

Anomalous propagators and the particle-particle correlation channel of many-body perturbation theory

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Table of Contents

1. Definitions, Hedin's equations and usual approximations
2. An alternative closed set of equations for G
3. The particle-particle Bethe-Salpeter equation
4. Conclusion and perspectives

Definitions, Hedin's equations and usual approximations

One-body Green's function

Definition

$$G(11') = \frac{1 = (\mathbf{r}_1, \sigma_1, t_1)}{\langle \Psi_0^N | \hat{T} \left[\hat{\psi}(1) \hat{\psi}^\dagger(1') \right] | \Psi_0^N \rangle}$$

Field operators **N-electron ground-state**

Charged excitations

Definition

$$G(11') = (-i) \langle \Psi_0^N | \hat{T} [\hat{\psi}(1) \hat{\psi}^\dagger(1')] | \Psi_0^N \rangle$$

Lehmann representation

$$\frac{x_1 = (\mathbf{r}_1, \sigma_1)}{G(\mathbf{x}_1 \mathbf{x}_{1'}; \omega) = \sum_S \frac{\mathcal{I}_S(\mathbf{x}_1) \mathcal{I}_S^*(\mathbf{x}_{1'})}{\omega - (E_0^N - E_S^{N-1}) - i\eta} + \sum_S \frac{\mathcal{A}_S(\mathbf{x}_1) \mathcal{A}_S^*(\mathbf{x}_{1'})}{\omega - (E_S^{N+1} - E_0^N) + i\eta}}$$

↑
S-th ionization potentials ↑
S-th electron affinities

How to compute G ?

The Dyson equation

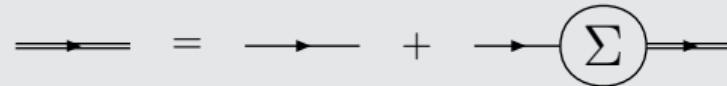
$$G(11') = G_0(11') + \int d(22') G_0(12) \Sigma(22') G(2'1')$$

 **Self-energy**

How to compute G ?

The Dyson equation

$$G(11') = G_0(11') + \int d(22') G_0(12) \Sigma(22') G(2'1')$$



How to compute G ?

The Dyson equation

$$G(11') = G_0(11') + \int d(22') G_0(12) \Sigma(22') G_0(2'1')$$
$$+ \int d(22'33') G_0(12) \Sigma(22') G_0(2'3) \Sigma(33') G_0(3'1') + \dots$$

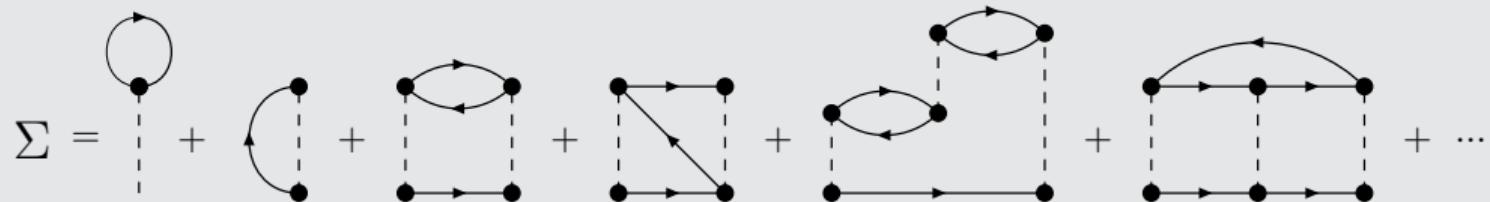


How to compute G ?

The Dyson equation

$$G(11') = G_0(11') + \int d(22') G_0(12) \Sigma(22') G(2'1')$$

An exact expression for the self-energy



Another exact formalism

Self-consistent set of equations

$$\textcolor{orange}{G}(11') = G_0(11') + G_0(12)\Sigma(22')\textcolor{orange}{G}(2'1')$$

$$\Sigma(11') = \Sigma_{\mathbb{H}}(11') + i \int d(22'33') V(12; 2'3) \textcolor{orange}{G}(2'3')\Gamma(3'3; 1'2)$$

$$\Gamma(12; 1'2') = \delta(12')\delta(1'2) + \int d(33'44') \frac{\delta\Sigma(11')}{\delta\textcolor{orange}{G}(33')} \textcolor{orange}{G}(34)\textcolor{orange}{G}(4'3')\Gamma(42; 4'2')$$

A few iterations

Initial condition

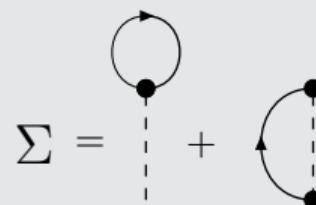
$$\Sigma^{(0)}(11') = 0$$

\Rightarrow

$$\frac{\delta \Sigma^{(0)}(11')}{\delta G(33')} = 0$$

First iteration

$$\Gamma^{(1)}(12; 1'2') = \delta(12')\delta(1'2) \quad \Sigma^{(1)}(11') = \Sigma_H(11') + i \int d(22') V(12; 2'1')G(2'2)$$



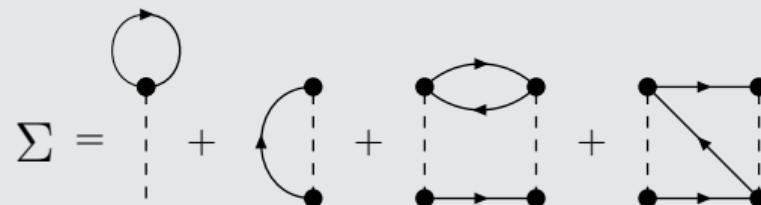
A few iterations

Second iteration

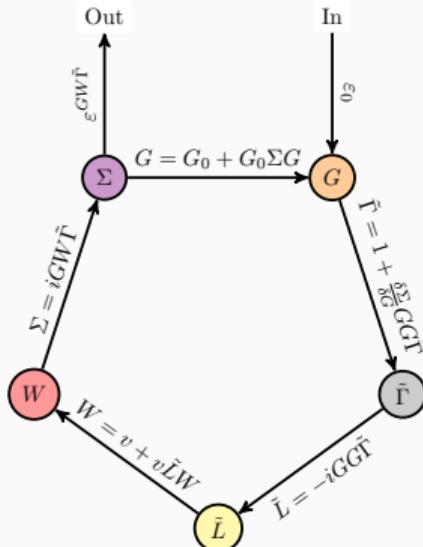
$$\frac{\delta \Sigma^{(1)}(11')}{\delta G(33')} = V(13'; 31') - V(13'; 1'3) = \bar{V}(13'; 31')$$

$$\Gamma^{(2)}(12; 1'2') = \delta(12')\delta(1'2) + \int d(33'44') \frac{\delta \Sigma^{(1)}(11')}{\delta G(33')} G(34)G(4'3')\Gamma^{(1)}(42; 4'2')$$

$$\Sigma^{(2)}(11') = \Sigma_{\text{Hx}}(11') + i \int d(22'33'44') V(12; 2'3)G(2'3')\bar{V}(3'4'; 41')G(42)G(34)$$



Hedin's Pentagon



Hedin, Phys Rev 139 (1965)
A796

The wonderful equations of Hedin

$$G(11') = G_0(11') + \int G_0(12) \Sigma(22') G(2'1') d(34)$$

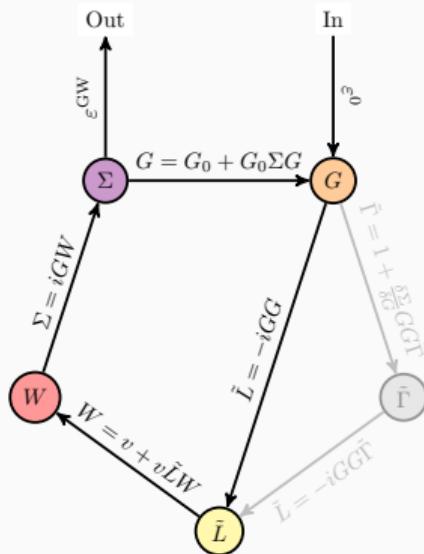
$$\underbrace{\tilde{\Gamma}(12; 1'2')}_{\text{vertex}} = \delta(12') \delta(1'2) + \int \frac{\delta \Sigma_{xc}(11')}{\delta G(33')} G(34) G(4'3') \tilde{\Gamma}(42; 4'2')$$

$$\underbrace{\tilde{L}(12; 1'2')}_{\text{polarizability}} = -i \int G(13) G(3'1') \tilde{\Gamma}(32; 3'2') d(33')$$

$$\underbrace{W(12; 1'2')}_{\text{screening}} = V(12; 1'2') + \int W(14; 1'4') \tilde{L}(3'4'; 34) V(23; 2'3')$$

$$\underbrace{\Sigma_{xc}(12)}_{\text{self-energy}} = i \int G(33') W(12'; 32) \tilde{\Gamma}(3'2; 1'2') d(22'3')$$

Hedin's Square



Hedin, Phys Rev 139 (1965)
A796

The GW approximation

$$\begin{aligned}\mathbf{G}(11') &= G_0(11') + \int G_0(12) \Sigma(22') \mathbf{G}(2'1') d(34) \\ \tilde{\Gamma}(12; 1'2') &= \underbrace{\delta(12') \delta(1'2)}_{\text{vertex}} \\ \tilde{L}(12; 1'2') &= -i \mathbf{G}(12') \mathbf{G}(21') \\ \underbrace{W(12; 1'2')}_{\text{screening}} &= V(12; 1'2') + \int W(14; 1'4') \tilde{L}(3'4'; 34) V(23; 2'3') \\ \underbrace{\Sigma_{xc}(12)}_{\text{self-energy}} &= i \int \mathbf{G}(32') W(12'; 31') d(2'3)\end{aligned}$$

Diagrammatic content of the GW approximation

The GW resummation

$$\Sigma = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \dots$$

The equation shows the diagrammatic representation of the Σ function as a sum of diagrams. The diagrams are composed of black dots representing vertices and arrows representing directed edges. The first term is a single loop with one vertex. Subsequent terms show more complex structures: a loop with two vertices, a square-like structure with two vertices and two internal loops, and so on, increasing in complexity. The ellipsis at the end indicates that the series continues indefinitely.

Diagrammatic content of the GW approximation

The GW resummation

$$\Sigma = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \dots$$

Diagram 1: A vertical dashed line with a solid dot at the top and a curved arrow forming a loop around it. A plus sign follows.

Diagram 2: A horizontal dashed line with a solid dot at each end, and a curved arrow forming a loop around the middle. A plus sign follows.

Diagram 3: Two horizontal dashed lines connected by a vertical dashed line. Each line has a solid dot at each end and a curved arrow forming a loop around the middle. A plus sign follows.

Diagram 4: Three horizontal dashed lines connected by two vertical dashed lines. Each line has a solid dot at each end and a curved arrow forming a loop around the middle. A plus sign follows.

Diagram 5: Four horizontal dashed lines connected by three vertical dashed lines. Each line has a solid dot at each end and a curved arrow forming a loop around the middle. A plus sign follows.

... indicates the series continues.

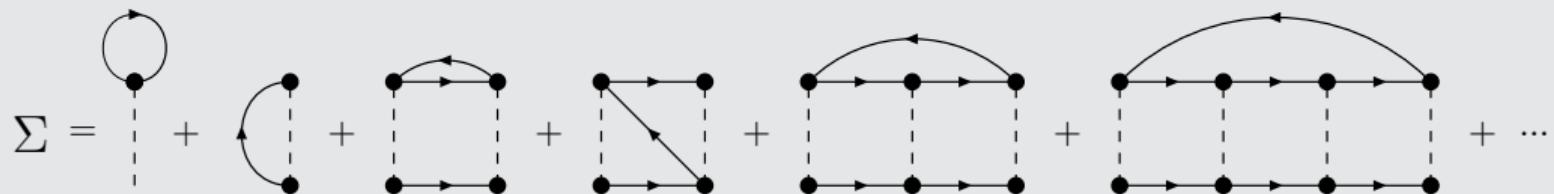
$$\Sigma = \text{Diagram 1} + \text{Diagram 2}$$

Diagram 1: A vertical dashed line with a solid dot at the top and a curved arrow forming a loop around it.

Diagram 2: A horizontal dashed line with a solid dot at each end, and a curved arrow forming a loop around the middle.

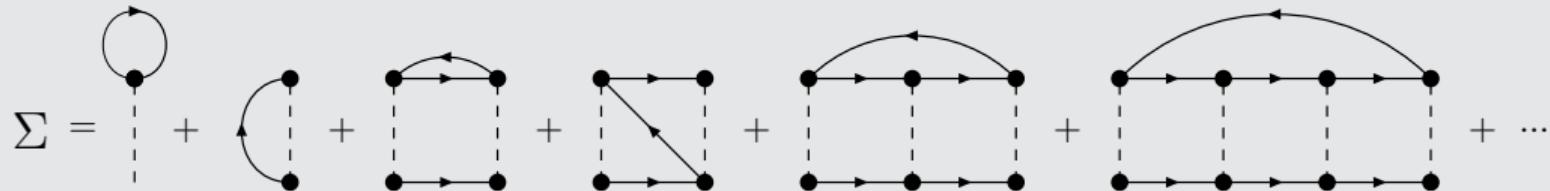
Some other resummation-based self-energies

Particle-particle T -matrix

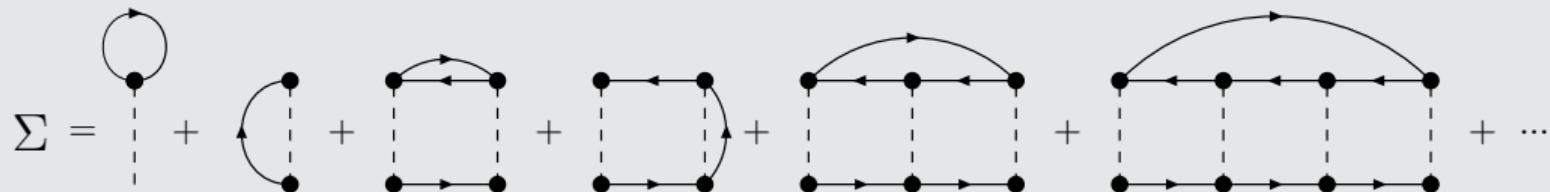


Some other resummation-based self-energies

Particle-particle T -matrix



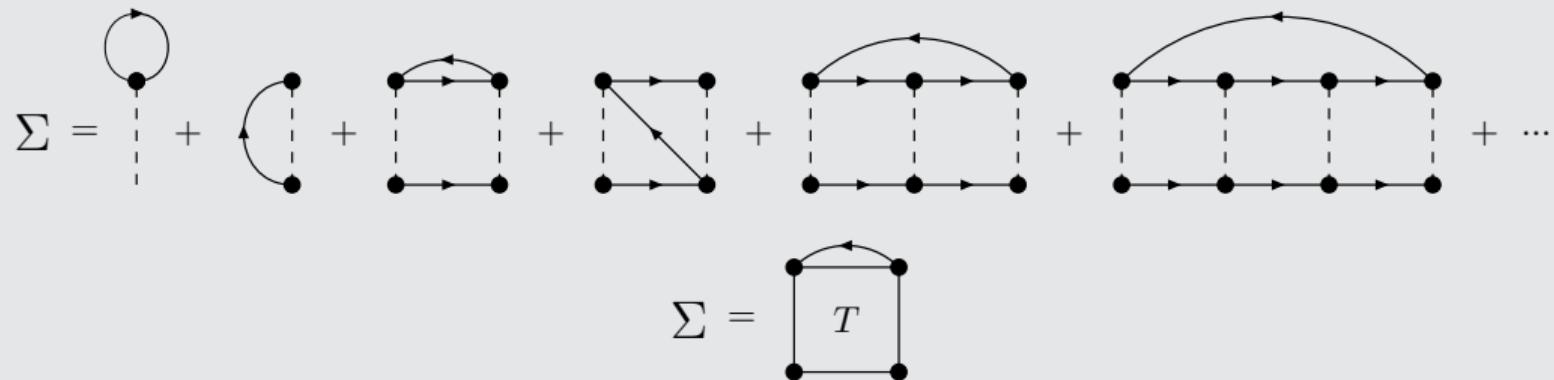
Electron-hole T -matrix



Romanelli, Bechstedt and Reining, Phys. Rev. B 85 (2012) 155131

Some other resummation-based self-energies

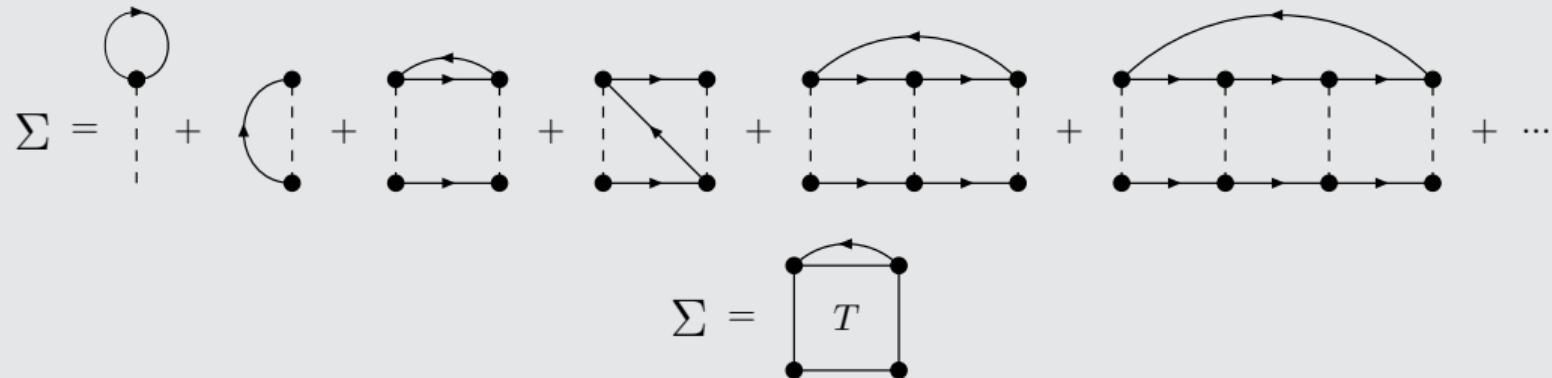
Particle-particle T -matrix



What's missing with respect to the GW self-energy?

Some other resummation-based self-energies

Particle-particle T -matrix

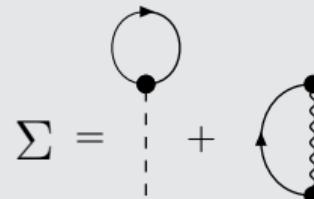


What's missing with respect to the GW self-energy?

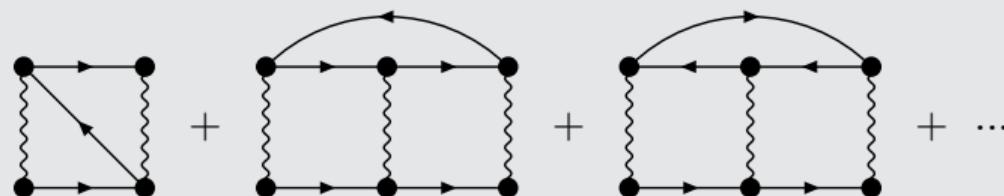
A systematic way to go beyond!

Vertex corrections to the GW self-energy

Zeroth iteration

$$\Sigma = \text{---} + \text{---}$$


First iteration

$$\text{---} + \text{---} + \text{---} + \dots$$


Mejuto-Zaera and Vlček, Phys. Rev. B 106 (2022) 165129

An alternative closed set of equations for G

Key step of the derivation

Self-energy and equation of motion

$$\Sigma(11') = -i \int d(33'44') V(13; 4'3') \underbrace{G_2(4'3'; 43)}_{\text{Two-body Green's function}} G^{-1}(41')$$

Key step of the derivation

Self-energy and equation of motion

$$\Sigma(11') = -i \int d(33'44') V(13; 4'3') \underset{\text{Two-body Green's function}}{\overbrace{G_2(4'3'; 43)}} G^{-1}(41')$$

The Schwinger relation

$$G_2(12; 1'2') = - \frac{\delta G(11'; [U])}{\delta U^{\text{eh}}(2'2)} \Big|_{U=0} + G(11')G(22')$$

↑
External potential

Key step of the derivation

Self-energy and equation of motion

$$\Sigma(11') = -i \int d(33'44') V(13; 4'3') \underset{\text{Two-body Green's function}}{\overbrace{G_2(4'3'; 43)}} G^{-1}(41')$$

The Schwinger relation

$$G_2(12; 1'2') = - \frac{\delta G(11'; [U])}{\delta U^{\text{eh}}(2'2)} \Big|_{U=0} + G(11')G(22')$$

↑
External potential

The external potential

$$\hat{\mathcal{U}}(t_1) = \int d(\mathbf{x}_1 \mathbf{x}_{1'} t'_1) \hat{\psi}^\dagger(\mathbf{x}_1) U^{\text{eh}}(11') \hat{\psi}(\mathbf{x}_{1'})$$

Alternative Schwinger

Another external potential ...

$$\hat{U}(t_1) = \frac{1}{2} \left(\int d(\mathbf{x}_1 \mathbf{x}_{1'} t'_1) \hat{\psi}(\mathbf{x}_1) U^{hh}(11') \hat{\psi}(\mathbf{x}_{1'}) + \int d(\mathbf{x}_1 d\mathbf{x}_{1'} t'_1) \hat{\psi}^\dagger(\mathbf{x}_{1'}) U^{ee}(11') \hat{\psi}^\dagger(\mathbf{x}_{1'}) \right)$$

Alternative Schwinger

Another external potential ...

$$\hat{U}(t_1) = \frac{1}{2} \left(\int d(\mathbf{x}_1 \mathbf{x}_{1'} t'_1) \hat{\psi}(\mathbf{x}_1) U^{hh}(11') \hat{\psi}(\mathbf{x}_{1'}) + \int d(\mathbf{x}_1 d\mathbf{x}_{1'} t'_1) \hat{\psi}^\dagger(\mathbf{x}_{1'}) U^{ee}(11') \hat{\psi}^\dagger(\mathbf{x}_{1'}) \right)$$

...leading to an alternative Schwinger relation

$$G_2(12; 1'2') = -2 \left. \frac{\delta G^{ee}(1'2')}{\delta U^{hh}(12)} \right|_{U=0}$$

Anomalous propagator

Description of a non-number conserving Hamiltonian

Anomalous propagators

$$G^{hh}(11') = (-i) \langle \Psi_0 | \hat{T} \left[\hat{\psi}(1) \hat{\psi}(1') \right] | \Psi_0 \rangle \quad G^{ee}(11') = (-i) \langle \Psi_0 | \hat{T} \left[\hat{\psi}^\dagger(1) \hat{\psi}^\dagger(1') \right] | \Psi_0 \rangle$$

Description of a non-number conserving Hamiltonian

Anomalous propagators

$$G^{hh}(11') = (-i) \langle \Psi_0 | \hat{T} \left[\hat{\psi}(1) \hat{\psi}(1') \right] | \Psi_0 \rangle \quad G^{ee}(11') = (-i) \langle \Psi_0 | \hat{T} \left[\hat{\psi}^\dagger(1) \hat{\psi}^\dagger(1') \right] | \Psi_0 \rangle$$

Nambu formalism and the Gorkov propagator

$$\mathbf{G}(11') = (-i) \langle \Psi_0 | \hat{T} \left[\begin{pmatrix} \hat{\psi}(1) \hat{\psi}^\dagger(1') & \hat{\psi}(1) \hat{\psi}(1') \\ \hat{\psi}^\dagger(1) \hat{\psi}^\dagger(1') & \hat{\psi}^\dagger(1) \hat{\psi}(1') \end{pmatrix} \right] | \Psi_0 \rangle = \begin{pmatrix} G^{he}(11') & G^{hh}(11') \\ G^{ee}(11') & G^{eh}(11') \end{pmatrix}.$$

Description of a non-number conserving Hamiltonian

Anomalous propagators

$$G^{hh}(11') = (-i) \langle \Psi_0 | \hat{T} [\hat{\psi}(1)\hat{\psi}(1')] | \Psi_0 \rangle \quad G^{ee}(11') = (-i) \langle \Psi_0 | \hat{T} [\hat{\psi}^\dagger(1)\hat{\psi}^\dagger(1')] | \Psi_0 \rangle$$

Nambu formalism and the Gorkov propagator

$$\mathbf{G}(11') = (-i) \langle \Psi_0 | \hat{T} \begin{bmatrix} \hat{\psi}(1)\hat{\psi}^\dagger(1') & \hat{\psi}(1)\hat{\psi}(1') \\ \hat{\psi}^\dagger(1)\hat{\psi}^\dagger(1') & \hat{\psi}^\dagger(1)\hat{\psi}(1') \end{bmatrix} | \Psi_0 \rangle = \begin{pmatrix} G^{he}(11') & G^{hh}(11') \\ G^{ee}(11') & G^{eh}(11') \end{pmatrix}.$$

Strategy

Derive a closed set of equations for the Gorkov propagator and then take the number-conserving limit.

The particle-particle Hedin's equations

A new set of equations

$$G(12) = G_0(12) + \int G_0(13)\Sigma(34)G(42) d(34)$$

$$\tilde{\Gamma}(12; 1'2') = \frac{1}{2} (\delta(1'2)\delta(2'1) - \delta(1'1)\delta(2'2)) - \left. \frac{\delta\Sigma_c^{ee}(1'2')}{\delta G^{ee}(33')} \right|_{U=0} G(43)G(4'3')\tilde{\Gamma}(12; 44')$$

$$\tilde{K}(12; 1'2') = iG(31')G(3'2')\tilde{\Gamma}(12; 33')$$

$$T(12; 1'2') = -\bar{V}(12; 1'2') - T(12; 33')\tilde{K}(33'; 44')\bar{V}(44'; 1'2')$$

$$\Sigma(11') = iG(2'2)T(12; 33')\tilde{\Gamma}(33'; 2'1')$$

The particle-particle vertex

The T -matrix as a first approximation

$$G(12) = G_0(12) + \int G_0(13)\Sigma(34)G(42) d(34)$$

$$\tilde{\Gamma}(12; 1'2') = \frac{1}{2} (\delta(1'2)\delta(2'1) - \delta(1'1)\delta(2'2))$$

$$\tilde{K}(12; 1'2') = \frac{i}{2} (G(12')G(21') - G(22')G(11'))$$

$$T(12; 1'2') = -\bar{V}(12; 1'2') - T(12; 33')\tilde{K}(33'; 44')\bar{V}(44'; 1'2')$$

$$\Sigma(11') = iG(2'2)T(12; 1'2')$$

The particle-particle vertex

The T -matrix as a first approximation

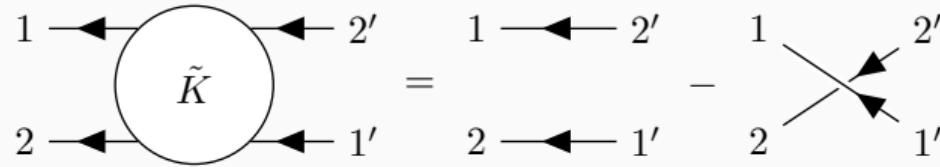
$$G(12) = G_0(12) + \int G_0(13)\Sigma(34)G(42) d(34)$$

$$\tilde{\Gamma}(12; 1'2') = \frac{1}{2} (\delta(1'2)\delta(2'1) - \delta(1'1)\delta(2'2))$$

$$\tilde{K}(12; 1'2') = \frac{i}{2} (G(12')G(21') - G(22')G(11'))$$

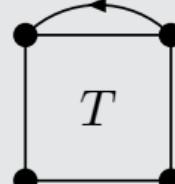
$$T(12; 1'2') = -\bar{V}(12; 1'2') - T(12; 33')\tilde{K}(33'; 44')\bar{V}(44'; 1'2')$$

$$\Sigma(11') = iG(2'2)T(12; 1'2')$$



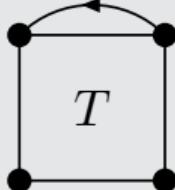
Vertex corrections to the GT self-energy

Zeroth iteration

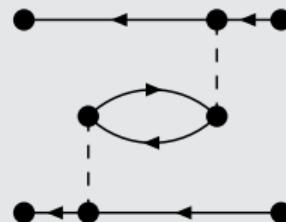
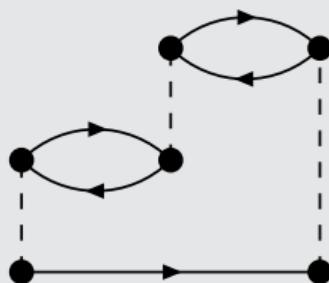
$$\Sigma = T$$
A diagram showing a square loop of four vertical segments connecting four black circular vertices. Inside the square, the letter 'T' is centered. Above the square, there is a curved arrow pointing from the top-left vertex to the top-right vertex, indicating a flow or correction path.

Vertex corrections to the GT self-energy

Zeroth iteration

$$\Sigma = T$$


Second iteration: outer and inner corrections

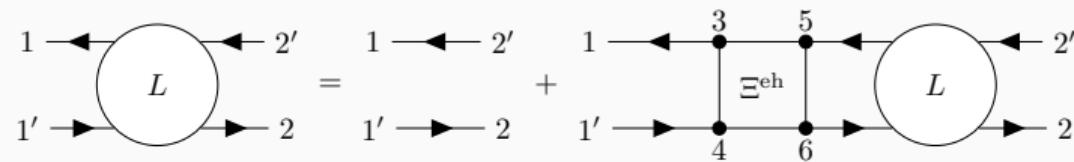


The particle-particle Bethe-Salpeter equation

Two-body Bethe-Salpeter equations

The electron-hole Bethe-Salpeter equation

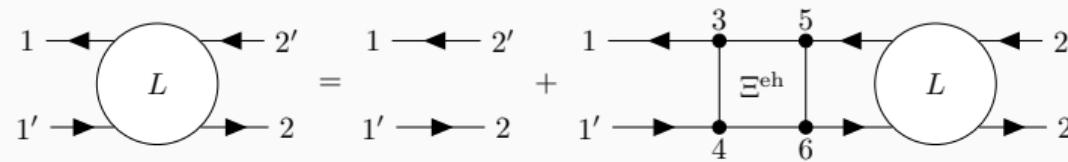
$$L(12; 1'2') = L_0(12; 1'2') + \int d(3456) L_0(14; 1'3) \Xi^{eh}(36; 45) L(52; 62').$$



Two-body Bethe-Salpeter equations

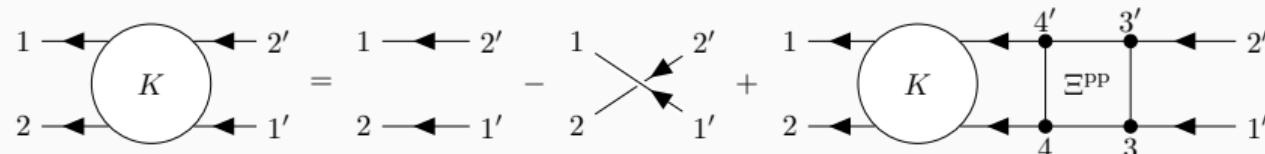
The electron-hole Bethe-Salpeter equation

$$L(12; 1'2') = L_0(12; 1'2') + \int d(3456) L_0(14; 1'3) \Xi^{eh}(36; 45) L(52; 62').$$



The particle-particle Bethe-Salpeter equation

$$K(12; 1'2') = K_0(12; 1'2') - \int d(3456) K(12; 56) \Xi^{pp}(56; 34) K_0(34; 1'2')$$



What's the difference?

The two kernels

$$\Xi^{\text{eh}}(12; 34) = \frac{\delta \Sigma^{\text{eh}}(13)}{\delta G^{\text{eh}}(42)} \Big|_{U=0}$$

What's the difference?

The two kernels

$$\Xi^{\text{eh}}(12; 34) = \left. \frac{\delta \Sigma^{\text{eh}}(13)}{\delta G^{\text{eh}}(42)} \right|_{U=0}$$

$$\int d(3'44') G(24) \Xi^{\text{pp}}(34; 3'4') K(3'4'; 1'2') = \\ \int d(3'44') G(41') \Xi^{\text{eh}}(34'; 43') L(3'2; 4'2')$$

Csanak, Taylor and Yaris, Adv. Atom. Mol. Phys. 7 (1971) 287-361

What's the difference?

The two kernels

$$\Xi^{eh}(12; 34) = \left. \frac{\delta \Sigma^{eh}(13)}{\delta G^{eh}(42)} \right|_{U=0}$$

$$\int d(3'44') G(24) \Xi^{pp}(34; 3'4') K(3'4'; 1'2') = \\ \int d(3'44') G(41') \Xi^{eh}(34'; 43') L(3'2; 4'2')$$

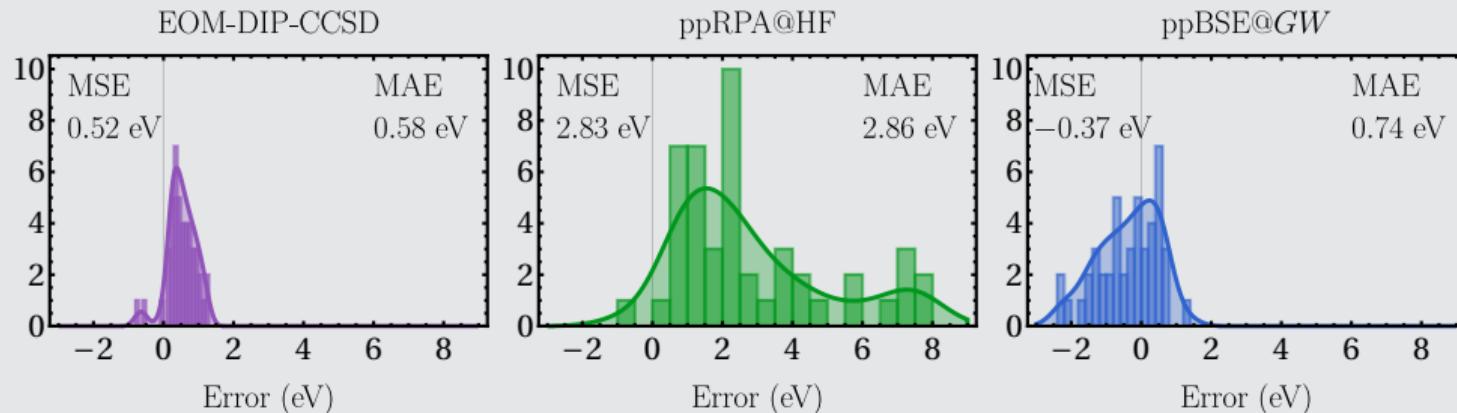
Csanak, Taylor and Yaris, Adv. Atom. Mol. Phys. 7 (1971) 287-361

A new expression for the particle-particle kernel

$$\Xi^{pp}(12; 34) = \left. \frac{\delta \Sigma^{ee}(34)}{\delta G^{ee}(12)} \right|_{U=0}$$

Valence double ionization potentials

Error distribution for 46 DIP of 23 small molecules



Conclusion and perspectives

Conclusion and perspectives

Conclusions

- A set of equations has been derived for the one-body propagator
- The pp T -matrix self-energy has no second-order term and the third order term might be really expensive
- Can we couple W and T thanks to the Nambu formalism?

Conclusion and perspectives

Conclusions

- A set of equations has been derived for the one-body propagator
- The pp T -matrix self-energy has no second-order term and the third order term might be really expensive
- Can we couple W and T thanks to the Nambu formalism?

Anomalous propagators are also useful for two-body equations

- Simple expression for the kernel of the particle-particle channel!
- Accuracy of the particle-particle Bethe-Salpeter for double ionization?
- “Spin-flip-like” strategy for neutral excited states?

Questions?

Gorkov-Hedin equations: effective interaction

Generalized T -matrix

$$T^{\text{he}} = \begin{array}{c} \bullet \\ \square \\ \bullet \end{array} + \begin{array}{c} \bullet \\ \square \\ \leftarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \leftarrow \leftarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \leftarrow \leftarrow \leftarrow \end{array} + \dots$$

$$T^{\text{hh}} = \begin{array}{c} \bullet \\ \square \\ \bullet \end{array} + \begin{array}{c} \bullet \\ \square \\ \leftarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \leftarrow \rightarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \leftarrow \rightarrow \leftarrow \end{array} + \dots$$

$$T^{\text{ee}} = \begin{array}{c} \bullet \\ \square \\ \bullet \end{array} + \begin{array}{c} \bullet \\ \square \\ \rightarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \rightarrow \leftarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \rightarrow \leftarrow \rightarrow \end{array} + \dots$$

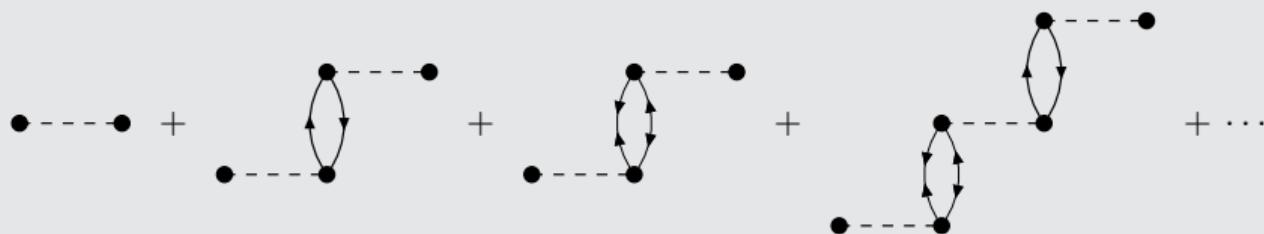
$$T^{\text{eh}} = \begin{array}{c} \bullet \\ \square \\ \bullet \end{array} + \begin{array}{c} \bullet \\ \square \\ \rightarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \rightarrow \leftarrow \end{array} + \begin{array}{c} \bullet \\ \square \\ \rightarrow \leftarrow \rightarrow \end{array} + \dots$$

Bozek, Phys Rev C 65 (2002) 034327

Self-energy

$$\Sigma(11') = i \int d(33') \begin{pmatrix} W(13'; 31')G^{he}(33') & -W(13'; 31')G^{hh}(33') \\ -W(31'; 13')G^{ee}(33') & W(31'; 13')G^{eh}(33') \end{pmatrix} \quad (1)$$

Screened interaction



Electron-hole propagator

$$L(\mathbf{x}_1 \mathbf{x}_2; \mathbf{x}_1' \mathbf{x}_2'; \omega) = \sum_{\nu>0} \frac{L_\nu^N(\mathbf{x}_2 \mathbf{x}_{2'}) R_\nu^N(\mathbf{x}_1 \mathbf{x}_{1'})}{\omega - (E_\nu^N - E_0^N - i\eta)} - \sum_{\nu>0} \frac{L_\nu^N(\mathbf{x}_2 \mathbf{x}_{2'}) R_\nu^N(\mathbf{x}_1 \mathbf{x}_{1'})}{\omega - (E_0^N - E_\nu^N + i\eta)} \quad (2)$$

Particle-particle interaction

$$K(\mathbf{x}_1 \mathbf{x}_2; \mathbf{x}_1' \mathbf{x}_2'; \omega) = \sum_{\nu} \frac{L_\nu^{N+2}(\mathbf{x}_1 \mathbf{x}_2) R_\nu^{N+2}(\mathbf{x}_1' \mathbf{x}_2')}{\omega - (E_\nu^{N+2} - E_0^N - i\eta)} - \sum_{\nu} \frac{L_\nu^{N-2}(\mathbf{x}_1' \mathbf{x}_2') R_\nu^{N-2}(\mathbf{x}_1 \mathbf{x}_2)}{\omega - (E_0^N - E_\nu^{N-2} + i\eta)} \quad (3)$$

Particle-hole and particle-particle RPA eigenvalue problem

phRPA

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^\dagger & \mathbf{A} \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix}, \quad (4)$$

$$A_{ia,bj}^{\text{RPA}} = (\epsilon_a - \epsilon_i) \delta_{ab} \delta_{ij} + \langle ib | aj \rangle \quad (5)$$

$$B_{ia,bj}^{\text{RPA}} = \langle ij | ab \rangle$$

ppRPA

$$\begin{pmatrix} \mathbf{C} & \mathbf{B} \\ \mathbf{B}^\dagger & \mathbf{D} \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix}, \quad (6)$$

$$C_{ab,cd}^{\text{RPA}} = (\epsilon_a + \epsilon_b) \delta_{ac} \delta_{bd} + \langle ab || cd \rangle$$

$$B_{ab,ij}^{\text{RPA}} = \langle ab || ij \rangle \quad (7)$$

$$D_{ij,kl}^{\text{RPA}} = -(\epsilon_i + \epsilon_j) \delta_{ik} \delta_{jl} + \langle ij || kl \rangle$$