Parquet equations for interacting and disordered electron systems: Self-energy and the role of the Ward identity

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> 20th Mardí Gras Conference, LSU, February 14, 2015



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Microscopic description & macroscopic consistency

- Thermodynamic consistency: from microscopic statistical mechanics to thermodynamic (macroscopic) phenomena
- Macroscopic conservation laws -- microscopic Ward identities
- Baym-Kadanoff construction -- 1P self-consistency for the self-energy
- Quantum critical phenomena -- divergence in two-particle functions
- To control 2P criticality -- a direct (diagrammatic) approach to 2P functions (not via self-energy)
- Parquet equations -- 2P self-consistency eliminating spurious (non-integrable) divergencies

How to make 2P (parquet) approach thermodynamically consistent?



Outline

1 Quantum many-body systems

- Thermodynamics & Green functions
- Bethe-Salpeter & parquet equations
- 2 Thermodynamically consistent many-body parquet approach
 - Schwinger-Dyson equation and Ward identity generally
 - Perturbing the self-energy
 - 2P approach Linearized Ward identity and Schwinger-Dyson equation
- Thermodynamic consistency in disordered systems
 2P reducibility and parquet equations in disordered systems
 Ward identity and the full 2P vertex

4 Conclusions



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Equilibrium Hamiltonian § general perturbation

Equilibrium hamiltonian: Tight-binding description

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

General perturbation: Normal & anomalous terms

$$\begin{split} \widehat{H}_{\text{ext}} &= \int d\mathbf{1} d\mathbf{2} \left\{ \sum_{\sigma} \eta_{\sigma}^{||}(1,2) c_{\sigma}^{\dagger}(1) c_{\sigma}(2) \quad \dots \text{ conserves charge § spin} \right. \\ &+ \left[\eta^{\perp}(1,2) c_{\uparrow}^{\dagger}(1) c_{\downarrow}(2) + \bar{\eta}^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}(1) \right] \quad \dots \text{ conserves charge} \\ &+ \sum_{\sigma} \left[\bar{\xi}_{\sigma}^{||}(1,2) c_{\sigma}(1) c_{\sigma}(2) + \xi_{\sigma}^{||}(1,2) c_{\sigma}^{\dagger}(1) c_{\sigma}^{\dagger}(2) \right] \quad \dots \text{ conserves spin} \\ &+ \left[\bar{\xi}^{\perp}(1,2) c_{\uparrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right\} \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\uparrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right\} \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\uparrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\uparrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\uparrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\uparrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\uparrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\downarrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}^{\dagger}(2) c_{\downarrow}^{\dagger}(1) \right] \dots \text{ changes charge § spin} \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}(2) c_{\downarrow}^{\dagger}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}(2) c_{\downarrow}(2) c_{\downarrow}(2) \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(1) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}(2) c_{\downarrow}(2) c_{\downarrow}(2) \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(2) c_{\downarrow}(2) + \xi^{\perp}(1,2) c_{\downarrow}(2) c_{\downarrow}(2) c_{\downarrow}(2) c_{\downarrow}(2) c_{\downarrow}(2) \right] \\ & = \left[\overline{\xi}_{\sigma}^{||}(1,2) c_{\downarrow}(2) c_{\downarrow}(2$$

Thermodynamics & Green functions - unrenormalized

 Thermodynamic potential with external sources (weak non-equilibrium)

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

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

$$G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\tau,\tau') = -\frac{1}{\hbar} \operatorname{Tr}\left\{\widehat{\rho}_{H} \mathcal{T}\left[c_{\mathbf{k}\sigma}^{\dagger}(\tau)c_{\mathbf{k}'\sigma'}(\tau')\right]\right\} = \frac{\delta\Omega[G^{(0)-1},H]}{\delta G^{(0)-1}(\mathbf{k},\tau;\mathbf{k}',\tau')}$$
$$\widehat{\rho}_{H} = \exp\left\{-\beta\widehat{H}\right\}/\operatorname{Tr}\exp\left\{-\beta\widehat{H}\right\}$$

■ 2P Green function

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



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

Green functions from a renormalized functional (Baym & Kadanoff)

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

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

IP Green function and self-energy (equilibrium)

$$G^{\alpha}(12) = \frac{\delta \Phi[G, H]}{\delta H_{\bar{\alpha}}(2, 1)} \bigg|_{H=0}, \qquad \Sigma^{\alpha}(12) = \frac{\delta \Phi[G, 0]}{\delta G_{\bar{\alpha}}(2, 1)}$$

2P Green and vertex functions (equilibrium)

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

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Fundamental relations between 1P § 2P GF

Dyson equation

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

Schwinger-Dyson equation -- projection of Schrödinger equation

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

Bethe-Salpeter equations

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

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 LSU (even asymptotically exact) theory

Necessity to control directly 2P functions

- Critical behavior and phase transitions due to singularities in Bethe-Salpeter equations
- Two-particle self-consistency needed to eliminate unphysical (non-integrable) singularities
- Stable equilibrium state in the critical region
 -- full control of 2P functions necessary
- BK approach does not work -- 2P vertex not explicitly known for the given self-energy (2P singularities not controlled)
- Inverse procedure to BK:
 - Direct (diagrammatic) approximation for 2P vertices
 - Introduce a two-particle self-consistency (when needed)
 - Construct a self-energy to the given 2P vertex
 - Ward identity generally lost

Thermodynamic consistency -- Ward identity to be reintroduced (macroscale)



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Bethe-Salpeter equation - electron-hole channel

Multiple simultaneous scatterings -- electron-hole ladder



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

$$\begin{split} \Gamma_{\sigma\sigma'}(k,k';q) &= \Lambda_{\sigma\sigma'}^{eh}(k,k';q) - \frac{1}{\beta\mathcal{N}}\sum_{q''}\Lambda_{\sigma\sigma'}^{eh}(k,k';q'') \\ &\times G_{\sigma}(k+q'')G_{\sigma'}(k'+q'')\Gamma_{\sigma\sigma'}(k+q'',k'+q'';q-q'') \end{split}$$

■ Decomposition of the full vertex: All = irreducible ∪ reducible (diagrams)

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



Bethe-Salpeter equation - electron-electron channel

Multíple símultaneous scatterings -- electron-electron ladder



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

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

■ Decomposition of the full vertex: All = irreducible ∪ reducible (diagrams)

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



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Vertex functions -- Parquet approach (two channels)

- Basic concept: 2P reducibility -- not uniquely defined
- Channel-dependent decompositions of the full vertex: $\Gamma_{\sigma\sigma'} = \Lambda^{ee}_{\sigma\sigma'} + \mathcal{K}^{ee}_{\sigma\sigma'} = \Lambda^{eh}_{\sigma\sigma'} + \mathcal{K}^{eh}_{\sigma\sigma'}$
- Fully irreducible vertex (diagrammatically): $\mathcal{I} = \Lambda^{eh} \cap \Lambda^{ee}$
- Existence (applicability) of the parquet decomposition:

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

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
- **I** Input to parquet equations: fully irreducible vertex \mathcal{I} , G_{σ}
- Output: 2PIR vertices Λ^{eh} and Λ^{ee}
- **I** No prescribed connection between Σ and Λ^{α} or Γ

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Parquet equations for interacting systems

- Non-locality in space & time -- parquet equations also locally
- IP propagators in the parquet equations: Self-energy from Schwinger-Dyson equation
 - Thermodynamic consistency not guaranteed: Singularity in the BSE does not break the symmetry of the self-energy
 - Parquet equations (2P approach) break down beyond the critical point (singularity in BSE)!
- Thermodynamic consistency only via Ward identity
- Full WI cannot be resolved
- WI does not determine the self-energy (energy not conserved) (unlike disordered systems)



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1P propagators § 2P vertices

Schwinger-Dyson equation: Self-energy and the full 2P vertex



Ward identity: Self-energy and 2P irreducible vertex



One can never fulfill both identities!



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Two-particle criticality

- Transition to an ordered state via a critical point -- divergence in a Bethe-Salpeter equation
- Magnetic order -- electron hole bubbles (local irreducible vertex)

$$\Gamma_{\uparrow\downarrow}(k,k';q) = \frac{\Lambda^U_{\uparrow\downarrow}}{1 - \Lambda^U_{\uparrow\downarrow}\chi_{\downarrow\downarrow}(k-k')\Lambda^U_{\downarrow\uparrow}\chi_{\uparrow\uparrow}(k-k')}$$
(1)

with
$$\chi_{\sigma\sigma'}(q) = (\beta N)^{-1} \sum_k G_{\sigma}(k) G_{\sigma'}(k+q)$$

• Critical point: $\Lambda^U_{\uparrow\downarrow} \chi_{\downarrow\downarrow}(0) = -1$

How to treat the theory beyond the critical point?

- Emergence of magnetic order spin-polarized self-energy
- Only in thermodynamically consistent theories



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Perturbed self-energy - magnetic ordering

- Repulsive particle interaction -- electron-hole scattering dominant
- Linear-response theory -- unperturbed Λ^{eh} (Λ^U) determines the self-energy
- Longitudinal magnetic order (eh bubbles): normal self-energy



Transversal (spin flip) magnetic order (eh ladders): self-energy anomalous only in the spin-polarized state

$$\Sigma_{\uparrow\downarrow}(\bar{\eta}^{\perp}) \doteq \begin{pmatrix} \uparrow & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\$$



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Perturbed self-energy - superconducting ordering

- Attractive particle interaction -- electron-electron scattering dominant
- Linear-response theory -- unperturbed Λ^{ee} determines the self-energy
- Triplet superconducting order (ee bubbles): anomalous self-energy § anomalous vertex (does not conserve spin)



Singlet superconducting order (ee ladders): anomalous self-energy



Linearized Ward identity

- WI resolved w.r.t. symmetry-breaking field only normal component
- Línearízed WI in the external magnetic field (longitudinal §



Mathematical expressions

$$egin{aligned} \Sigma_{\uparrow}(k) &= rac{1}{eta N} \sum_{q} \Lambda^U_{\uparrow\downarrow}(k,k;q) G_{\downarrow}(k+q) \ \Sigma_{\uparrow\downarrow}(k) &= rac{1}{eta N} \sum_{k'} \Lambda^{eh}_{\uparrow\downarrow}(k,k';0) G_{\uparrow\downarrow}(k') \end{aligned}$$

Vertex depends quadratically on the perturbing (magnetic) field

LSU

SDE in the thermodynamically consistent approach

Linearized WI: symmetry of the self-energy gets broken at the divergence in the BSE for a zero eigenvalue of

 $M_{k,k'} = \delta_{k,k'} + \Lambda_{\uparrow\downarrow}(k,k';0)G_{\uparrow}(k')G_{\downarrow}(k')$

■ 1P propagators should use Σ from LWI in all equations with 2P functions: BSE, SDE

Schwinger-Dyson equation with $\Gamma_{\sigma\sigma'}$ and G_σ from the parquet equations determines the physical (thermodynamic) self-energy



SDE in the thermodynamically consistent approach

Linearized WI: symmetry of the self-energy gets broken at the divergence in the BSE for a zero eigenvalue of

 $M_{k,k'} = \delta_{k,k'} + \Lambda_{\uparrow\downarrow}(k,k';0)G_{\uparrow}(k')G_{\downarrow}(k')$

■ 1P propagators should use Σ from LWI in all equations with 2P functions: BSE, SDE

Schwinger-Dyson equation with $\Gamma_{\sigma\sigma'}$ and G_{σ} from the parquet equations determines the physical (thermodynamic) self-energy

$$egin{aligned} \Sigma_{\uparrow}(k) &= rac{U}{eta N} \sum_{k'} G_{\downarrow}(k') \left[1 - rac{1}{eta N} \sum_{k'} G_{\downarrow}(k'') G_{\uparrow}(k+k'-k'')
ight. \ & imes \Gamma_{\uparrow\downarrow}(k',k'';k-k'')
ight] \end{aligned}$$

LSU

Parquet equations for disordered electrons

- Quenched disorder § no ee interaction
 - -- no dynamics, energy conserved
- Equilibrium thermodynamics
 - -- renormalization of the dispersion relation
- Non-equilibrium -- Linear Response Theory (Kubo formalism)
 - Equilibrium two-particle Green function needed
 - Multiple scattering on impurities
 - Local scatterings -- mean field (CPA)
 - Nonlocal scatterings -- electron-electron and electron-hole simultaneous propagation distinguishable
 - Two-particle self-consistency -- via parquet equations (beyond CPA)
 - Vertex function not fully compatible with the ward identity
- Thermodynamic consistency -- corrections to the vertex from the parquet equations so that Ward identity is obeyed



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Model description of scatterings on impurities

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

$$\widehat{H}_{AD} = \sum_{\langle ij
angle} t_{ij}c_i^{\dagger}c_j + \sum_i V_ic_i^{\dagger}c_i$$

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)

$$F_{av} = -k_B T \Big\langle \ln \operatorname{Tr} \exp \Big\{ -eta \widehat{H}_{AD}(t_{ij}, V_i) \Big\} \Big\rangle_{av}$$

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



Two-particle reducibility and parquet decomposition

- Distinction between electron and holes necessary for parquet equations -- non locality in time or space
- Static theory -- non-local scatterings (beyond local mean-field)
- Expansion beyond MFT: non-local (off-diagonal) 1PGF

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

- Dístinguíshable two-particle reducibility
- Local díagrams -- fully irreducible
- Electron-hole simultaneous propagation: $\overline{G}(E_+, \mathbf{k})\overline{G}(E_-, \mathbf{q} + \mathbf{k})$
- Electron-electron simultaneous propagation: $\overline{G}(E_+, \mathbf{k})\overline{G}(E_-, \mathbf{q} \mathbf{k})$



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Bethe-Salpeter and the parquet equations (no WI)

BS equation with multiple nonlocal eh scatterings

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

BS equation with multiple nonlocal ee scatterings

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

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

Parquet equation

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

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



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

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



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ward identity

- 2P vertex from parquet equations (or other 2P constructions) does not fully obey Ward identity
- IP propagators in 2P approaches are input
- Vollhardt-Wölfle identity (continuity equation) ($\mathbf{k}_{\pm} = \mathbf{k} \pm \mathbf{q}/2$)

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

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

• WI guaranteed in 2P approaches (parquets) only for $\omega = 0$ and q = 0

$$\Lambda_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) \neq \overline{\Lambda}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q})$$



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vertex for the ward identity § self-energy

- Self-energy in the 1P propagator of the parquet equations $(E_{\pm} = E \pm i0^{+})$ $\Im \Sigma(E_{+}, \mathbf{k}) = \frac{1}{N} \sum_{\mathbf{k}'} \Lambda_{\mathbf{k}\mathbf{k}'}(E_{+}, 0) \Im G(E_{+}, \mathbf{k}')$ $\Re \Sigma(E_{+}, \mathbf{k}) = \Sigma_{\infty} + P \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\Im \Sigma(\omega_{+}, \mathbf{k})}{\omega - E}$
- vertex Λ -- irreducible also locally (eh and ee processes indistinguishable)
- \blacksquare Irreducible vertex for the ward identity from the vertex of the parquet equations $\overline{\Lambda}$

$$\Lambda_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}\mathbf{k}''}(\mathbf{q}) + \frac{1}{N} \sum_{\mathbf{k}''} \bar{\Lambda}_{\mathbf{k}\mathbf{k}''}(\mathbf{q}) \left[G_{+}(\mathbf{k}'') \left\langle G_{-} \right\rangle + \left\langle G_{+} \right\rangle G_{-}(\mathbf{k}_{-}) \right]$$

 $-\left\langle {{\it G}_{+}} \right
angle \left\langle {{\it G}_{-}}
ight
angle
ight
angle \Lambda_{{f k}^{\prime\prime}{f k}^{\prime}}({f q})$

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



New quantities to define a vertex compatible with WI

$$\begin{split} \Delta G_{\mathbf{k}}(\omega,\mathbf{q}) &= G(E_{+},\mathbf{k}_{+}) - G(E_{-},\mathbf{k}_{-}) \\ \Delta \Sigma_{\mathbf{k}}(\omega,\mathbf{q}) &= \Sigma_{\mathbf{k}_{+}}(E_{+},\mathbf{k}_{+}) - \Sigma(E_{-},\mathbf{k}_{-}) \\ R_{\mathbf{k}}(\omega,\mathbf{q}) &= \frac{1}{N} \sum_{\mathbf{k}'} \Lambda_{\mathbf{k}\mathbf{k}'}(\omega,\mathbf{q}) \Delta G_{\mathbf{k}'}(\omega,\mathbf{q}) - \Delta \Sigma_{\mathbf{k}}(\omega,\mathbf{q}) \\ \left\langle \Delta G(\omega,\mathbf{q})^{2} \right\rangle &= \frac{1}{N} \sum_{\mathbf{k}} \Delta G_{\mathbf{k}}(\omega,\mathbf{q})^{2} \end{split}$$

 $E_{\pm} = E \pm \omega/2 \pm i0^+$, $\mathbf{k}_{\pm} = \mathbf{k} \pm \mathbf{q}/2$

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

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

Conclusions 1

Parquet approach -- many-body & general

- Applicability of parquet approach
 -- distinguishability of electrons and holes
- Dynamical or nonlocal scatterings
- Intermediate coupling -- a divergence in a BS equation (RPA pole)
- To go beyond the pole -- 1P order parameter is to be introduced
- Thermodynamic consistency between 1P propagators § 2PI vertex in parquet equations
- Linearized Ward identity -- self-energy in 1P propagators in parquet equations
- Schwinger-Dyson equation -- determines the physical self-energy (not self-consistent in parquet equations)



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Conclusions II

Parquet approach -- dísordered systems

- Parquet approach only to nonlocal vertices
 -- beyond mean field (CPA)
- Electron-hole symmetry on 2P level leads to a single nonlinear integral equation
- 2P vertex does not obey ward identity
- Ward identity induces restriction of the irreducible vertex in 2P space
- Corrections to 2PIR vertex to restore WI
- Full 2P vertex from a Bethe-Salpeter equation with a restricted irreducible vertex and WI corrections
- Physical quantities from the full vertex obeying WI



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