Green functions in the renormalized many-body perturbation theory

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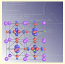

Outline

1. Many-body interacting electrons
2. Renormalized perturbation theory
    - Static renormalizations
    - Dynamical corrections & Green functions
    - Fundamental equations
3. 1P approach - renormalization of perturbation expansion
    - Baym-Kadanoff construction
    - Ambiguity in relating 1P & 2P functions
4. 2P approach – Mean-field theory with 2P self-consistency
    - 2P vertex & 2P self-consistency
    - Reduced parquet equations - effective interaction
    - One-particle functions and self-energies
5. Conclusions

Systems of interacting quantum particles

1. Indistinguishable particles – exchange interaction
   Individual quantum particles cannot be followed
   Coherent many-body state (fluid) instead

2. Measurable only asymptotic (scattering) states
   Theoretical picture – separable quasiparticles

3. Thermodynamics is coupled with dynamics due to non-trivial quantum many-body vacuum

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Major question: How do quasiparticles emerge from the many-body coherent state?

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Perturbation theory: A relation between interacting and renormalized non-interacting systems

Representing quantum many-body systems

- Fock space of quantum states – Bose & Fermi statistics
- Grand canonical statistical ensemble ($N \approx 10^{23}$)
- Basis: (anti)symmetrized products of eigenstates of the one-particle Hamiltonian $\widehat{H}_0$
- Creation & annihilation operators: $a^\dagger_\alpha, a_\alpha$
- Fundamental commutation relations

$$\left[a_\alpha, a^\dagger_\beta\right]_\pm \equiv a_\alpha a^\dagger_\beta \pm a^\dagger_\beta a_\alpha = \delta_{\alpha,\beta}$$

- Particle interaction $\widehat{V}$ – bare dynamical scattering potential in the Fock space built on eigenstates of $\widehat{H}_0$

Interacting fermions – generic Hamiltonians

- Single-orbital Hubbard (tight-binding) model for
  long-range many-body fluctuations

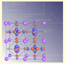
$$\widehat{H}_H = \sum_{\mathbf{k},\sigma} \epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_i \widehat{n}_{i\uparrow} \widehat{n}_{i\downarrow}$$

- Falicov-Kimball model for static
  thermally equilibrated fluctuations

$$\widehat{H}_{FK} = -t \sum_{<ij>} c^\dagger_i c_j + \sum_i \epsilon_i f^\dagger_i f_i + U \sum_i c^\dagger_i c_i f^\dagger_i f_i$$

- Single impurity Anderson model for
  local quantum fluctuations

$$\widehat{H}_{SIAM} = -t \sum_{<ij>\sigma} c^\dagger_{i\sigma} c_{j\sigma} + E_f \sum_\sigma f^\dagger_\sigma f_\sigma + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow + \sum_{i,\sigma} \left(V_i c^\dagger_{i\sigma} f_\sigma + V^*_i f^\dagger_\sigma c_{i\sigma} \right)$$



Quantum fluctuations

Quantum fluctuations: $\left[\Delta\widehat{H}, \widehat{H}_0\right] \neq 0$

Effect of correction $\Delta\widehat{H} = \widehat{H}_I + \widehat{H}_{ext}$
to be determined

$\widehat{H}_0$ – Exact Solution

$\widehat{H}_{ext}$ – Linear Response Theory

$\widehat{H}_I$ – Perturbation Theory

Thermodynamic potential & perturbation

- Grand potential

$$\Omega[H_0, H_I, H_{ext}] = -\beta^{-1} \log \mathrm{Tr}\left[\exp\left\{-\beta\left(\widehat{H}_0 - \mu\widehat{N} + \underbrace{\widehat{H}_I + \widehat{H}_{ext}}_{\text{perturbation}}\right)\right\}\right]$$

- External perturbation for accessible (quantum) phases

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

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

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

$$+ \sum_\sigma \left[\bar{\xi}^{||}_\sigma(1,2)c_\sigma(1)c_\sigma(2) + \xi^{||}_\sigma(1,2)c^\dagger_\sigma(1)c^\dagger_\sigma(2)\right] \Big\}$$

with $1 = (\mathbf{R}_1, \tau_1)$ and η, ξ symmetry-breaking fields

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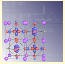

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Weak-coupling mean-field approximation

- Gibbs-Bogoljubov inequality

$$\Omega\left\{\widehat{H}\right\} \leq \Omega\left\{\widehat{H}_0\right\} + \left\langle \Delta\widehat{H}\right\rangle_0$$

- Hartree-Fock parameters (unrestricted)

$$\widehat{H}_0 = \sum_{\mathbf{k},\sigma} \epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{i}\sigma} \left(E_{\mathbf{i}\sigma} - \mu - \sigma h_{\mathbf{i}}\right) \widehat{n}_{\mathbf{i}\sigma}$$

$$\langle \Delta\widehat{H}\rangle_0 = \sum_{\mathbf{i}} \left[U n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} - \sum_{\sigma} E_{\mathbf{i}\sigma} n_{\mathbf{i}\sigma}\right]$$

where $n_{\mathbf{i}\sigma} = \langle \widehat{n}_{\mathbf{i}\sigma}\rangle_0$

- Parameters $E_{\mathbf{i}\sigma}$ minimize the r.h.s. of GB inmequlity
- Homogeneous solution: $E_\sigma = U n_{-\sigma}$

Strong-coupling mean-field approximation

- Decomposition of the full Hamiltonian

$$\widehat{H} = \sum_\alpha \lambda_\alpha \widehat{H}_\alpha$$

- Convexity of the thermodynamic potential ($\sum_\alpha \lambda_\alpha = 1$)

$$\sum_\alpha \lambda_\alpha \Omega\left\{\widehat{H}_\alpha\right\} \leq \Omega\left\{\widehat{H}\right\}$$

- Sum of two Falicov-Kimball models

$$\lambda_\alpha \widehat{H}_\alpha = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + \lambda_\alpha \sum_{\mathbf{i}\sigma} (E^\alpha_\sigma - \mu_\sigma)\, \widehat{n}_{\mathbf{i}\sigma} + U\lambda_\alpha \sum_{\mathbf{i}} \widehat{n}_{\mathbf{i}\uparrow}\widehat{n}_{\mathbf{i}\downarrow}$$

- Restriction: $\sum_\alpha \lambda_\alpha E^\alpha_\sigma = 0$
- Infinite spatial dimensions (mean-field solution) – thermodynamically consistent Hubbard III

Averaged quantum fluctuations – Fermi liquid theory I

- Adiabatic switching of interaction – number of low-lying excitations identical with the Fermi gas
- Quasiparticle excitations $\delta n_{\mathbf{k},\sigma}(t)$ with Fermi statistics
- Macroscopic (time averaged) energy functional – Landau scattering function $f(\mathbf{k},\mathbf{k}';\sigma,\sigma')$

$$E[\delta n_{\mathbf{k},\sigma}] = \sum_{\mathbf{k},\sigma} \left(\epsilon(\mathbf{k}) + V_{\mathbf{k}\sigma}\right) \overline{\delta n_{\mathbf{k},\sigma}(t)} + \frac{1}{2V} \sum_{\mathbf{k}\mathbf{k}',\sigma\sigma'} f(\mathbf{k},\mathbf{k}';\sigma,\sigma') \overline{\delta n_{\mathbf{k},\sigma}(t)\delta n_{\mathbf{k}',\sigma'}(t)}$$

Averaged quantum fluctuations – Fermi liquid theory II

- Ergodic theorem: $\overline{\delta n_{\mathbf{k},\sigma}(t)} = \langle \delta n_{\mathbf{k},\sigma} \rangle$
- Linear, Hartree decoupling

$$\overline{\delta n_{\mathbf{k},\sigma}(t)\delta n_{\mathbf{k}',\sigma'}(t)} = \langle \delta n_{\mathbf{k},\sigma} \rangle \langle \delta n_{\mathbf{k}',\sigma'} \rangle$$

- Fermi statistics

$$\langle \delta n_{\mathbf{k},\sigma} \rangle = \frac{1}{\exp\{-\beta(\epsilon_{\mathbf{k}} + V_{\mathbf{k}\sigma} + U_{\mathbf{k},\sigma})\} + 1} - \theta(k_F - k)$$

- Effective interaction due to external perturbations $V_{\mathbf{k}\sigma}$

$$U_{\mathbf{k},\sigma} = \frac{1}{V} \sum_{\mathbf{k}',\sigma'} f(\mathbf{k}, \mathbf{k}'; \sigma, \sigma') \langle \delta n_{\mathbf{k}',\sigma'} \rangle$$

Landau scattering function f either experiment (phenomenology) or perturbations theory (microscopic)

Many-body perturbation theory – Green functions

- Unperturbed Hamiltonian $\widehat{H}_0 = \sum_{\mathbf{k}\sigma} \left(\epsilon(\mathbf{k}) - \mu - \sigma h\right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$
- Time-dependent operators $c_{\mathbf{k}\sigma}(\tau) = \exp\{\tau \widehat{H}_0\} c_{\mathbf{k}\sigma} \exp\{-\tau \widehat{H}_0\}$

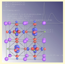
$$c^\dagger_{\mathbf{k}\sigma}(\tau) = \exp\{\tau \widehat{H}_0\} c^\dagger_{\mathbf{k}\sigma} \exp\{-\tau \widehat{H}_0\}$$

- Notice: $c^\dagger_{\mathbf{k}\sigma}(\tau) \neq c_{\mathbf{k}\sigma}(\tau)^\dagger = c^\dagger_{\mathbf{k}\sigma}(-\tau)$
- Green functions - general matrix elements

$$G_{(n)}(1,\ldots,n,\bar{n},\ldots,\bar{1}) = \frac{(-1)^n}{\hbar^n}$$

$$\frac{1}{\mathcal{Z}} \mathrm{Tr}_0 \mathcal{T} \left[c\,(1) \ldots c\,(n), c^\dagger(\bar{n}) \ldots c^\dagger(\bar{1}) \exp\left\{ -\int_0^\beta d\tau \widehat{H}_I(\tau) \right\} \right]$$

- Trace: $\mathrm{Tr}_0 \widehat{X} = \mathrm{Tr}\left[\widehat{X} \exp\{-\beta(\widehat{H}_0\}\right]$
- Partition sum: $\mathcal{Z} = \mathrm{Tr}_0 \mathcal{T} \exp\left\{ -\int_0^\beta d\tau \widehat{H}_I(\tau) \right\}$



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Matsubara formalism – diagonal bare propagators

- Unperturbed Green function in a diagonal form

$$G^{(0)}_\sigma(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu + \sigma h - \epsilon(\mathbf{k})}$$

- Functional-integral representation of the partition sum

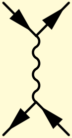
$$\mathcal{Z}\left[G^{(0)}, U\right] = \int \mathcal{D}\psi\mathcal{D}\psi^* \exp\left\{\sum_{\mathbf{k}}\sum_{n\sigma} e^{i\omega_n 0^+}\psi^*_{n\sigma}(\mathbf{k})\left[\underbrace{i\omega_n + \mu + \sigma h - \epsilon(\mathbf{k})}_{G^{(0)}_\sigma(\mathbf{k},i\omega_n)^{-1}}\right]\psi_{n\sigma}(\mathbf{k}) - U\sum_i \int_0^\beta d\tau\ \underbrace{\widehat{n}^d_\uparrow(\tau,\mathbf{R}_i)\widehat{n}^d_\downarrow(\tau,\mathbf{R}_i)}_{\text{dynamical scatterer}}\right\}$$

$\psi^*_{n\sigma}(\mathbf{k})$ and $\psi_{n\sigma}(\mathbf{k})$ are Grassmann variables

Perturbation expansion - graphical representation

Perturbation theory – expansion in the interaction strength

- Particle propagator $\bar{1}$  1
- Hole propagator 1  $\bar{1}$
- Interaction (photon exchange)



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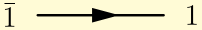
- Particle propagator 

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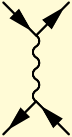
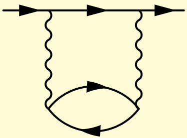
- Interaction (photon exchange) 
- 1P Scattering 

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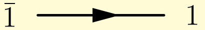

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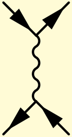
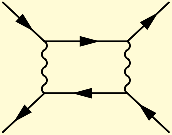


- 2P Scattering



1P & 2P Green functions

- Density matrix: $\widehat{\rho}_H = \exp\left\{-\beta\widehat{H}\right\} / \mathrm{Tr}\exp\left\{-\beta\widehat{H}\right\}$
- One-particle Green function (propagator)

$$G(1\bar{1}) = -\frac{1}{\hbar}\mathrm{Tr}\left\{\widehat{\rho}\,\mathcal{T}\left[\widehat{\psi}_{\sigma_1}(\mathbf{R}_1,\tau_1)\,\widehat{\psi}_{\sigma_{\bar{1}}}(\mathbf{R}_{\bar{1}},\tau_{\bar{1}})^\dagger\right]\right\}$$

- Two-particle Green function

$$G_{(2)}(1\bar{1},3\bar{3}) = \frac{1}{\hbar^2}\mathrm{Tr}\left\{\widehat{\rho}\,\mathcal{T}\left[\widehat{\psi}_{\sigma_1}(\mathbf{R}_1,\tau_1)\widehat{\psi}_{\sigma_3}(\mathbf{R}_3,\tau_3)\widehat{\psi}_{\sigma_{\bar{3}}}(\mathbf{R}_{\bar{3}},\tau_{\bar{3}})^\dagger\widehat{\psi}_{\sigma_{\bar{1}}}(\mathbf{R}_{\bar{1}},\tau_{\bar{1}})^\dagger\right]\right\}$$

Schwinger, Dyson & Schwinger-Dyson equations

- Schwinger equation - matching 1P & 2P GF

$$G(1,\bar{1}) = G^{(0)}(1,\bar{1}) + \int d\bar{2}d2\, G^{(0)}(1,\bar{2})U(\bar{2}-2)G_{(2)}(\bar{1}\bar{2},22^{+})$$

- Dyson equation - self energy Σ (dynamical 1P scatterer)

$$G(1,\bar{1}) = G^{(0)}(1-\bar{1}) + \int d3d\bar{3}\, G^{(0)}(1-\bar{3})\Sigma(\bar{3},3)G(3,\bar{1})$$

- Two-particle vertex Γ

$$G_{(2)}(1\bar{1},3\bar{3}) = G(1,\bar{1})G(3,\bar{3}) + \int d1'd\bar{1}'d3'd\bar{3}'\, G(1,\bar{1}')G(1'\bar{1})\Gamma(1'\bar{1}',3'\bar{3}')G(3,\bar{3}')G(3'\bar{3})$$

Schwinger-Dyson equation: 2P vertex Γ & self-energy Σ used in the Schwinger equation

Irreducibility in Green functions

Dynamical scatterers – irreducible functions (vertices)

- 1P reducibility – cutting one particle line splits the diagram in two
  1P irreducible 1P GF – self-energy Σ
  1P irreducible 2P GF – 2P vertex Γ
- 2P reducibility – cutting two particle lines splits the diagram in two
- Three types of 2P irreducibility – 2PIR vertices Λ^{α} (2P dynamical scatterers)
  - Electron-hole irreducibility: Λ^{eh}
  - Electron-electron (hole-hole) irreducibility: Λ^{ee}
  - Electron-hole irreducibility of vacuum pairs: Λ^{U}

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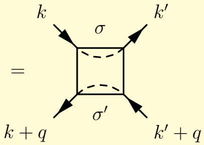
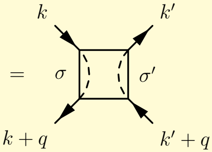
Direct and transpose 2P vertex

- Direct Γ and transpose Γ^t vertices

$\Gamma_{\sigma\sigma'}(k, k'; q) =$



$\Gamma^t_{\sigma\sigma'}(k, k'; q) =$



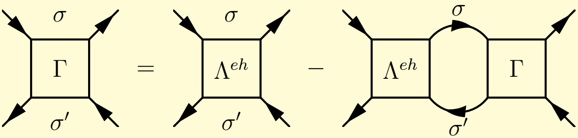
four-vector notation: $k = (\mathbf{k}, i\omega_n)$ for fermions,
$q = (\mathbf{q}, i\nu_m)$ for bosons

- Charge & spin are conserved in normal vertices
- Symmetry relation: $\Gamma^t_{\sigma\sigma}(k, k'; q) = -\Gamma_{\sigma\sigma}(k, k+q; k'-k)$

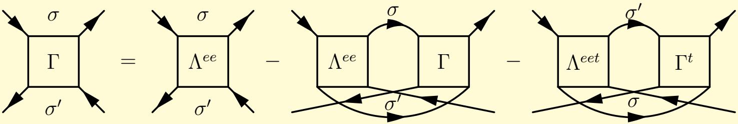
2P scatterings – Bethe-Salpeter equations

2P irreducible vertices – Bethe-Salpeter equations I

- Electron-hole Bethe-Salpeter equation

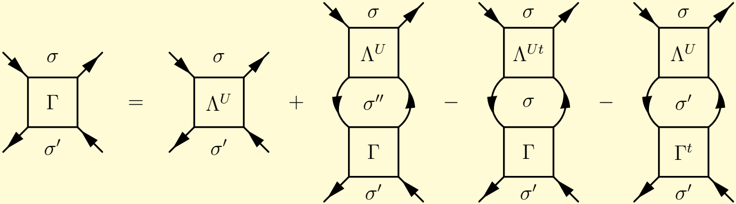


- Electron-electron Bethe-Salpeter equation



2P irreducible vertices – Bethe-Salpeter equations II

- Bethe-Salpeter equation with virtual electron-hole pairs (mixes normal and transpose vertices)



- Double-prime spin indices are dummy (integration) variables

1P & 2P renormalizations

Renormalizations of the perturbation expansion : self-consistent equations for irreducible functions

- 1P self-consistency: $\Sigma[G^{(0)}, U] \to \Sigma[G, U]$
  $\Lambda^{\alpha}[G^{(0)}, U] = \Lambda^{\alpha}[G, U]$
- 2P self-consistency: $\Sigma[G, U] \to \Sigma[G, \Lambda^{\alpha}]$
  $\Lambda^{\alpha}[G, U] \to \Lambda^{\alpha}[G, \Lambda^{\beta}]$
- 1P propagator

$$G_{\sigma}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu_{\sigma} - \epsilon(\mathbf{k}) - \Sigma_{\sigma}(\mathbf{k}, i\omega_n)}$$

$(\mu_{\sigma} = \mu + \sigma h)$

1P self-consistency not enough to control critical behavior!

Baym-Kadanoff – 1P self-consistency

- Renormalized grand potential – generating functional

$$\frac{1}{N}\Omega[G,\Sigma] = -\frac{1}{\beta N}\sum_{\sigma,\omega_n,\mathbf{k}} e^{i\omega_n 0^+}\left\{\ln\left[i\omega_n + \mu_\sigma - \epsilon(\mathbf{k}) - \Sigma_\sigma(\mathbf{k}, i\omega_n)\right]\right.$$
$$\left. + G_\sigma(\mathbf{k}, i\omega_n)\Sigma_\sigma(\mathbf{k}, i\omega_n)\right\} + \Phi[G,U]$$

- Equilibrium from stationarity conditions

$$\frac{\delta\Omega[G,\Sigma]}{\delta G_\sigma(\mathbf{k}, i\omega_n)} = 0 = \frac{\delta\Omega[G,\Sigma]}{\delta\Sigma_\sigma(\mathbf{k}, i\omega_n)}$$

- Luttinger-Ward functional $\Phi[G,U]$ from renormalized PT
- Irreducible vertices from the Luttinger-Ward functional

$$\Sigma_\sigma(k) = \frac{\delta\Phi[G,U]}{\delta G_\sigma(k)}\,, \quad \Lambda_{\sigma\sigma'}(k,k';q) = \frac{\delta\Sigma_\sigma(k,k')}{\delta G_{\sigma'}(k'+q,k+q)}$$

Conservation laws – Ward identities

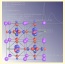
- Particle-mass conservation – continuity equation – integral Ward identity

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

- Particle-interaction conservation – mass and charge of electron indivisible – sum rule

$$\frac{\partial\Omega(U,\mu_{\mathbf{i}\sigma})}{\partial U} = \sum_{\mathbf{i}}\left[\frac{\delta^2\Omega}{\delta\mu_{i\Uparrow}\delta\mu_{i\Downarrow}} + \frac{\delta\Omega}{\delta\mu_{i\Uparrow}}\frac{\delta\Omega}{\delta\mu_{i\Downarrow}}\right] = \sum_i\left\{\frac{k_B T}{4}\left[\kappa_{ii}-\chi_{ii}\right] + n_{i\Uparrow}n_{i\Downarrow}\right\}$$

with local compressibility κ_{ii} and susceptibility χ_{ii}



Schwinger-Dyson equation vs. Ward identity

Two ways to connect 1P and 2P vertices

- Schwinger-Dyson equation

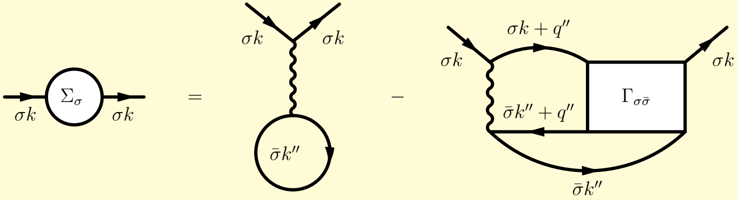
$$\Sigma_\sigma(\mathbf{k}, i\omega_n) = \frac{U}{2}(n - \sigma m) - \frac{U}{N^2}\sum_{\mathbf{k}'',\mathbf{q}} \frac{1}{\beta^2}\sum_{\omega_l,\nu_m} G_\sigma(\mathbf{k}'', i\omega_l) G_{\bar\sigma}(\mathbf{k}'' + \mathbf{q}, i\omega_l + i\nu_m) \times \Gamma_{\sigma\bar\sigma}(\mathbf{k}'', i\omega_l, \mathbf{k}, i\omega_n; \mathbf{q}, i\nu_m) G_{\bar\sigma}(\mathbf{k} + \mathbf{q}, i\omega_n + i\nu_m)$$

$(\bar\sigma = -\sigma)$

Schwinger-Dyson equation vs. Ward identity

Two ways to connect 1P and 2P vertices

- Schwinger-Dyson equation



Schwinger-Dyson equation vs. Ward identity

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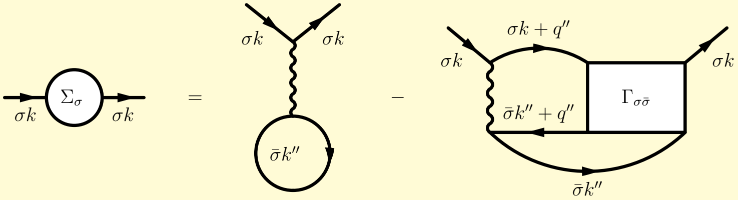
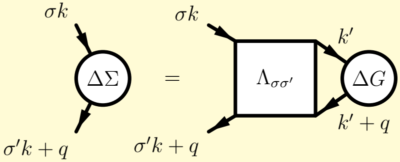


- Ward identity



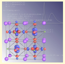
Ambiguity in the perturbation theory I

- Ward identity imposes restriction on 2P vertex in the Schwinger-Dyson equation
- Gauge transformation: dynamical interaction $U(\mathbf{q}, i\nu_m)$ and chemical potential $\mu_\sigma(\mathbf{k}, i\omega_n)$

$$\underbrace{\frac{\delta\Phi[U,G]}{\delta U(\mathbf{q}, i\nu_m)}}_{\text{Schwinger-Dyson}} = \underbrace{-\frac{1}{\beta N}\sum_{\mathbf{k},\omega_n}\frac{\delta G_\sigma(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_m)}{\delta\mu_{-\sigma}(\mathbf{k}, i\omega_n)}}_{\text{Ward}}$$

- Exact solution for self-energy (Schwinger field theory)

$$\Sigma = U\left\langle G - G\left[1 + \frac{\delta\Sigma}{\delta G}GG\star\right]^{-1}\frac{\delta\Sigma}{\delta G}GG\right\rangle$$



Ambiguity in the perturbation theory II

- Exact solution for *eh* irreducible vertex

$$\Lambda^{eh}_{\sigma\bar{\sigma}} = U - U\left[1 + G_\sigma G_{\bar{\sigma}} \Lambda^{eh}_{\sigma\bar{\sigma}} \star\right]^{-1} G_\sigma \left\{ \Lambda^{eh}_{\sigma\bar{\sigma}} + G_{\bar{\sigma}} \frac{\delta \Lambda^{eh}_{\sigma\bar{\sigma}}}{\delta G_{\bar{\sigma}}} \right\} \times \left[1 + \star G_\sigma G_{\bar{\sigma}} \Lambda^{eh}_{\sigma\bar{\sigma}}\right]^{-1} \circ G_{\bar{\sigma}}$$

- Electron-hole $\star$ and electron-electron $\circ$ channels coupled

No approximate solution complies with indivisibility of charge and mass

Either single self-energy with two vertices or vice versa
Baym-Kadanoff – single self-energy & two vertices

Example: Simple approximations I

- Luttinger-Ward for Hartree approximation

$$\Phi_{Hartree}[G,U] = \frac{U}{N^2}\sum_{\mathbf{k},\mathbf{k}'}\frac{1}{\beta^2}\sum_{\omega_n\omega_{n'}} e^{i(\omega_n+\omega_{n'})0^+} G_\uparrow(\mathbf{k},i\omega_n)G_\downarrow(\mathbf{k}',i\omega_{n'})$$

- Self-energy from stationarity of $\Omega[G,\Sigma]$ =SDE

$$\Sigma_\sigma^{Hartree}(\mathbf{k},i\omega_n) = U\frac{1}{\beta N}\sum_{\omega_{n'},\mathbf{k}'} e^{i\omega_n 0^+} G_{\bar\sigma}(\mathbf{k}',i\omega_n') = Un_{\bar\sigma}$$

- Dyson equation from stationarity of $\Omega[G,\Sigma]$

$$G_\sigma(\mathbf{k},i\omega_n) = \frac{1}{i\omega_n + \mu_\sigma - \epsilon(\mathbf{k}) - Un_{\bar\sigma}}$$

Example: Simple approximations II

- Irreducible vertex from WI (second variation of $\Omega[G, \Sigma]$)

$$\Lambda^{Hartree}_{\sigma\sigma'} = \frac{\delta\Sigma_\sigma}{\delta G_{\sigma'}} = U\delta_{\sigma',\bar{\sigma}}$$

- Full 2P vertex from Bethe-Salpeter equation

$$\Gamma^{WI}_{\uparrow\downarrow}(\mathbf{q}, i\nu_m) = \frac{U}{1 + U\phi_{\uparrow\downarrow}(\mathbf{q}, i\nu_m)}$$

- Electron-hole bubble

$$\phi_{\uparrow\downarrow}(\mathbf{q}, i\nu_m) = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\beta}\sum_{\omega_n}\left[G_\downarrow(\mathbf{k}+\mathbf{q}, i\omega_{n+m}) + G_\downarrow(\mathbf{k}-\mathbf{q}, i\omega_{n-m})\right] G_\uparrow(\mathbf{k}, i\omega_n)$$

Example: Simple approximations III

$$\Gamma^{WI}_{\uparrow\downarrow} \neq \Gamma^{SDE}_{\uparrow\downarrow} = 0$$

- Spectral self-energy – Bethe-Salpeter in Schwinger-Dyson with $\Lambda^{Hartree}_{\uparrow\downarrow}$: $\Gamma^{WI}_{\uparrow\downarrow} \to \Gamma^{SDE}_{\uparrow\downarrow}$

$$\Sigma^{Sp}_{\sigma}(\mathbf{k},\omega_+) = \frac{U}{N}\sum_{\mathbf{q}} P\int_{-\infty}^{\infty}\frac{dx}{\pi}\left\{ b(x) G_{\bar\sigma}(\mathbf{k}+\mathbf{q},\omega_+ + x) \times \Im\left[\frac{1}{1+U\phi_{\uparrow\downarrow}(\mathbf{q},x_+)}\right] - \frac{f(x+\omega)}{1+U\phi_{\uparrow\downarrow}(\mathbf{q},x_-)}\Im G_{\bar\sigma}(\mathbf{k}+\mathbf{q},x+\omega_+)\right\}$$

with $x_\pm = x \pm i0^+$ and $\bar\sigma = -\sigma$

Example: Simple approximations IV

- RPA propagator

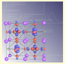
$$G(\mathbf{k},\omega_+) = \frac{1}{\omega_+ + \mu - \epsilon(\mathbf{k}) - \Sigma^{Sp}(\mathbf{k},\omega_+)}$$

- FLEX Luttinger-Ward

$$\Phi_{FLEX}[G,U] = \frac{1}{N}\sum_{\mathbf{q}} P\int_{-\infty}^{\infty}\frac{d\omega}{\pi} b(\omega)\Im\left[U\phi_{\uparrow\downarrow}(\mathbf{q},\omega_+)\right.$$
$$\left. - \ln\left(1 + U\phi_{\uparrow\downarrow}(\mathbf{q},\omega_+)\right)\right]$$

- New irreducible FLEX vertex: $\Lambda^{FLEX}_{\sigma\sigma'} = \delta\Sigma^{Sp}_{\sigma}/\delta G_{\sigma'} \neq U$

Unique 2P vertex is essential for unique criticality



2P approach to many-body systems I

2PIR vertex Λ replaces Φ/Σ as the generating functional of renormalized approximations

- Singular vertex Γ from the Bethe-Salpeter equation with regular irreducible vertex Λ
- Critical symmetry-breaking field η separates 1P functions
- Odd and even 1P functions

$$\Delta_\eta G(\mathbf{k}, i\omega_n) = \frac{1}{2}\left[G_\sigma(\mathbf{k}, i\omega_n; \eta) - G_{\bar\sigma}(\mathbf{k}, i\omega_n; -\eta)\right]$$

$$\bar{G}_\eta(\mathbf{k}, i\omega_n) = \frac{1}{2}\left[G_\sigma(\mathbf{k}, i\omega_n; \eta) + G_{\bar\sigma}(\mathbf{k}, i\omega_n; -\eta)\right]$$

- 2P functions only with even symmetry

2P approach to many-body systems II

- Odd self-energy – order parameter
  – from linearized Ward identity

$$\Delta_\eta \Sigma(\mathbf{k}, i\omega_n) = \frac{1}{\beta N} \sum_{\mathbf{k}', \omega_{n'}} \bar{\Lambda}_\eta(\mathbf{k}, i\omega_n, \mathbf{k}', i\omega_{n'}; 0, 0) \Delta_\eta G(\mathbf{k}', i\omega_{n'})$$

- Even self-energy – quantum dynamics
  – from Schwinger-Dyson equation

$$\bar{\Sigma}_\eta(\mathbf{k}, i\omega_n) = \frac{U}{2} n - \frac{U}{2N^2} \sum_\sigma \sum_{\mathbf{k}'\mathbf{q}} \frac{1}{\beta^2} \sum_{\omega_{n'}\nu_m} G_{\bar{\sigma}}(\mathbf{k} + \mathbf{q}, i\omega_n + i\nu_m)$$
$$\times G_\sigma(\mathbf{k}', i\omega_{n'}) \bar{\Gamma}_\eta(\mathbf{k}, i\omega_n, \mathbf{k}', i\omega_{n'}; \mathbf{q}, i\nu_m) G_{\bar{\sigma}}(\mathbf{k}' + \mathbf{q}, i\omega_{n'} + i\nu_m)$$

Vertex Γ_η from the critical Bethe-Salpeter equation with Λ_η

2P self-consistency – parquet equations

2P self-consistency to suppress spurious critical behavior

- Critical channel – electron-hole multiple scatterings
- Screening channel – electron-electron multiple scatterings
- Parquet equation – inequivalent 2P irreducibilities

$$\Gamma = \Lambda^\alpha + \mathcal{K}^\alpha = \mathcal{I}_l + \sum_{\alpha=1}^{l} \mathcal{K}^\alpha$$

- Two-channel parquet equations

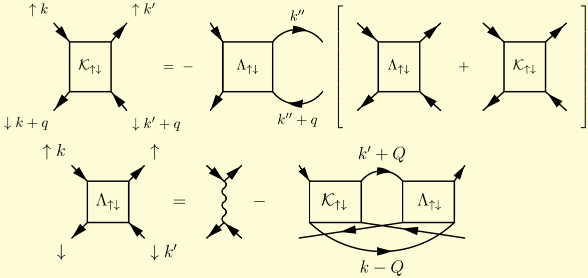
$$\mathcal{K}^\alpha = -\Lambda^\alpha GG \star (\mathcal{K}^\alpha + \Lambda^\alpha)$$
$$\Lambda^\alpha = \mathcal{I}\left[1 - GG \circ (\mathcal{K}^\alpha + \Lambda^\alpha)\right] - \mathcal{K}^\alpha GG \circ (\mathcal{K}^\alpha + \Lambda^\alpha)$$

Parquet equations with $\mathcal{I} = U$ suppress critical points

Reduced parquet equations ($\mathcal{I} = U$)

Suppress the terms of the parquet equations destroying the critical behavior

- Reduced parquet equations (spin singlet) graphically



dummy variables Q and k''

Mean-field approximation – effective interaction I

Irreducible vertex $\Lambda(k, k')$ approximated by a constant Λ

- Reducible vertex

$$\mathcal{K}(\mathbf{q}, i\nu_m) = -\frac{\Lambda^2 \phi(\mathbf{q}, i\nu_m)}{1 + \Lambda\phi(\mathbf{q}, i\nu_m)}$$

with $\phi(\mathbf{q}, i\nu_m) = \frac{1}{2\beta N}\sum_{\sigma,\mathbf{k},i\omega_n} G_{\bar{\sigma}}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_m) G_\sigma(\mathbf{k}, i\omega_n)$

- Irreducible vertex – inconsistent with a constant

$$\left[1 - \frac{\Lambda^2}{N}\sum_{\mathbf{q}}\frac{1}{\beta}\sum_{\nu_m}\phi(-\mathbf{q}, -i\nu_m) \times \frac{G_\uparrow(\mathbf{k}+\mathbf{q}, i\omega_{n+m}) G_\downarrow(\mathbf{k}'-\mathbf{q}, i\omega_{n'-m})}{1 + \Lambda\phi(-\mathbf{q}, -i\nu_m)}\right]\Lambda = U$$

Mean-field approximation – effective interaction II

Only approximate solutions – various options

- Local mean-field of metals at low temperatures – fermionic variables from Fermi energy

$$\Lambda \equiv \Lambda(0_+, 0_-) = \frac{U}{1 + \Lambda^2 K X}$$

$$K = -\phi(\mathbf{0}, 0) = \int_{-\infty}^{\infty} \frac{dx}{\pi} f(x) \Im \left[G(x_+)^2 \right]$$

- Screening integral

$$X = \int_{-\infty}^{\infty} \frac{dx}{\pi} \left\{ \frac{\Re\left[G(x_+) G(-x_+)\right]}{\sinh(\beta x)} \Im \left[\frac{1}{1 + \Lambda \phi(-x_+)} \right] - f(x) \Im \left[\frac{G(x_+) G(-x_+)}{1 + \Lambda \phi(-x_+)} \right] \right\}$$

Mean-field approximation – effective interaction III

- General lattice systems – Normalized averaging over irrelevant fermionic variables

$$\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{k}'}\frac{1}{\beta^2}\sum_{\omega_n,\omega_{n'}} G_\downarrow(-\mathbf{k},-i\omega_n)G_\uparrow(-\mathbf{k}',-i\omega_{n'})\left\{\left[1-\frac{\Lambda^2}{N}\sum_{\mathbf{q}}\frac{1}{\beta}\sum_{\nu_m}\phi(\mathbf{q},i\nu_m)\frac{G_\uparrow(\mathbf{k}+\mathbf{q},i\omega_{n+m})G_\downarrow(\mathbf{k}'-\mathbf{q},i\omega_{n'-m})}{1+\Lambda\phi(\mathbf{q},i\nu_m)}\right]\Lambda-U\right\}=0$$

- Solution

$$\Lambda=\frac{U\left(n^2-m^2\right)}{n^2-m^2+4\Lambda^2\mathcal{X}}$$

Mean-field approximation – effective interaction IV

- Charge and spin densities

$$n = \frac{2}{\beta N} \sum_{\mathbf{k},\omega_n} \bar{G}_\eta(\mathbf{k}, i\omega_n) e^{i\omega_n 0^+}$$

$$m = \frac{2}{\beta N} \sum_{\mathbf{k},\omega_n} \Delta G_\eta(\mathbf{k}, i\omega_n) e^{i\omega_n 0^+}$$

- Screening integral

$$\mathcal{X} = -\frac{1}{N} \sum_{\mathbf{q}} \frac{\psi(\mathbf{q}, i\nu_m)\psi(-\mathbf{q}, -i\nu_m)\phi(-\mathbf{q}, -i\nu_m)}{1 + \Lambda\phi(-\mathbf{q}, -i\nu_m)} > 0$$

- Critical point: $0 = 1 + \Lambda\phi(\mathbf{q}_0, 0)$

Mean-field approximation – effective interaction V

- Electron-electron bubble (spin-independent)

$$\psi(\mathbf{q},\omega_+) = \frac{1}{2N}\sum_{\sigma}\sum_{\mathbf{k}}\frac{1}{\beta}\sum_{\omega_n} G_{\bar{\sigma}}(\mathbf{q}+\mathbf{k}, i\omega_{m+n})G_{\sigma}(-\mathbf{k},-i\omega_n)$$

Only integrable singularities allowed due to self-consistent screening of the interaction

Freedom in selecting the equation for Λ does not change qualitatively the critical behavior

1P propagators – magnetic order

- Thermodynamic propagators (only static corrections)

$$G_\sigma(\mathbf{k},\omega_+) = \frac{1}{\omega_+ + \mu_\sigma - \epsilon(\mathbf{k}) + \sigma\Lambda\frac{m}{2} - U\frac{n}{2}}$$

used to determine thermodynamic properties (2P vertex)

- Full renormalized propagators

$$\mathcal{G}_\sigma(\mathbf{k},i\omega_n) = \frac{1}{i\omega_n + \mu_\sigma - \epsilon(\mathbf{k}) - \sigma\Delta\Sigma - U\frac{n}{2} - \bar{\Sigma}(\mathbf{k},i\omega_n)}$$

determines all physical (measurable) quantities

Fully 1P & 2P self-consistent theory: $G \to \mathcal{G}$

Self-energies

- Odd self-energy w.r.t. magnetic field – order parameter

$$\Delta\Sigma = -\Lambda[U; n, m]m/2$$

- Dynamical (spectral) self-energy

$$\bar{\Sigma}(\mathbf{k}, \omega_+) = -\frac{U\Lambda}{N}\sum_{\mathbf{q}} P\int_{-\infty}^{\infty}\frac{dx}{\pi}\left\{b(x)\bar{\mathcal{G}}(\mathbf{k}+\mathbf{q}, \omega_+ + x)\right.$$
$$\left.\times\Im\left[\frac{\bar{\Phi}(\mathbf{q}, x_+)}{1+\Lambda\phi(\mathbf{q}, x_+)}\right] - \frac{f(x+\omega)\bar{\Phi}(\mathbf{q}, x_-)}{1+\Lambda\phi(\mathbf{q}, x_-)}\Im\bar{\mathcal{G}}(\mathbf{q}+\mathbf{k}, x+\omega_+)\right\}$$

- Full self-energy: $\Sigma_\sigma(\mathbf{k}, \omega_+) = Un/2 + \sigma\Delta\Sigma + \bar{\Sigma}(\mathbf{k}, \omega_+)$

Both self-energies from the same vertex Λ

Physical quantities – spectral representation

- Charge density

$$n = -\frac{1}{N}\sum_{\mathbf{k}}\sum_{\sigma}\int_{-\infty}^{\infty}\frac{dx}{\pi}f(x)\Im\mathcal{G}_{\sigma}(\mathbf{k},x_+)$$

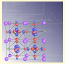
- Spin density

$$m = -\frac{1}{N}\sum_{\mathbf{k}}\sum_{\sigma}\sigma\int_{-\infty}^{\infty}\frac{dx}{\pi}f(x)\Im\mathcal{G}_{\sigma}(\mathbf{k},x_+)$$

- Two-particle bubble (even symmetry)

$$\bar{\Phi}(\mathbf{q},\omega_+) = -\frac{1}{2N}\sum_{\sigma}\sum_{\mathbf{k}}\int_{\infty}^{\infty}\frac{dx}{\pi}f(x)\left[\mathcal{G}_{\bar{\sigma}}(\mathbf{k}+\mathbf{q},x+\omega_+)\right.$$

$$\left.+\mathcal{G}_{\bar{\sigma}}(\mathbf{k}-\mathbf{q},x-\omega_+)\right]\Im\mathcal{G}_{\sigma}(\mathbf{k},x_+)$$



Conclusions I - Renormalizations

Many-body perturbation theory

- Spectrum of the full Hamiltonian unknown
- Fundamental objects – asymptotic states (quasiparticles)
- Interaction only perturbatively – source of scatterings
- Static renormalizations – mean-field theories
- Dynamical corrections – Green functions
- Renormalized perturbation theory – self-consistent determination of irreducible functions
- 1PIR vertex (Self-energy) – mass renormalization
- 2PIR vertices – charge renormalization

Conclusions II – Green functions

Ambiguous way to relate 1P and 2P Green functions

Two many-body approaches

- 1P approach – single self-energy & two 2P vertices
  - Inconsistent (ambiguous) critical behavior
  - Ordered phase does not match the disordered one
- 2P approach – single 2PIR vertex Λ & two self-energies
  - Unique criticality
  - Symmetry-breaking field splits the self-energy
  - Odd self-energy from WI – thermodynamic order parameter
  - Even self-energy from SDE – spectra & dynamics

Mean-field theory with 2P self-consistency:
analytically controlled approximation
interpolating between weak and strong coupling
& suppressing spurious poles (phase transitions)

Conclusions II – Green functions

Schwinger-Dyson equation & Ward identity incompatible with single self-energy and single 2P vertex

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