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

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

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

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

Ward identities

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

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Unrestricted Ward identities – consequences

- Formal definition of "quantum diffusion" $D_{\alpha\beta}(\mathbf{q},\omega)$:

$$\sigma_{\alpha\beta}(\mathbf{q},\omega) = -e^2 D_{\alpha\beta}(\mathbf{q},\omega)\left[\chi(\mathbf{q},\omega) - \chi(\mathbf{q},0)\right]$$

- Einstein relation – hydrodynamic regime: $\omega \to 0,\ q/\omega \to 0$

$$\sigma(\omega) = e^2 D(\omega)\int_{-\infty}^{\infty}\frac{dE}{\pi}\frac{df(E)}{dE}\Im G^R(E) = e^2 D(\omega)\left(\frac{\partial n}{\partial\mu}\right)_T$$

- Electron-hole correlation function (diffusive regime: $q \to 0,\ \omega/q \to 0$)

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

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

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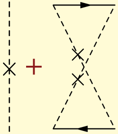
Analyticity vs. Ward identity (perturbatively)

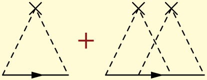
- Vertex from analyticity (stability) -- second order

$\Lambda_C^{eh} =$



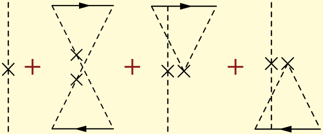
- Self-energy -- second order

$\Sigma_{WI} =$



- Vertex from Ward identity -- second order

$\Lambda_{WI}^{eh} =$



Analyticity vs. Ward identity (non-perturbatively)

- Specific difference: $\Delta W(\omega) = \frac{1}{N}\sum_{\mathbf{k}}[\Sigma^R(\mathbf{k}, E-\omega) - \Sigma^R(\mathbf{k}, E+\omega)]$
- Representation via Ward identity (finite frequencies)

$$\Delta W(\omega) = \frac{-1}{N^2}\sum_{\mathbf{k}\mathbf{k}'}\left\{2i\left[\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) - \Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E-\omega, E)\right]\Im G^R(\mathbf{k}', E)\right.$$
$$\left.+\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E)\left[G^R_{\mathbf{k}'}(E+\omega) - G^R_{\mathbf{k}'}(E)\right] - \Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E-\omega, E)\left[G^R_{\mathbf{k}'}(E-\omega) - G^R_{\mathbf{k}'}(E)\right]\right\}$$

- Singular part (diffusion pole via eh symmetry emerges in Λ^{ee})

$$\Lambda^{sing}_{\mathbf{k}\mathbf{k}'}(z_+, z_-, \mathbf{0}) \doteq \frac{2\pi n_F \lambda}{-i\Delta z\, sign\,(\Im\Delta z) + D(\mathbf{k}+\mathbf{k}')^2}$$

- Dimensional dependence

$$\Delta W^{sing}_d(\omega) \approx K\lambda n_F^2 \times \begin{cases} \frac{1}{\omega}\left|\frac{\omega}{Dk_F^2}\right|^{d/2} & \text{for } d \neq 4l, \\ \frac{1}{\omega}\left|\frac{\omega}{Dk_F^2}\right|^{d/2} \ln\left|\frac{Dk_F^2}{\omega}\right| & \text{for } d = 4l, \end{cases}$$

Mean-field solution from high spatial dimensions

- Full vertex from high dimensional asymptotics

$$\Gamma^{MF}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \Lambda_0 \left[\frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \Lambda_0 \chi(\mathbf{q})} + \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{k} + \mathbf{k}' + \mathbf{q})}{1 - \Lambda_0 \chi(\mathbf{k} + \mathbf{k}' + \mathbf{q})} \right]$$

$\Lambda_0 = \bar{\Lambda}_0 / (1 + \bar{\Lambda}_0 G_+ G_-)$

- General form of the low-energy electron-hole correlation function

$$\Phi^{RA}_E(\mathbf{q}, \omega) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} G^{(2)}_{\mathbf{k}\mathbf{k}'}(E + \omega + i0^+, E - i0^+; \mathbf{q}) \approx \frac{2\pi n_F / A_E}{-i\omega + D^0_E / A_E \mathbf{q}^2}$$

- Weight of the low-energy singularity: $2\pi n_F / A_E$

$$A_E = 1 + 2i \Im G^R(E) \left. \frac{\partial \Lambda^{RA}_0(E + \omega, E)}{\partial \omega} \right|_{\omega = 0} \geq 1$$

- Bare diffusion constant

$$D^0_E = -\frac{2}{\Im G^R(E)} \frac{1}{N} \sum_{\mathbf{k}} v(\mathbf{k})^2 \Im G^R(\mathbf{k}, E)^2 > 0$$

Anderson localization -- vanishing of diffusion

- If $A_E > 1$ -- Ward identity not satisfied dynamically $(\omega \neq 0)$
- Increasing disorder strength $(A_E \to \infty)$:

$$n_E = \frac{n_F}{A_E} \to 0, \quad D = \frac{D_E^0}{A_E} \to 0$$

- Anderson localization transition: $A_E = \infty$

The number n_E of extended states at the Fermi energy vanishes

- Order parameter in the localized phase

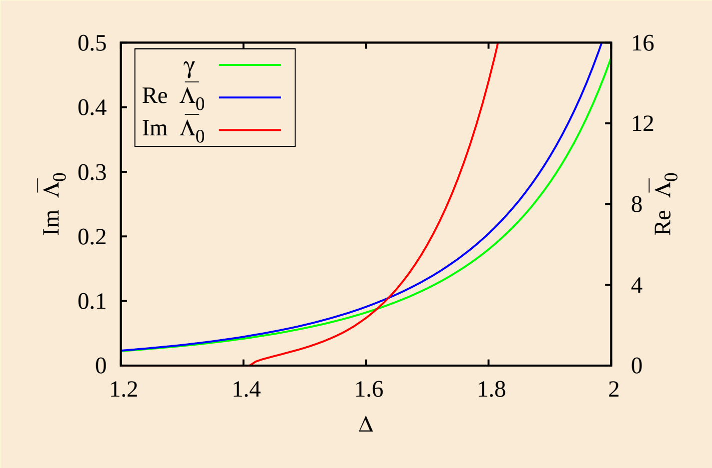
$$\Im\Lambda_0^+ = \lim_{\omega\searrow 0} \Lambda_0^{RA}(E+\omega, E) = \xi^{-2} \geq 0$$

ξ -- localization length

Electron-hole symmetry broken

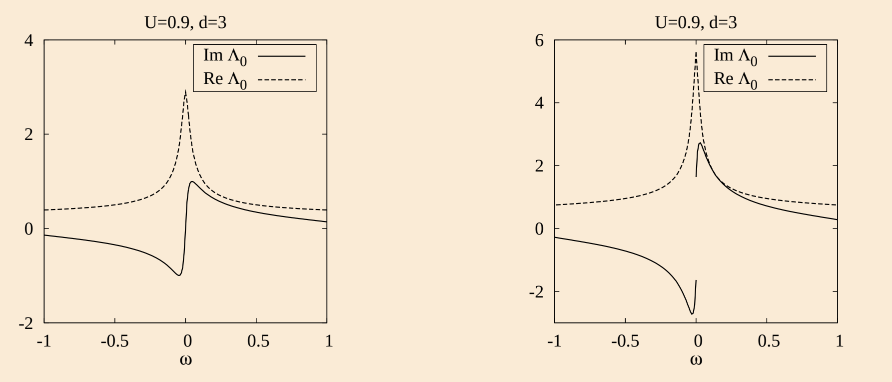
Anderson localization transition

CPA full local vertex γ and the vertex from parquet equations $\overline{\Lambda}_0$ (3d binary alloy, symmetric case)



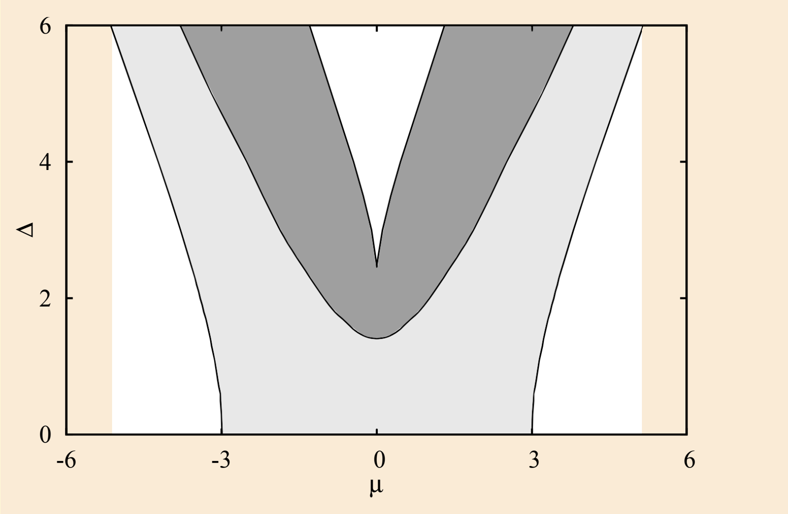
Anderson localization transition

Vertex function - metallic & localized phase



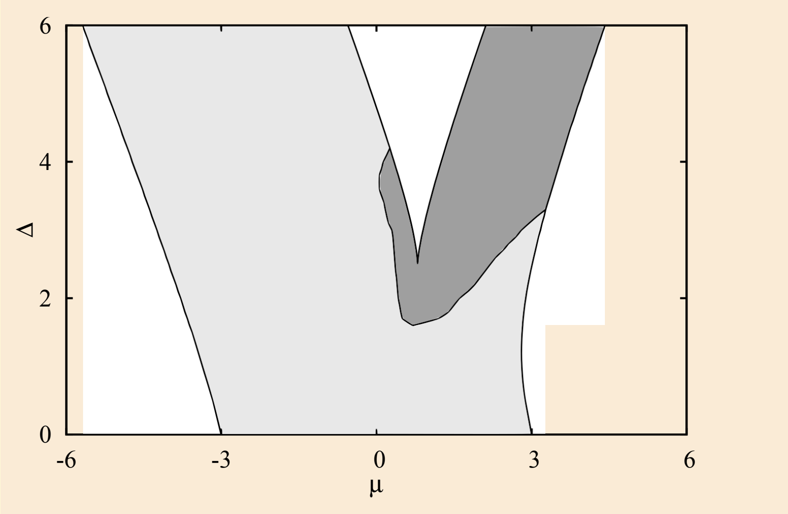
Anderson localization transition

Binary alloy in 3d -- symmetric distribution ($c = 0.5$)



Anderson localization transition

Binary alloy in 3d -- asymmetric distribution ($c = 0.2$)



Conclusions I

Parquet approach -- many-body & general

- Applicability of parquet approach
  -- distinguishability of electrons and holes
- Dynamical or nonlocal scatterings
- Intermediate coupling -- a singularity in BS equations (RPA pole)
- Simplification in the critical region - neglecting finite fluctuations, keeping only critical ones
- One-particle self-consistency -- thermodynamic self-energy (linearized Ward identity)
- Possible LRO & symmetry breaking in strong coupling (thermodynamic consistency needed)

Conclusions II

Parquet approach -- disordered systems

- Parquet approach only to nonlocal vertices -- beyond mean field (CPA)
- Electron-hole symmetry on 2P level leads to a single nonlinear integral equation
- Simplification in high spatial dimensions -- explicit asymptotic solution
- Anderson localization -- new solution for nonlocal irreducible vertex; its phase as an order parameter
- Ward identities obeyed only in the static limit $\omega = 0$
- Weight of the diffusion pole (density of extended states) decreases to zero when approaching ALT ($n_F/A_E \to 0$)
- No diffusion pole in the localized phase

References - additional reading

Vertex functions & parquet approach -- generally

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2. V. Janiš and J. Kolorenč, Mean-field theories for disordered electrons: Diffusion pole and Anderson localization, Phys. Rev. B71, 245106 (2005).
3. V. Janiš and V. Pokorný, Renormalized perturbation theories of Anderson localization: Self-consistent two-particle vertices, Ann. Phys. (Berlin) 523, 715 (2011).

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2. V. Janiš and J. Kolorenč, Conservation laws in disordered electron systems: Thermodynamic limit and configurational averaging, Phys. Stat. Sol. (b) 241, 2032 (2004).
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