Multiple Scattering and Many-Body Green Functions

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THE MULTIPLE SCATTERING GREEN'S FUNCTION APPROACH TO ELECTRONIC STRUCTURE AND SPECTROSCOPY CALCULATIONS,

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Outline

Fundamental QM problem – Schrödinger equation

Single quantum particle in an external potential

- Hamiltonian operator in the Hilbert state space

$$\widehat{H} = \widehat{H}_0 + \widehat{V}$$

- Quantum dynamics: $[\widehat{H}_0, \widehat{V}] \neq 0$
- Stationary Schrödinger equation

$$\left(\widehat{H}_0 + \widehat{V}\right)|\Psi_E\rangle = E|\Psi_E\rangle$$

- Bound ($E < 0$) & scattering ($E > 0$) states

When spectrum of the full Hamiltonian is unavailable – Perturbative methods to be employed

Time-independent scattering theory

- Unperturbed particle

$$\widehat{H}_0 \left|\phi_\alpha\right\rangle = E_\alpha \left|\phi_\alpha\right\rangle$$

- Lippmann-Schwinger equation

$$\left|\Psi_E^{(\pm)}\right\rangle = \left|\phi\right\rangle + \left(E - \widehat{H}_0 \pm i\eta\right)^{-1} \widehat{V} \left|\Psi_E^{(\pm)}\right\rangle$$

- Operator form – T-matrix:

$$\widehat{T}(z) = \widehat{V} + \widehat{V}\left(z - \widehat{H}_0\right)^{-1} \widehat{T}(z)$$

- T-matrix in the basis of $\widehat{H}_0$

$$\left\langle \phi_\alpha \left| \widehat{T}(z) \right| \phi_\beta \right\rangle \equiv T_{\alpha\beta}(z) = V_{\alpha\beta} + \sum_\gamma \frac{V_{\alpha\gamma} T_{\gamma\beta}(z)}{z - E_\gamma}$$

Multiple scattering – T-matrix & dynamical renormalization of the scattering potential

Time-dependent potential – Green functions

- Bare (unperturbed) propagator – Green function

$$\left(i\hbar\frac{d}{dt} - \widehat{H}_0\right)\widehat{G}^{\pm}(t) = \widehat{I}\delta(t)$$

- Full propagator with the scattering potential

$$\left(i\hbar\frac{d}{dt} - \widehat{H}_0 - \widehat{V}(t)\right)\widehat{\mathcal{G}}^{\pm}(t, t_0) = \widehat{I}\delta(t - t_0)$$

- Lippmann-Schwinger equation for Green functions
  – interaction (Dirac) picture

$$\widehat{\mathcal{G}}^{\pm}(t, t') = \widehat{G}^{\pm}(t - t') + \int_{-\infty}^{\infty} dt''\widehat{G}^{\pm}(t - t'')\widehat{V}_D(t'')\widehat{\mathcal{G}}^{\pm}(t'', t')$$

Systems of interacting quantum particles

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

2. Scattering states – normal thermodynamic phase
   Bound states – ordered thermodynamic phase

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

Scattering events - via Feynman local (particle) space-time picture & Feynman diagrams
Real & virtual scatterings

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Representing quantum many-body systems

- Fock space of quantum states – Bose & Fermi statistics
- 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

Interacting fermions – generic Hamiltonians

- Interacting electrons – second quantization

$$\widehat{H} = \sum_{\alpha\beta} \left\langle \psi_\alpha \left| \widehat{H}_0 \right| \psi_\beta \right\rangle c^\dagger_\alpha c_\beta + \frac{1}{2} \sum_{ij} \sum_{\alpha\beta\gamma\delta} \left\langle \psi_\alpha \psi_\gamma \left| \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \right| \psi_\delta \psi_\beta \right\rangle c^\dagger_\alpha c^\dagger_\gamma c_\delta c_\beta$$

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

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

- Single impurity Anderson model for local quantum fluctuations

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

Thermodynamic potential & perturbation

- Grand potential

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

- External perturbation for accessible (quantum) phases

$$\begin{aligned} \widehat{H}_{ext} = \int d1d2 \Big\{ & \sum_\sigma \eta^{||}_\sigma(1,2) c^\dagger_\sigma(1) c_\sigma(2) \ldots \text{conserves charge \& spin} \\ & + \left[\eta^\perp(1,2) c^\dagger_\uparrow(1) c_\downarrow(2) + \bar{\eta}^\perp(1,2) c^\dagger_\downarrow(2) c_\uparrow(1) \right] \ldots \text{conserves charge} \\ & + \left[\bar{\xi}^\perp(1,2) c_\uparrow(1) c_\downarrow(2) + \xi^\perp(1,2) c^\dagger_\downarrow(2) c^\dagger_\uparrow(1) \right] \ldots \text{conserves spin} \\ & + \sum_\sigma \left[\bar{\xi}^{||}_\sigma(1,2) c_\sigma(1) c_\sigma(2) + \xi^{||}_\sigma(1,2) c^\dagger_\sigma(1) c^\dagger_\sigma(2) \right] \Big\} \end{aligned}$$

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

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Interaction representation (Dirac picture)

- Unperturbed Hamiltonian $\widehat{H}_0 = \sum_{\mathbf{k}\sigma} (\epsilon(\mathbf{k}) - \mu - \sigma h)\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$
- 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

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

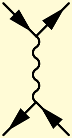
- Functional-integral representation of the partition sum

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

$\psi^*_{n\sigma}(\mathbf{k})$ 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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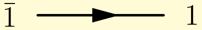
- Particle propagator 

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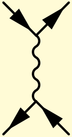
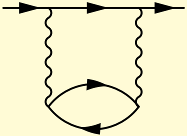
- Interaction (photon exchange) 
- 1P Scattering 

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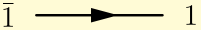
- Particle propagator 

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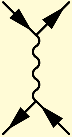
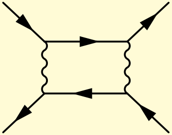
- Interaction (photon exchange) 
- 2P Scattering 

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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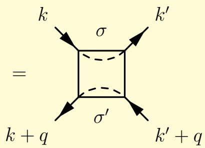
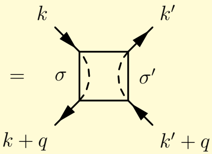
Direct and transpose 2P vertex

- Direct Γ and transpose Γ^t vertices

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

$\Gamma^{t}_{\sigma\sigma'}(k,k';q) =$ 

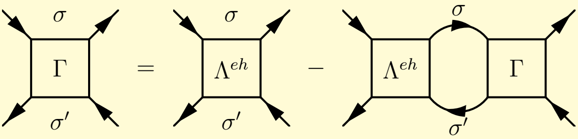
four-vector notation: $k = (\mathbf{k}, i\omega_n)$ for fermions,
$q = (\mathbf{q}, i\nu_m)$ for bosons

- Charge & spin are conserved in normal vertices
- Symmetry relation: $\Gamma^{t}_{\sigma\sigma}(k,k';q) = -\Gamma_{\sigma\sigma}(k,k+q;k'-k)$

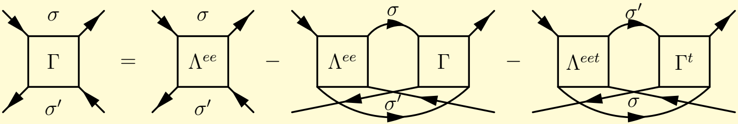
2P scatterings – Bethe-Salpeter equations

2P irreducible vertices – Bethe-Salpeter equations I

- Electron-hole Bethe-Salpeter equation

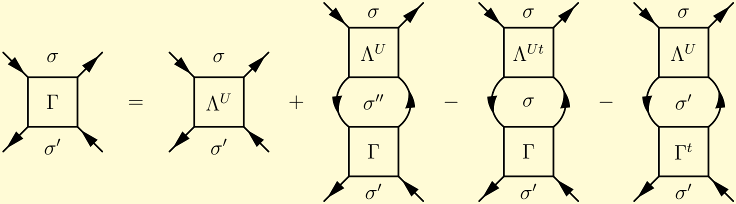


- Electron-electron Bethe-Salpeter equation



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 scatterings

Multiple scatterings in many-body systems: renormalization of 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

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

- 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 – no external sources of particle interaction – sum rule

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

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

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

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

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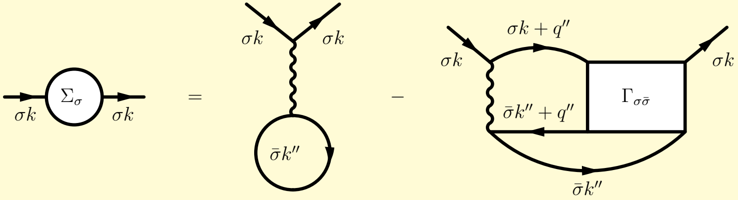

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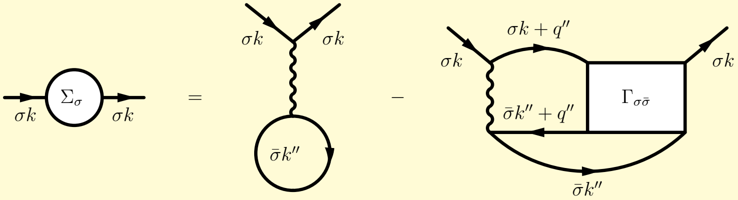

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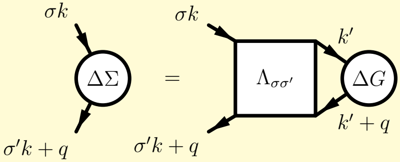

Ambiguity in the perturbation theory

- 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 $\mu_\sigma(\mathbf{k}, i\omega_n)$

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

- No approximate solution complies with indivisibility of charge and mass
- Either single self-energy with two vertices or vice versa

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Byam-Kadanoff – single self-energy & two vertices

Example: Hartree approximation I

- Renormalized functional of the grand potential

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

$$\left. + G_\sigma(\mathbf{k}, i\omega_n)\Sigma_\sigma(\mathbf{k}, i\omega_n)\right\} + U\prod_\sigma\left[\frac{1}{\beta N}\sum_{\omega_n,\mathbf{k}} e^{i\omega_n 0^+} G_\sigma(\mathbf{k}, i\omega_n)\right]$$

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

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

Example: Hartree approximation II

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

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

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

$$\Lambda_{\sigma\sigma'} = \frac{\delta \Sigma_\sigma}{\delta G_{\sigma'}} = U \delta_{\sigma', \bar{\sigma}}$$

- Full 2P vertex from Bethe-Salpeter equation

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

Example: Hartree approximation III

- Electron-hole bubble

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

- Schwinger-Dyson equation = Stationarity of $\Omega[G,\Sigma]$

$$\Sigma_{\sigma} = U n_{\bar{\sigma}}$$

- Vertex from SDE: $\Gamma^{SDE} = 0$

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

Unique 2P vertex is essential for unique criticality

2P approach to many-body systems I

2PIR vertex Λ – 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

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

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

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

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

$$\mathcal{K}^\alpha = -\Lambda^\alpha GG \star (\mathcal{K}^\alpha + \Lambda^\alpha)$$

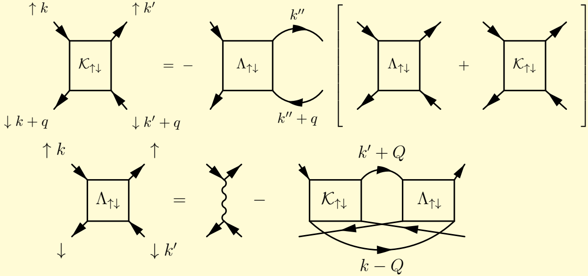
$$\Lambda^\alpha = \mathcal{I}\left[1 - GG \circ (\mathcal{K}^\alpha + \Lambda^\alpha)\right] - \mathcal{K}^\alpha GG \circ (\mathcal{K}^\alpha + \Lambda^\alpha)$$

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

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

with $\phi_{\uparrow\downarrow}(\mathbf{q}, i\nu_m) = \frac{1}{\beta N}\sum_{\mathbf{k}, i\omega_n} G_\uparrow(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_m)G_\downarrow(\mathbf{k}, i\omega_n)$

- Averaging over irrelevant redundant fermionic variables (non-universal & not uniquely defined)

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

Mean-field approximation – effective interaction II

- Charge and spin densities

$$n = \frac{1}{\beta N}\sum_{\sigma}\sum_{\mathbf{k},\omega_n} G_{\sigma}(\mathbf{k}, i\omega_n)e^{i\omega_n 0^+}$$

$$m = \frac{1}{\beta N}\sum_{\sigma}\sigma\sum_{\mathbf{k},\omega_n} G_{\sigma}(\mathbf{k}, i\omega_n)e^{i\omega_n 0^+}$$

- 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 III

- Electron-hole bubble (even symmetry)

$$\phi(\mathbf{q}, i\nu_m) = \frac{1}{2N}\sum_{\sigma}\sum_{\mathbf{k}}\frac{1}{\beta}\sum_{\omega_n}\left[G_{\bar{\sigma}}(\mathbf{k}+\mathbf{q}, i\omega_{n+m}) + G_{\bar{\sigma}}(\mathbf{k}-\mathbf{q}, i\omega_{n-m})\right] G_{\sigma}(\mathbf{k}, i\omega_n)$$

- Electron-electron bubble (spin-independent)

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

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

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

$$\mathcal{G}_\sigma(\mathbf{k},i\omega_n) = \frac{1}{i\omega_n + \mu_\sigma - \epsilon(\mathbf{k}) - \sigma\Delta\Sigma - \bar{\Sigma}_0 - \bar{\Sigma}(\mathbf{k},i\omega_n)}$$

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

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

- Static Hartree term: $\bar{\Sigma}_0 = Un/2$
- Dynamical (spectral) self-energy

$$\bar{\Sigma}(\mathbf{k}, \omega_+) = -\frac{U\Lambda}{N}\sum_{\mathbf{q}} P\int_{-\infty}^{\infty}\frac{dx}{\pi}\left\{b(x)\bar{\mathcal{G}}(\mathbf{k}+\mathbf{q}, \omega_+ + x)\right.$$

$$\left.\times\Im\left[\frac{\bar{\Phi}(\mathbf{q}, x_+)}{1+\Lambda\phi(\mathbf{q}, x_+)}\right] - \frac{f(x+\omega)\bar{\Phi}(\mathbf{q}, x_-)}{1+\Lambda\phi(\mathbf{q}, x_-)}\Im\bar{\mathcal{G}}(\mathbf{q}+\mathbf{k}, x+\omega_+)\right\}$$

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

- Full self-energy: $\Sigma_\sigma(\mathbf{k}, \omega_+) = \bar{\Sigma}_0 + \sigma\Delta\Sigma + \bar{\Sigma}(\mathbf{k}, \omega_+)$

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)

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

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

Conclusions I – Scatterings

Particle scatterings in many-body systems

- Spectrum of the full Hamiltonian unknown
- Fundamental objects – asymptotic states (quasiparticles)
- Interaction only perturbatively – source of scatterings
- Green functions describe propagation of quasiparticles
- Single particle scattering on (virtual) excitations of quantum vacuum – 1P irreducibility & self-energy – mass renormalization
- Two-particle scatterings via mutual photon exchange – 2P irreducibility & multiple 2PIR vertex functions – charge renormalization

Multiple scatterings – renormalization of irreducible Green functions with 1P & 2P self-consistencies

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Multiple scatterings – renormalization of irreducible Green functions with 1P & 2P self-consistencies

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 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

Conclusions II - Green functions

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

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References – 2P self-consistent approach

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