Two-particle renormalizations in many-fermion perturbation theory

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Perturbaton theory

- Systematic tool for developing analytically controlled approximations
- Diagrammatic representation – appealing physical interpretation
- Microscopic understanding of physical phenomena
- Modern approach – diagrammatic input into exact equations of motion

Model calculations

- Long-range length scales only
- Collective response and cooperative behavior
- More advaced methods can be developed and explored

Layout

1. *Diagrammatic renormalizations*
2. *Thermodynamic quantities in renormalized theories*
3. *One-particle (mass) renormalizations – Baym-Kadanoff*
4. *Two-particle renormalizations – non-self-consistent & self-consistent*
5. *Parquet equations – charge renormalization*
6. *Solution of simplified parquet equations*
7. *Conclusions & perspectives*

Need for a renormalized perturbation expansion

- **Effects of "irrelevant" (noncritical) part of PT**
  - ✗ Fermi liquid – weak-coupling quasiparticle picture, "mass renormalization"
  - ✗ Mean-field global bahavior – Hartree, Gutzwiller, DMFT
- **Strong dynamical fluctuations (without apparent thermodynamic order)**
  - ✓ Non-Fermi-liquid behavior
  - ✓ Mott-Hubbard MIT
- **Collective critical phenomena (in particular in low dimensions)**
  - ✔ Thermodynamic (quantum) phase transitions – phase stability
  - ✔ Formation and condensation of bound and resonant states

Demands and restrictions on diagrammatic renormalizations

- Thermodynamic consistence – generating thermodynamic potential
- Absence of unphysical behavior – no spurious poles
- Macroscopic conservation laws should be obeyed
- Causality should be acomplished
- No double counting of diagrams
- Controllable theory – anchor points (exact limits), “small parameters”

Model & input parameters

One-band model Hamiltonian

$$\widehat{H}_H = \sum_{\mathbf{k}\sigma} \left(\epsilon(\mathbf{k}) - \mu + \sigma B\right) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} \widehat{n}_{\mathbf{i}\uparrow} \widehat{n}_{\mathbf{i}\downarrow} \tag{1}$$

Multi-orbital Hubbard Hamiltonian

$$H^{\mathrm{Hubb}} = \sum_{\mathbf{R}\lambda,\mathbf{R}'\lambda'} t_{\mathbf{R}\lambda,\mathbf{R}'\lambda'}\, a^{+}_{\mathbf{R}\lambda}\, a_{\mathbf{R}'\lambda'} + \sum_{\mathbf{R},\lambda,\lambda'} U_{\mathbf{R}\lambda\lambda'}\, n_{\mathbf{R}\lambda}\, n_{\mathbf{R}\lambda'} \tag{2}$$

LMTO input (lattice structure)

$$H^{\mathrm{LMTO}}_{\mathbf{R}\lambda,\mathbf{R}'\lambda'} = C_{\mathbf{R}\lambda\lambda'}\, \delta_{\mathbf{R}\mathbf{R}'} + \Delta^{1/2}_{\mathbf{R}\lambda}\, S^{\gamma}_{\mathbf{R}\lambda,\mathbf{R}'\lambda'}\, \Delta^{1/2}_{\mathbf{R}'\lambda'} \tag{3}$$

where $\lambda = (L\sigma) = (\ell m\sigma)$ is the spinorbital index

Relevant input parameters:

t – hopping amplitude (kinetic energy, particle mass)
U – Coulomb interaction (particle charge squared)
μ – chemical potential (Fermi energy, particle number)

Thermodynamic quantities and external perturbations

Grand potential

$$\Omega(t, U; T, \mu) = -k_B T \ln \mathrm{Tr} \exp -\beta(\widehat{H} - \mu \widehat{N}\}) \tag{4}$$

- External sources used to disturb equilibrium
- Stability with respect to small perturbations – linear response
- Quantum systems allow for "anomalous" nonconserving sources

$$\widehat{H} \longrightarrow \widehat{H} + \widehat{H}_{ext}$$

$\eta^{||}$ - conserving source (spin, charge density)
$\xi^{||}$ - adds spin and charge
$\eta^{\perp}$ - adds spin, preserves charge
$\xi^{\perp}$ - adds charge, preserves spin

complex fields - anomalous responses

$$
\begin{aligned}
\widehat{H}_{ext} = \int d1d2 \Big\{ \sum_\sigma \Big[& \eta^{||}_\sigma(1,2) c^\dagger_\sigma(1) c_\sigma(2) \\
& + \bar{\xi}^{||}_\sigma(1,2) c_\sigma(1) c_\sigma(2) + \xi^{||}_\sigma(1,2) c^\dagger_\sigma(1) c^\dagger_\sigma(2) \Big] \\
& + \Big[\eta^{\perp}(1,2) c^\dagger_\uparrow(1) c_\downarrow(2) + \bar{\eta}^{\perp}(1,2) c^\dagger_\downarrow(2) c_\uparrow(1) \Big] \\
& + \Big[\bar{\xi}^{\perp}(1,2) c_\uparrow(1) c_\downarrow(2) + \xi^{\perp}(1,2) c^\dagger_\downarrow(2) c^\dagger_\uparrow(1) \Big] \Big\} \quad (5)
\end{aligned}
$$

where labels $1 = (\mathbf{r}_1, \tau_1)$, $2 = (\mathbf{r}_2, \tau_2)$, etc

Generalized susceptibilities – criteria for local stability from two-particle functions

$$
\widehat{\chi}^\alpha = \frac{\delta^2 \Phi[H_{ext}]}{\delta H_\alpha \delta H_{\bar{\alpha}}} \geq 0
$$

α – channel index

At instability (divergence in χ^α) – LRO sets in

Order parameters – Legendre conjugates to the relevant external sources H_α

Summation of diagrams

Bare expansion in $G^{(0)}$

Diagrams summed term by term in powers of the interaction strength: unbiased PT thermodynamic potential $\Omega[G^0, U]$ – suitable in situations with large diagram cancellations

Renormalized summations in G – conserving approximations

Naive: Closed connected diagrams, free of self-energy insertions, in the 1P renormalized propagator directly for a thermodynamic potential – explicit generating Luttinger-Ward functional $\Phi[G, U]$; thermodynamic Φ-derivable approximations

Standard: One-particle irreducible diagrams: self-energy functional approximated

$$\Sigma[G] = \frac{\delta \Phi[G, U]}{\delta G}$$

Equation of motion – Dyson, diagrammatic input via Σ

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

Baym-Kadanoff formal construction

Perturbation expansion in renormalized quantities only (one-particle level)

Free energy

$$\Omega\left\{G^{(0)-1}, U\right\} = -\beta^{-1}\ln\left[\mathsf{Z}\left\{J; G^{(0)-1}, U\right\}\right]$$
$$= -\beta^{-1}\ln\int \mathcal{D}\varphi\mathcal{D}\varphi^{*}\exp\left\{\varphi^{*}\left[G^{(0)-1}-J\right]\varphi + U\left[\varphi,\varphi^{*}\right]\right\} \quad (6)$$

Replacement in PT: $G^{(0)-1} \to G^{-1} + \Sigma$, (Dyson equation) in Ω

Variational approach: new functional $\Psi[G,\Sigma]$ defined from

$$\frac{\delta\beta\Psi}{\delta\Sigma} = \frac{\delta\beta\Omega}{\delta G^{(0)-1}} + \left[G^{(0)-1} - \Sigma\right]^{-1} \quad (7)$$

$$\frac{\delta\beta\Psi}{\delta G} = \frac{1}{G^2}\frac{\delta\beta\Omega}{\delta G^{(0)-1}} - G^{-1} \quad (8)$$

Explicit functional

$$\Psi\left[G,\Sigma,U\right] = \Omega\left\{G^{-1}+\Sigma, U\right\} - \beta^{-1}\mathrm{tr}\ln G - \beta^{-1}\mathrm{tr}\ln\left[G^{(0)-1} - \Sigma - J\right] \quad (9)$$

Variational conditions:

$$\frac{\delta\Psi\left[G,\Sigma\right]}{\delta G} = 0 \qquad\qquad \frac{\delta\Psi\left[G,\Sigma\right]}{\delta\Sigma} = 0$$

Approximations expressed entirely in terms of renormalized quantities G, Σ

Φ-derivability

$\Psi[G,\Sigma,U]$ not suitable for approximations – Σ to be excluded via Legendre transform

$$\Phi[G,U] = \Omega\left\{G^{-1}+\Sigma, U\right\} - \beta^{-1}\mathrm{tr}\ln G + \Sigma G \tag{10}$$

Theory is Φ-derivable if $\Phi[G,U]$ is found explicitly in closed form, i.e., variational equation

$$\Sigma[G] = \frac{\delta\Phi[G,U]}{\delta G}$$

must be resolved for Φ as a functional of the renormalized propagator G

Practically only weak-coupling theories are Φ-derivable

Dynamical mean-field theory

Separation of **site** diagonal and off-diagonal parts

$$G = G^{diag}\left[d^0\right] + G^{off}\left[d^{-1/2}\right], \qquad \Sigma = \Sigma^{diag}\left[d^0\right] + \Sigma^{off}\left[d^{-3/2}\right]$$

Mean-field functional

$$\Psi\left[G,\Sigma\right] = \Omega\left\{G^{diag\ -1} + \Sigma^{diag}\right\} - \beta^{-1}\text{tr}\ln G^{diag} - \beta^{-1}\text{tr}\ln\left[G^{(0)-1} - \Sigma^{diag} - J\right] \tag{11}$$

where $G(\mathbf{k}, i\omega_n) \rightarrow G^{diag}(i\omega_n)$, $\Sigma(\mathbf{k}, i\omega_n) \rightarrow \Sigma^{diag}(i\omega_n)$

Only **local** correlations matter in the generating functional

Lattice structure enters only due to the bare propagator:

$$G^{(0)-1}(\mathbf{k}, i\omega_n) = i\omega_n + \mu + \sigma B - \epsilon(\mathbf{k}) \tag{12}$$

Application of DMFT:

- Exact asymptotic formulas for $d \to \infty$ used in $d = 3$
- Only density of states (DOS) matters:

  $\rho(E) = -\frac{1}{\pi N} \sum_{\mathbf{k}} \mathrm{Im}\, G(\mathbf{k}, E + i0^{+})$
- Momentum summations in internal vertices independent
- **Nonlocal** quantities irrelevant in the thermodynamic potential

What about correlation functions?

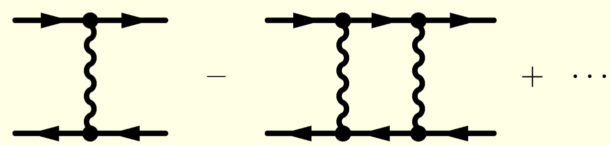
- Correlation functions determine stability of a DMFT
- Generally nonolocal quantities (LRO exists) – cavity (loop) field
- Irreducible vertex functions – local but not unique
- Various (2P channel-dependent) leading-order corrections

Two-particle functions

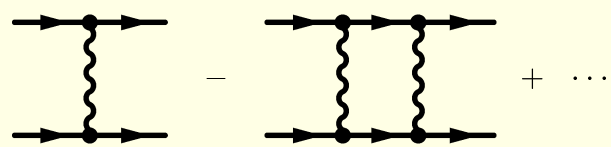
Advanced scheme for PT: Approximations at the two-particle level: 2P irreducible vertices aproximated diagrammatically – cannot be disconnected by cutting a pair of 1P propagators

2P irreducibility three (independent) two-particle scattering channels – beyond static local theory (atomic limit)

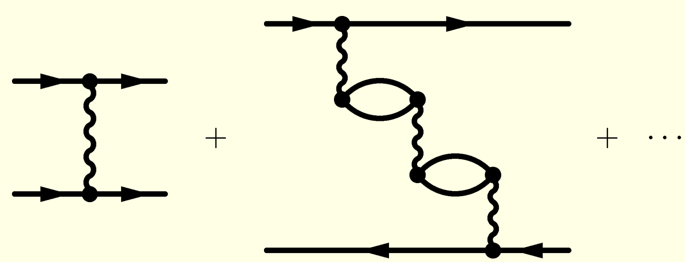
eh ladders



ee ladders



eh bubbles

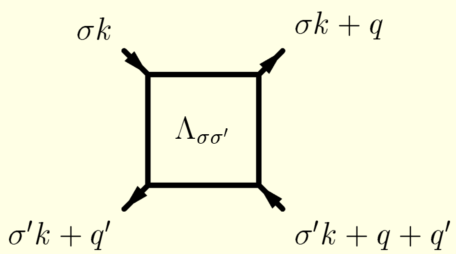


Characterization of 2P channels

2nd variations in external sources lead to specific 2P reducible functions:

- $\eta^{||}$ - interaction ch. (bubble chain, polarization bubbles), longitudinal susceptibilities, LRO
- $\eta^{\perp}$ - electron-hole ch. (singlet e-h scatterings), transverse susceptibilities, (anomalous) LRO
- $\xi^{\perp}$ - electron-electron ch. (singlet e-e scatterings), superconductivity, anomalous GF

Labelling of two-particle functions in momentum space $\Lambda_{\sigma\sigma'}(k, q, q')$:



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

Channel-dependent (linear) multiplication schemes

eh-channel (RPA)

$$\left[\widehat{X}GG \circ \widehat{Y}\right]_{\sigma\sigma'}(k,k';q) = \frac{1}{\beta\mathcal{N}}\sum_{q''} X_{\sigma\sigma'}(k;q'',q)G_\sigma(k+q'')G_{\sigma'}(k+q+q'') \times Y_{\sigma\sigma'}(k+q'';k'-k-q'';q)$$

ee-channel (TMA)

$$\left[\widehat{X}GG \bullet \widehat{Y}\right]_{\sigma\sigma'}(k,k';q) = \frac{1}{\beta\mathcal{N}}\sum_{q''} X_{\sigma\sigma'}(k;q'',q+q'-q'')G_\sigma(k+q'')G_{\sigma'}(k+q+q'-q'') \times Y_{\sigma\sigma'}(k+q'',q-q'';q'-q'')$$

U-channel (shielded interaction, GWA)

$$\left[\widehat{X}GG \star \widehat{Y}\right]_{\sigma\sigma'}(k,k';q) = \frac{1}{\beta\mathcal{N}}\sum_{\sigma''k''} X_{\sigma\sigma''}(k;q,q'')G_{\sigma''}(k+q'')G_{\sigma''}(k+q+q'') \times Y_{\sigma''\sigma'}(k+q'';q,k'-k-q'')$$

Two-particle renormalizations

Two-particle irreducible vertices Λ^α approximated diagrammatically

Equations of motion for the full 2P vertex Γ

Bethe-Salpeter equations – channel dependent, generically

$$\Gamma(k;q,q') = \Lambda^\alpha(k;q,q') - [\Lambda^\alpha GG \odot \Gamma](k;q,q') \quad (13)$$

used to calculate Γ from a known Λ

Schwinger-Dyson equation – Schrödinger equation for Green functions

$$\Sigma_\sigma(k) = \frac{U}{\beta N}\sum_{k'} G_{-\sigma}(k') - \frac{U}{\beta^2 N^2}\sum_{k'q} G_\sigma(k+q)G_{-\sigma}(k'+q)\Gamma_{\sigma-\sigma}(k+q;q,k'-k)G_{-\sigma}(k') \quad (14)$$

used to calculate Σ from Γ

Non-self-consistent 2P renormalizations – FLEX

Ring diagrams $(\Lambda^{U}_{\uparrow\downarrow} = U)$

$$\Gamma^{Ring}_{\uparrow\downarrow}(k;q,q') = \frac{U}{1 - U^2 X_{\uparrow\uparrow}(q) X_{\downarrow\downarrow}(q)} \tag{15}$$

$$X_{\sigma\sigma'}(q) = \frac{1}{\beta\mathcal{N}} \sum_{k''} G_{\sigma}(k'') G_{\sigma'}(k'' + q)$$

Ladder diagrams $(\Lambda^{eh}_{\uparrow\downarrow} = U \quad \vee \quad \Lambda^{ee}_{\uparrow\downarrow} = U)$

$$\Gamma^{RPA}_{\uparrow\downarrow}(k;q,q') = \frac{U}{1 + U X_{\uparrow\downarrow}(q')} \tag{16}$$

$$\Gamma^{TMA}_{\uparrow\downarrow}(k;q,q') = \frac{U}{1 + U Y_{\uparrow\downarrow}(2k + q + q')} \tag{17}$$

$$Y_{\sigma\sigma'}(q) = \frac{1}{\beta\mathcal{N}} \sum_{k''} G_{\sigma}(k'') G_{\sigma'}(q - k")$$

Self-consistent 2P renormalizations – Parquet approach

Completely 2P irreducible function I: irreducible in all 2P channles (disconnected by cutting at least three fermion lines)

Parquet approach: I determined diagrammatically, Λ^α from defining equations

Topological nonequivalence of different 2P channels (beyond local static theory, atomic limit):

$$\Gamma = \Lambda^\alpha + \mathcal{K}^\alpha, \qquad \Lambda^\alpha = I + \sum_{\alpha' \neq \alpha} \mathcal{K}^{\alpha'} \tag{18}$$

Parquet equations: Reducible functions $\mathcal{K}^\alpha$ in (18) replaced by the solutions of the respective Bethe-Salpeter equations

Genuine charge renormalization $U \longrightarrow \Lambda$ in perturbation theory:

$$\Lambda^\alpha = L^\alpha \left[I[U; G, \Lambda]; \Lambda, G \right] \tag{19}$$

Parquet method – simultaneous renormalization of m and U

- 1P renormalization – 1P irreducible function

$$G = G_0 + G_0 \Sigma G$$

- 2P renormalization – vertex function

$$\Gamma = \Lambda^\alpha - \Lambda^\alpha G G \Gamma$$

Λ^α – 2P irreducible vertex – ambiguously defined

- Parquet equations – topological nonequivalence of the choice of 2P irreducibility – completely 2P-IR vertex I

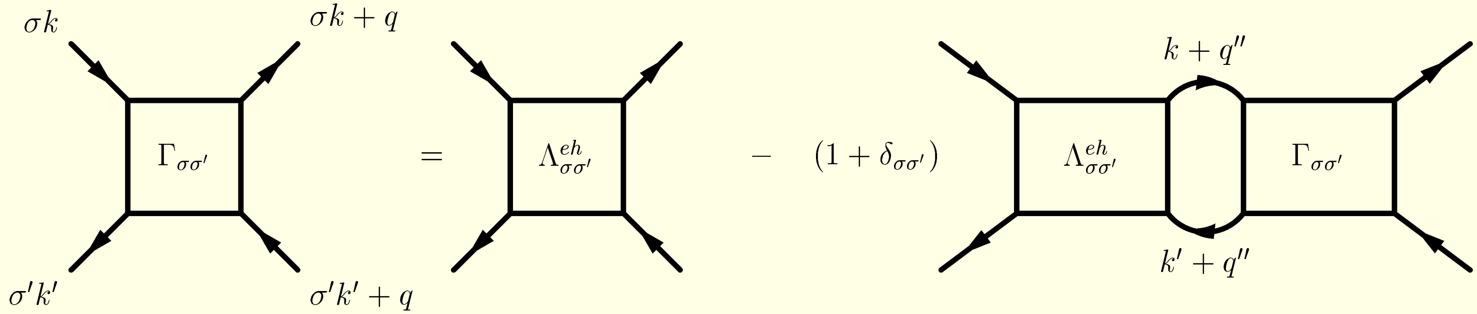
$$\Lambda^\alpha = I + \sum_{\alpha' \neq \alpha} [\Gamma - \Lambda^{\alpha'}]$$

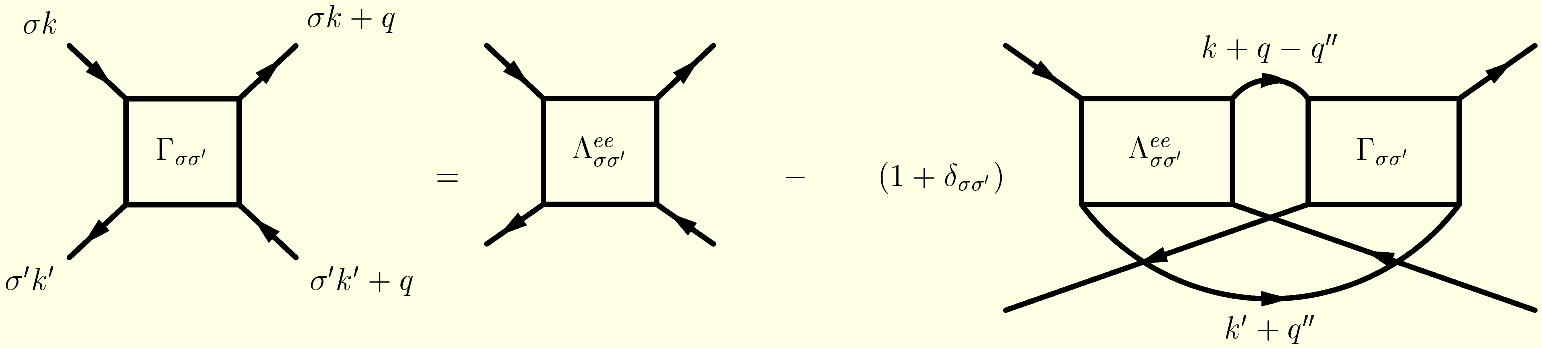
- Schwinger-Dyson equation of motion

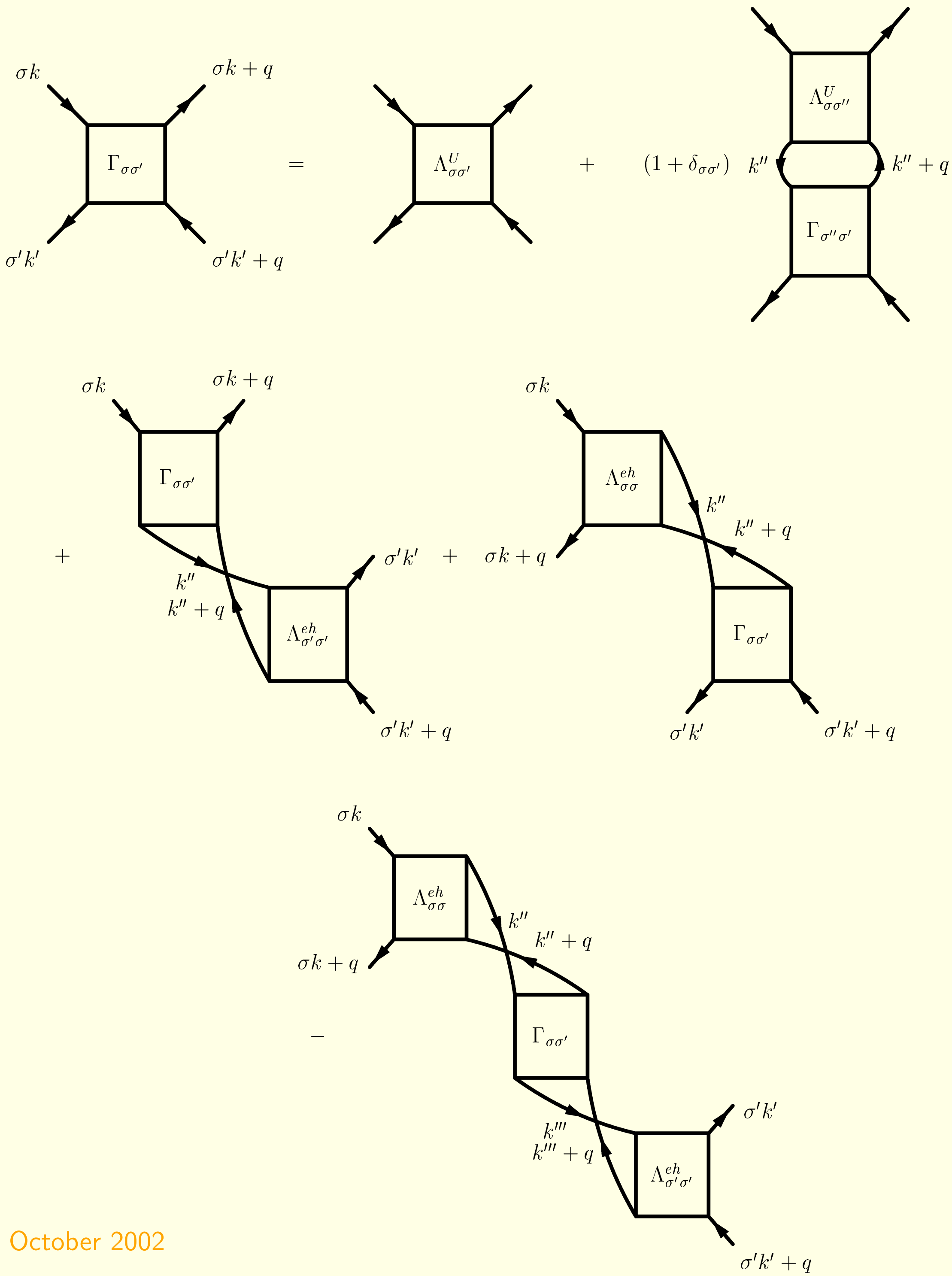
$$\Sigma = UG - UG\Gamma GG$$

Close system of equations with a diagrammatic input – completely 2P-IR function: $I = U + \Delta I[G, \Lambda]$

Parquet diagrams – Bethe-Salpeter equations







σk
$\sigma k + q$
$\Gamma_{\sigma\sigma'}$
$\sigma' k'$
$\sigma' k' + q$
$=$
$\Lambda^U_{\sigma\sigma'}$
$+$
$(1 + \delta_{\sigma\sigma'})$
$\Lambda^U_{\sigma\sigma''}$
k''
$k'' + q$
$\Gamma_{\sigma''\sigma'}$
$+$
σk
$\sigma k + q$
$\Gamma_{\sigma\sigma'}$
k''
$k'' + q$
$\Lambda^{eh}_{\sigma'\sigma'}$
$\sigma' k'$
$\sigma' k' + q$
$+$
σk
$\Lambda^{eh}_{\sigma\sigma}$
k''
$k'' + q$
$\sigma k + q$
$\Gamma_{\sigma\sigma'}$
$\sigma' k'$
$\sigma' k' + q$
$-$
σk
$\Lambda^{eh}_{\sigma\sigma}$
k''
$k'' + q$
$\sigma k + q$
$\Gamma_{\sigma\sigma'}$
k'''
$k''' + q$
$\Lambda^{eh}_{\sigma'\sigma'}$
$\sigma' k'$
$\sigma' k' + q$

Simplified parquet equations – approximate diagonalization

Each vertex (2P) function has three (four)-momentum variables – problem not tractable (N. Bickers – high temperatures), approximations necessary

Approximations:

- Keep only relevant variables for which possible singularities may appear
- Incoming fermion variable (k) in the vertex function essentially irrelevant
- Only spin-singlet potentially singular vertex functions (eh and U (noncrossed) channels)

$$\overline{\Lambda^U}_L(x,q) = \frac{U\delta(x) + \overline{\langle \Lambda^{eh} G_\uparrow G_\downarrow \rangle}_L(x,q)\left[U\delta(x) - \overline{\Lambda^{eh}}_L(x,q)\right]}{1 + \overline{\langle \Lambda^{eh} G_\uparrow G_\downarrow \rangle}_L(x,q)} \tag{20}$$

$$\overline{\Lambda^{eh}}_R(q,x) = \frac{U\delta(x) - \prod_\sigma \overline{\langle \Lambda^{eh} G_\sigma G_\sigma \rangle}_R(q,x)\left[U\delta(x) - \overline{\Lambda^U}_R(q,x)\right]}{1 - \prod_\sigma \overline{\langle \Lambda^{eh} G_\sigma G_\sigma \rangle}_R(q,x)} \tag{21}$$

Only the first part $U\delta(x)$ – quasi-algebraic equations for one-variable vertex functions

One-variable simplified parquet equations

Two singlet eh channels – only the (conserving) variable in each channel kept, analytic structure of the FLEX

horizontal transfer momentum for Λ^{eh}, vertical transfer momentum for Λ^{U}

$$\Lambda^{eh}(q) = \frac{U}{1 - \left\langle \frac{UG_\uparrow G_\uparrow}{1+\langle \Lambda^{eh} G_\uparrow G_\downarrow \rangle} \right\rangle (q) \left\langle \frac{UG_\downarrow G_\downarrow}{1+\langle \Lambda^{eh} G_\uparrow G_\downarrow \rangle} \right\rangle (q)} \tag{22}$$

$$\Lambda^{U}(q) = \frac{U}{1 + \left\langle \frac{UG_\uparrow G_\downarrow}{1-\langle \Lambda^{U} G_\uparrow G_\uparrow \rangle \langle \Lambda^{U} G_\downarrow G_\downarrow \rangle} \right\rangle (q)} \tag{23}$$

$$\langle \Gamma G_\sigma G_{\sigma'} \rangle (q) = \frac{1}{\beta N} \sum_k \Gamma(k) G_\sigma(k) G_{\sigma'}(k+q) \tag{24}$$

Self-energy from the Schwinger-Dyson equation:

$$\Sigma^{U}_{\sigma}(k) = -\,U \sum_q \frac{G_{-\sigma}(k+q) \left\langle U G_\uparrow G_\downarrow \right\rangle (q)}{1 + \left\langle \frac{U}{1-\langle \Lambda^{U} G_\uparrow G_\uparrow \rangle \langle \Lambda^{U} G_\downarrow G_\downarrow \rangle} \, G_\uparrow G_\downarrow \right\rangle (q)} \tag{25}$$

Solution of the simplified parquet equations (DMFT)

Weak-coupling $U \lessapprox w$ – very close to FLEX

Intermediate coupling $U > w$ – new nonperturbative solution for 2P IR vertices $\Lambda^{eh}, \Lambda^{U}$
two real solutions split into the complex plane in an effort to avoid a nonintegrable pole in BS-equations – complex conjugate solutions

Symmetry breaking at the two-particle level: $\Lambda(z) \neq \Lambda(z^*)^*$

Order parameters – anomalous 2P vertex: $\Gamma_{anom}(\omega) = (\Gamma(\omega + i\eta) - \Gamma^*(\omega - i\eta))/2$

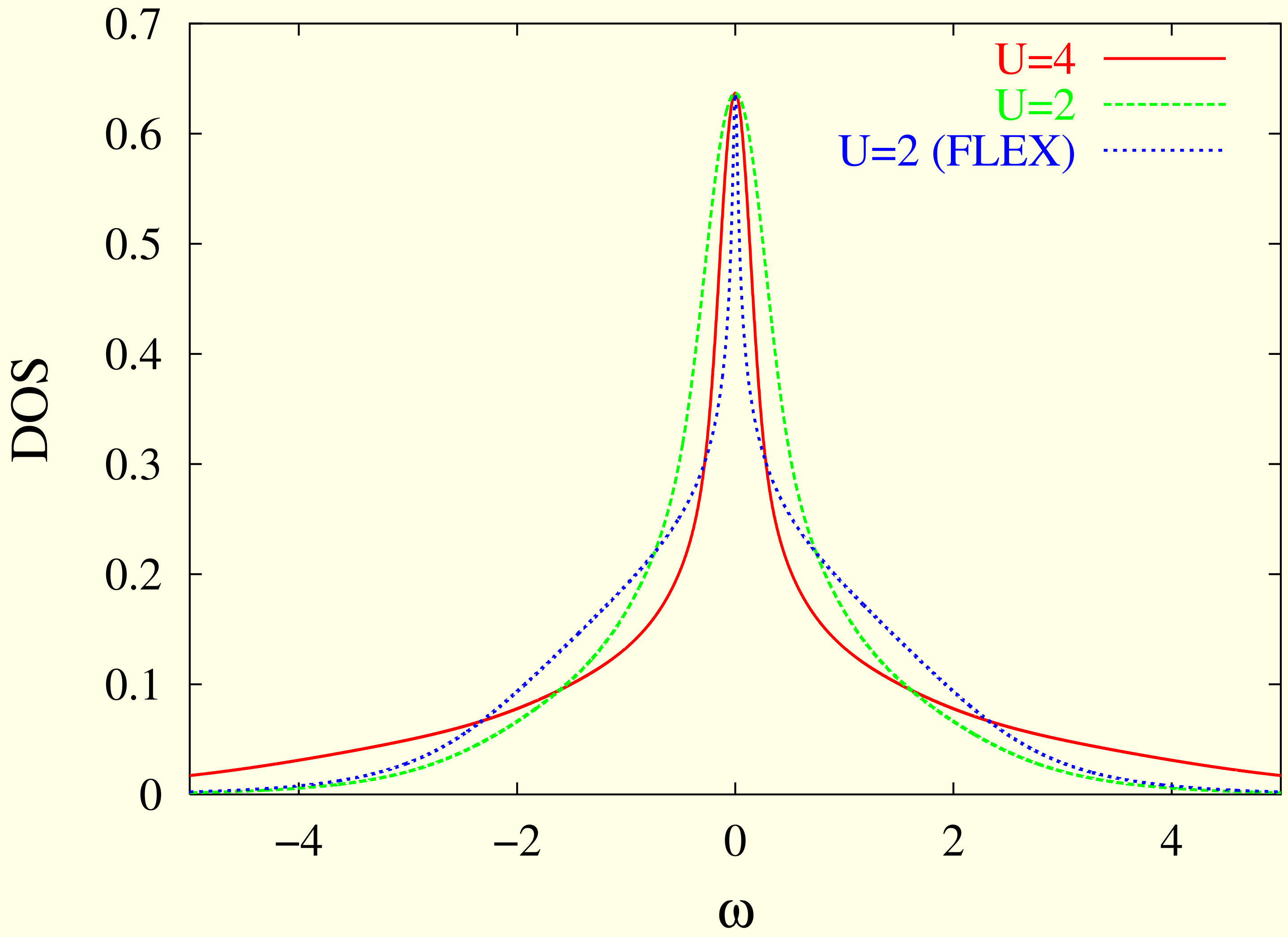
Physical (measurable) quantities: $\Gamma_{reg}(\omega) = (\Gamma(\omega + i\eta) + \Gamma^*(\omega - i\eta))/2$

Effective particle interaction $\Lambda(0)$ gets complex! No divergence in the vertex functions!

Interpretation: resonant pair states
Im $U_{eff} > 0$ – absorption to bound state
Im $U_{eff} < 0$ – emission from bound state

QM analogy with tunneling ($E_{kin} < U$, real $\longrightarrow$ complex momentum)

Half-filled Hubbard model in the DMFT limit – simplified parquet (with symmetry breaking) and FLEX



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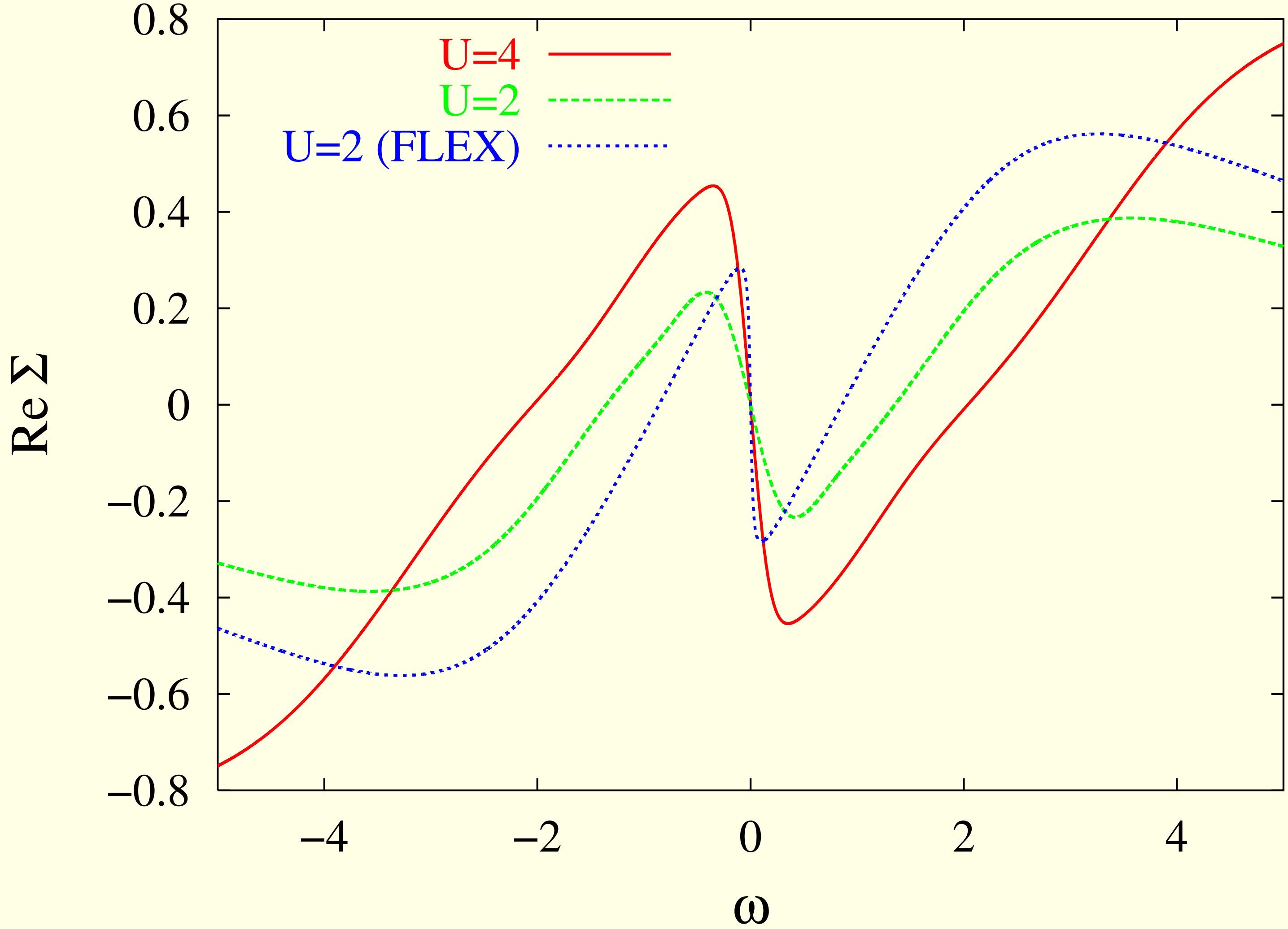

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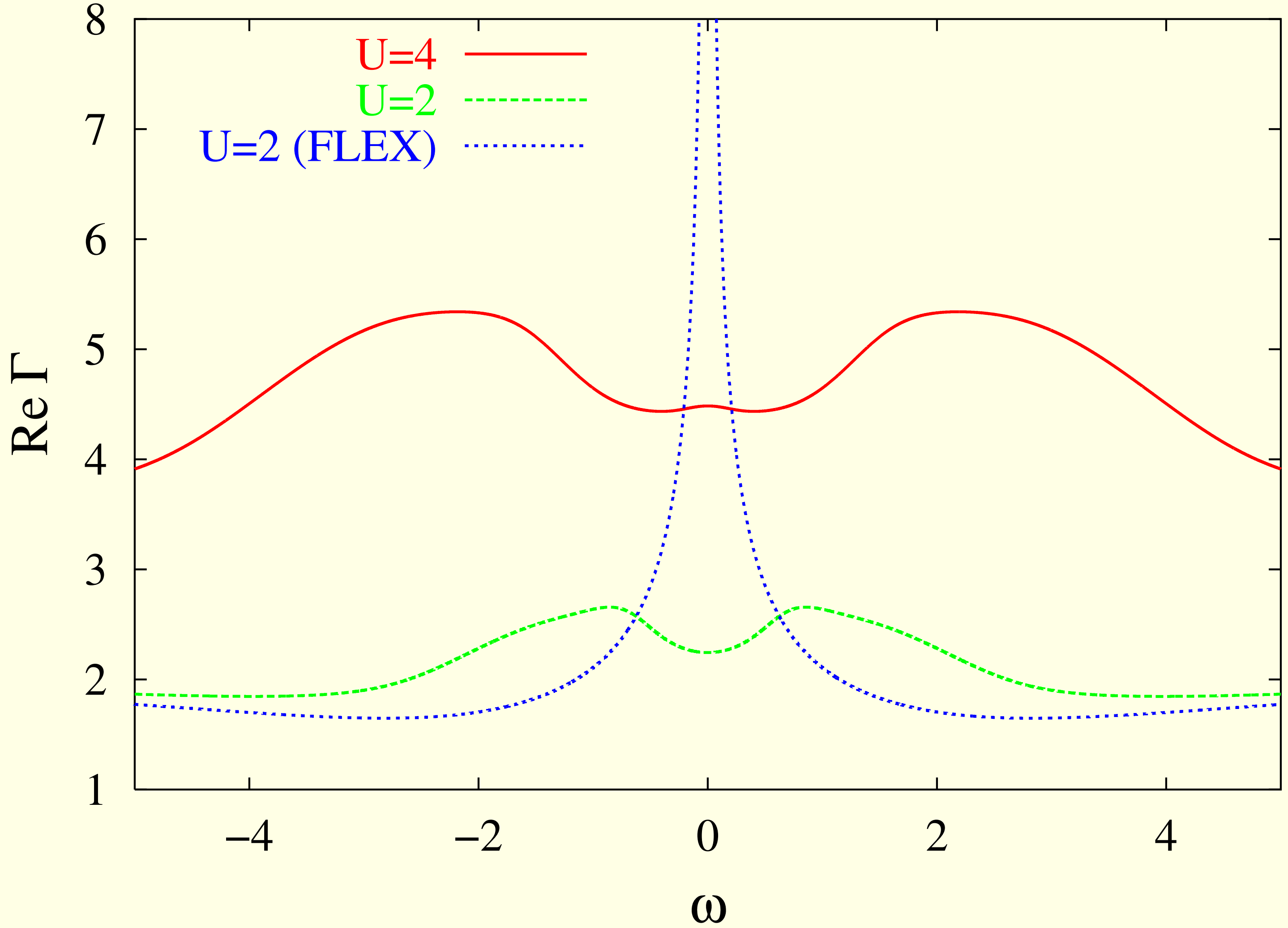

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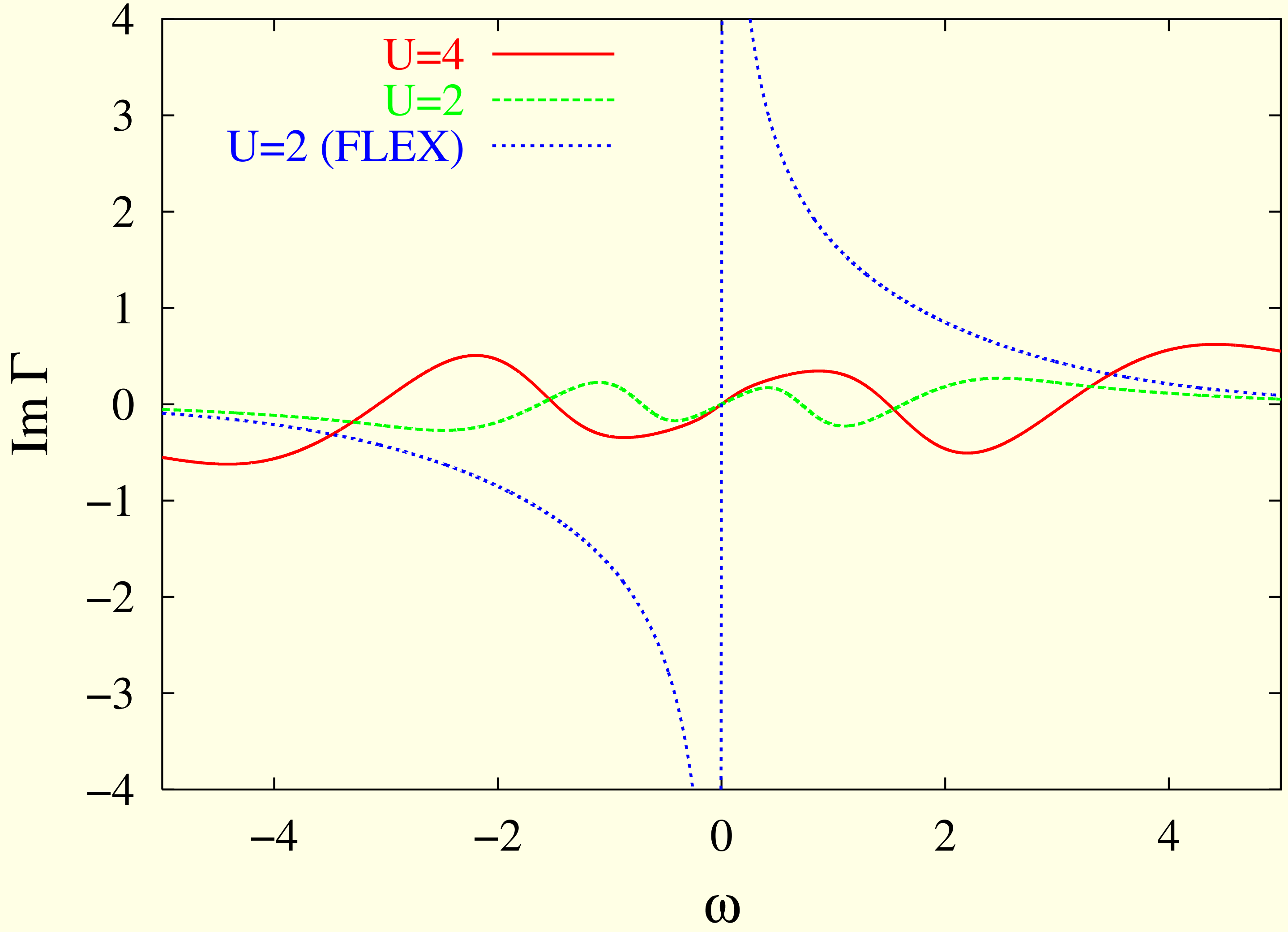

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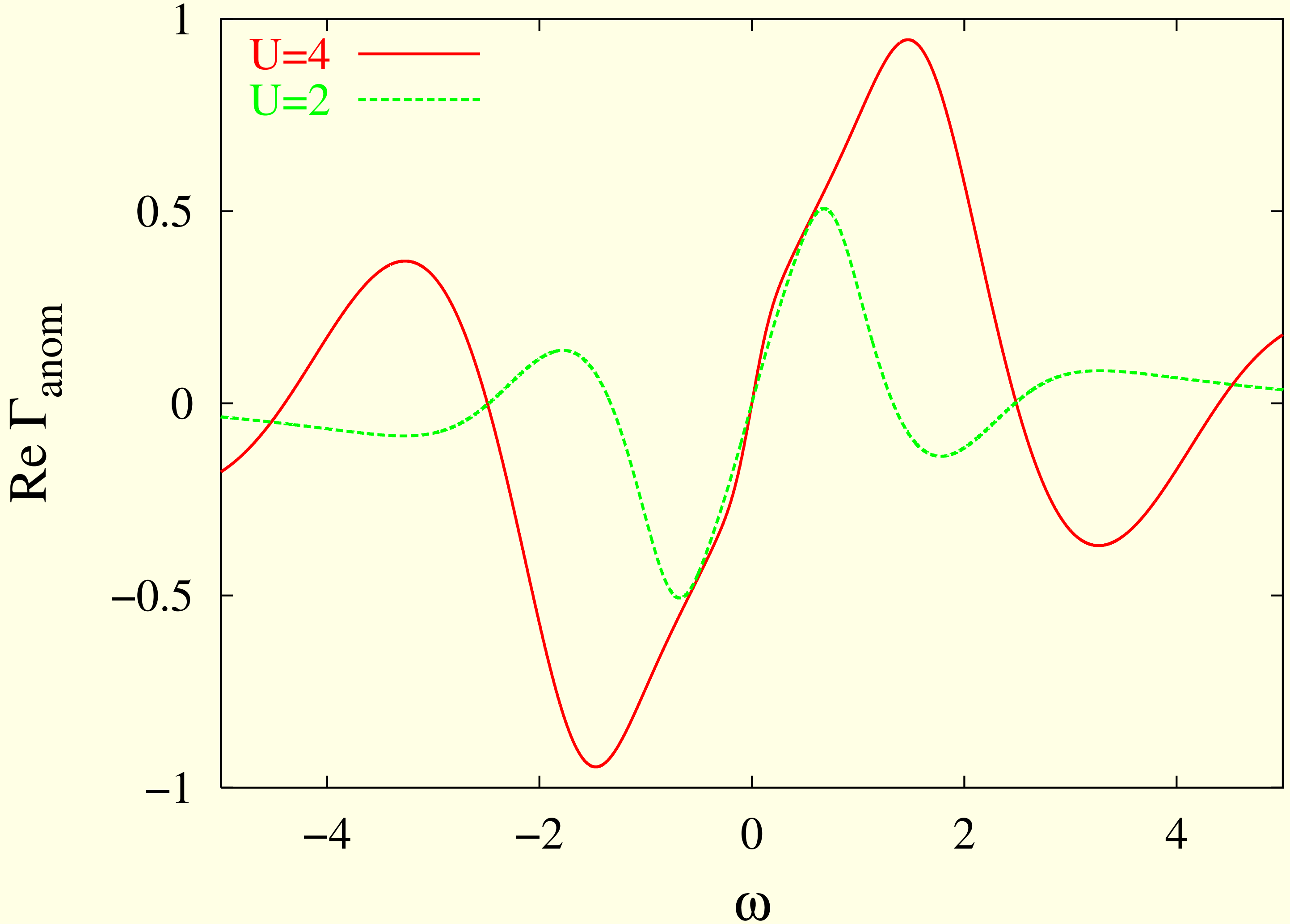

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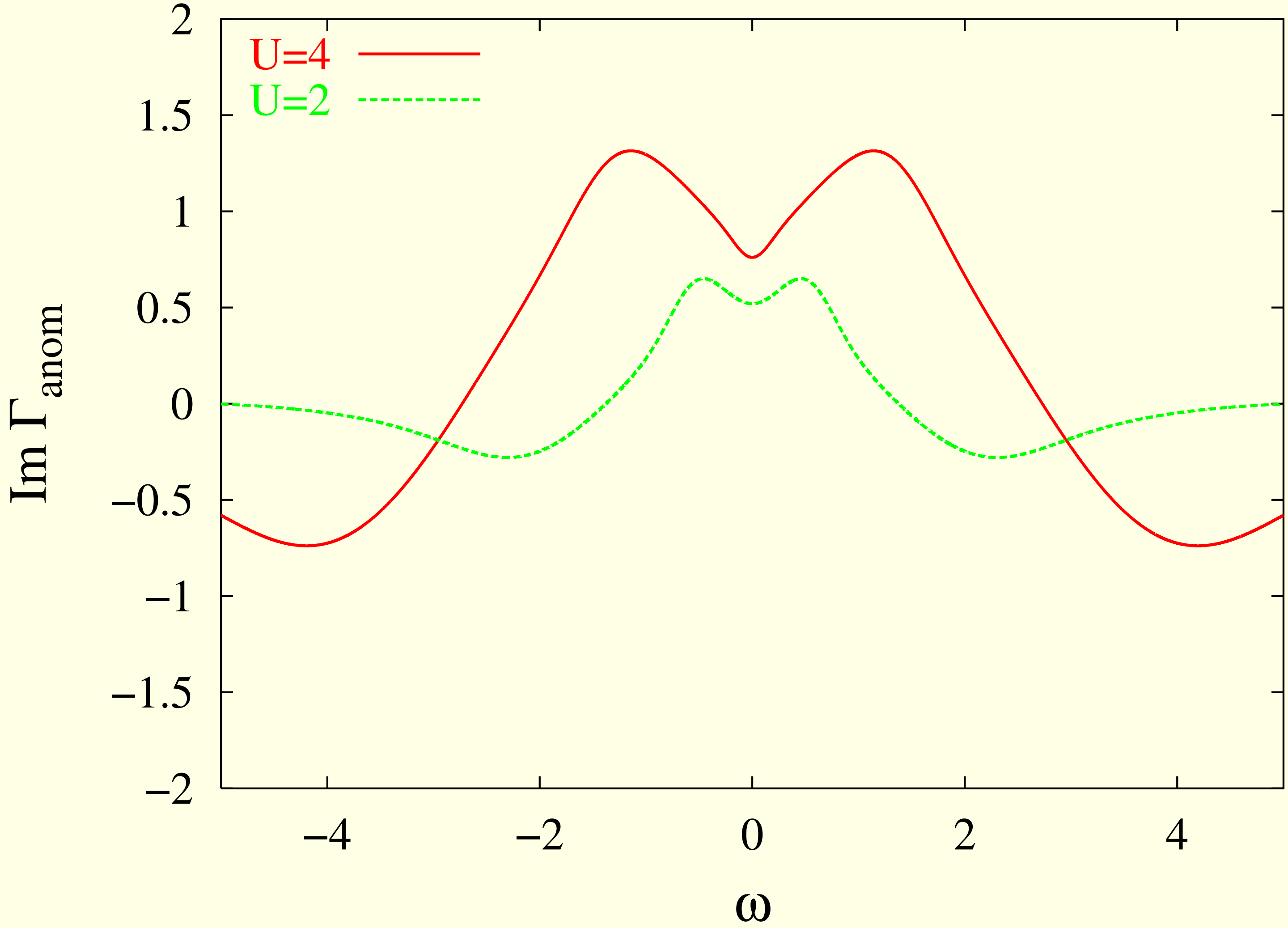

FLEX vs. Parquet equations

FLEX

- Straightforward approach – analytic solution accessible (Bethe-Salpeter equation algebraic)
- Good in $d > 2$ and weak coupling only
- Fails in critical regions – singularity only in one channel
- Nonintegrable singularities may exist

Parquet equations

- ✔ (Nonlinear integral) equations for irreducible vertex functions (effective interaction) – only approximate solutions
- ✔ Nonperturbative solutions – singularities and bifurcation points (new phases with 2P order parameters)
- ✔ Only integrable singularities – important in low dimensions
  - $d > d_l$ broken symmetry – 1P anomalous vertex Σ – condensation of bound pairs
  - $d \leq d_l$ breakdown of mirror symmetry $\Lambda(q) \neq \Lambda^*(q^*)$ – 2P anomalous vertices – effective complex interaction $\Lambda(0)$ – resonant pair states

Conclusions

- ✔ Renormalized PT: diagrammatic (perturbative) input into a set of equations of motion
- ✔ One-particle (mass) renormalizations: Fermi-liquid regime with dominant fermionic excitations
- ✔ Two-particle (charge) renormalizations: Critical regions with singularities in the Bethe-Salpeter equations
- ✔ Two-particle self-consistence (parquet): low-dimensional dynamical systems with critical behavior (integrability of singularities not guaranteed)
- ✞ Extrapolation only from weak to intermediate coupling
- ✞ Not yet reliable (understood) in the strong-coupling regime –properties of the new 2P phase, symmetry-breaking field, etc.
- ✞ Conflict between Schwinger-Dyson & Ward – both cannot be obeyed simultaneously

Perspectives

Model

- Ward identity used for determining Σ from Λ (replacing Schwinger-Dyson)
- More detailed analysis of the new 2P quantum phase
- Disordered systems – new phase related to Anderson localization

Realistic

- FLEX generalized to multi-orbital Hubbard – U, J, various degrees of self-consistence
- Parquet – not yet mature for applications, still to be explored at the model level