

# Quantum kinetic equations

## Lecture #2

Michael Bonitz, Karsten Balzer

Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu  
Kiel, 24098 Kiel, Germany

December 3, 2008

# Outline

- 1 Self-energy concept
  - Hierarchy decoupling
- 2 Approximations and Feynman diagrams
  - Conserving approximations
  - Feynman diagrams
- 3 Single-time kinetic equations
  - Boltzmann equation
- 4 Conclusion
  - Conclusion

Kadanoff-Baym/Keldysh equations ▶ more

## Kadanoff-Baym/Keldysh equations (KBE)—Review

$$\begin{aligned} \left( i \frac{\partial}{\partial t_1} - H^1(1) \right) G(1, \bar{1}) &= \delta_{\mathcal{C}'}(1 - \bar{1}) \pm i \int_{\mathcal{C}'} d2 W(1 - 2) G_{12}(1, 2; \bar{1}, 2^+) \\ \left( -i \frac{\partial}{\partial t_{\bar{1}}} - H^1(\bar{1}) \right) G(1, \bar{1}) &= \delta_{\mathcal{C}'}(1 - \bar{1}) \pm i \int_{\mathcal{C}'} d2 W(\bar{1} - 2) G_{12}(1, 2; \bar{1}, 2^+) \end{aligned}$$

- $H^1(1) = -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}_1}^2 + V(1) - \mu \hat{N}$  denotes the single-particle Hamiltonian
- The upper sign refers to bosons the lower one refers to fermions, and the temporal integrations are taken over the Schwinger/Keldysh time contour  $\mathcal{C}'$
- KBE not closed but coupled to higher orders via the 2-particle Green's function  $G_{12}(1, 2; \bar{1}, \bar{2})$
- *Martin-Schwinger (MS) hierarchy*: The  $n$ -particle Green's function generally requires information from the  $(n \pm 1)$ -particle Green's function

# MS Hierarchy decoupling

Idea: Express 2-particle Green's function  $G_{12}$  in terms of products of 1-particle Green's functions

$$G_{12}(1, 2; \bar{1}, \bar{2}) = [G(\cdot, \cdot)G(\cdot, \cdot)](1, 2; \bar{1}, \bar{2}) + \Delta_{\text{corr}}(1, 2; \bar{1}, \bar{2})$$

with corrections  $\Delta_{\text{corr}}(1, 2; \bar{1}, \bar{2})$  ( $\Rightarrow$  correlation contributions)

- Simplest example: *Hartree-Fock* approximation (first order)

$$G_{12}(1, 2; \bar{1}, \bar{2}) \approx \overset{\text{Fock (exchange)}}{G(1, \bar{1}) G(2, \bar{2}) \pm G(1, \bar{2}) G(2, \bar{1})} + \overset{\text{Hartree (classical mean-field)}}{\dots}$$

# Formal MS hierarchy decoupling

Introduce self-energy  $\Sigma$ :

$$\pm i \int_{\mathcal{C}'} d2 W(1-2) G_{12}(1, 2; \bar{1}, 2^+) \stackrel{!}{=} \int_{\mathcal{C}'} d2 \Sigma[G, W](1, 2) G(2, \bar{1})$$

Remarks:

- All interaction effects are now contained in the self-energy  $\Sigma[G, W](1, \bar{1})$
- The self-energy appears as a functional of the interaction potential  $W(1, \bar{1})$  and the 1-particle Green's function  $G(1, \bar{1})$ , and thus varies on the Schwinger/Keldysh contour  $\mathcal{C}' \rightarrow \Sigma^{\geq}, \Sigma^{1/\Gamma}$ , and  $\Sigma^M$ .
- In general, the pair interaction enters  $\Sigma$  as infinite summations
- A diagrammatic expansion of  $\Sigma$  (known from ground state theory) can be extended to finite temperature and nonequilibrium situations

# Conserving approximations

Definition: Approximations for  $G_{12}$  which conserve total energy, momentum and angular momentum [when calculated from  $G(1, \bar{1})$ ] are denoted as *conserving approximations*.

How can one guarantee that a self-energy gives a conserving approximation for the Green's function?

- Conservation of total energy and momentum if
  - (A)  $G(1, \bar{1})$  satisfies the general equations of motions (KBE),
  - (B) the approximation for  $G_{12}$  satisfies the symmetry condition

$$G_{12}(1, 2; 1^+, 2^+) = G_{12}(2, 1; 2^+, 1^+).$$

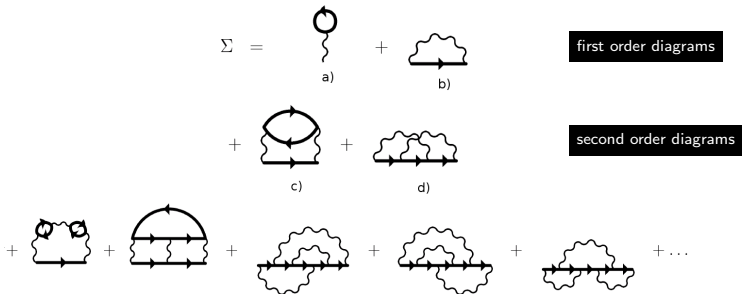
[G. Baym, and L.P. Kadanoff, Phys. Rev **124**, 287 (1961)]

- Conclusion:  $\Phi$ -derivable self-energy ▶ more

$$\Sigma(1, \bar{1}) = \frac{\delta\Phi[G]}{\delta G(\bar{1}, 1)}.$$

How  $\Phi$  can be constructed? [J.M. Luttinger, and J.C. Ward Phys. Rev. **118**, 1417 (1960)]

# Lowest-order $\Sigma$ -diagrams



**Figure:** Self-energy (Feynman) diagrams. First order in the interaction  $W(1, \bar{1})$ : a) Hartree, b) Fock. Second order in  $W(1, \bar{1})$ : c) & d) second Born terms.

- Waved lines ( $1 \rightsquigarrow \bar{1}$ ) indicate the interaction  $W(1 - \bar{1})$ , whereas solid lines ( $1 \rightarrow \bar{1}$ ) denote the *full* nonequilibrium Green's function  $G(1, \bar{1})$
- All self-energy terms contain an infinite summation of diagrams.

# Interpretation of $\Sigma$ -diagrams

Contributions of first order in the interaction  $W$ :



**Figure:** First order self-energies: Hartree (class. mean-field) term [left], Fock (exchange) term [right].

Hartree-Fock self-energy  $\Sigma^{\text{HF}} = \Sigma^{\text{H}} + \Sigma^{\text{F}}$

$$\Sigma^{\text{H}}(1, \bar{1}) = \pm i \delta_{\mathcal{C}}(1 - \bar{1}) \int_{\mathcal{C}} d2 W(1 - 2) G(2, 2^+)$$

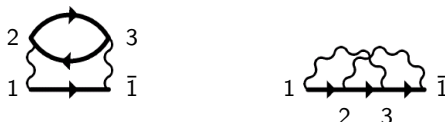
$$\Sigma^{\text{F}}(1, \bar{1}) = i G(1, \bar{1}) W(1^+ - \bar{1})$$

- Note the time-ordering and recall  $1^+ = t_1 \rightarrow t_1 + \epsilon > 0$
- Contributions of order  $n$  take a sign of  $(-i)^n$ , the direct (Hartree) term has an additional minus sign only for fermions



# Interpretation of $\Sigma$ -diagrams

Contributions of second order in the interaction  $W$ :



**Figure:** Second (order) Born diagrams, composed of two interaction lines and three Green's functions. Direct term [left], exchange term [right].

Second Born contributions  $\Sigma^{2\text{ndB}} = \Sigma_1^{2\text{ndB}} + \Sigma_2^{2\text{ndB}}$

$$\Sigma_2^{2\text{ndB}}(1, \bar{1}) = \pm (-i)^2 \int_{\mathcal{C}} d2 d3 G(1, \bar{1}) W(1^+ - 2) W(\bar{1} - 3) G(3, 2) G(2, 3^+)$$

$$\Sigma_1^{2\text{ndB}}(1, \bar{1}) = (-i)^2 \int_{\mathcal{C}} d2 d3 G(1, 2) W(1 - 3^+) G(2, 3) G(3, \bar{1}) W(2^+ - \bar{1})$$

- $\Sigma_1^{2\text{ndB}}$  and  $\Sigma_2^{2\text{ndB}}$  are to be added to the Hartree-Fock self-energy  $\Sigma^{\text{HF}}$

Equation of motion for  $G^*(1, \bar{1})$ ,  $* \in \{M, >, <, \uparrow, \downarrow\}$ 

Keldysh/Kadanoff-Baym equations:

$$\left( i \frac{\partial}{\partial t_1} - H^1(1) \right) G(1, \bar{1}) = \delta_{\mathcal{C}'}(1 - \bar{1}) + \int_{\mathcal{C}'} d2 \Sigma(1, 2) G(2, \bar{1})$$

together with its adjoint equation including the derivative  $\partial_{\bar{1}}$

- $G(1, \bar{1})$  is a  $3 \times 3$ -matrix of the form

$$\left( \begin{array}{cc|c} G^{++} & G^{+-} & G^{+\downarrow} \\ G^{-+} & G^{--} & G^{-\downarrow} \\ \hline G^{\uparrow+} & G^{\uparrow-} & G^{\uparrow\downarrow} \end{array} \right) = \left( \begin{array}{cc|c} G^c & G^< & G^{\downarrow} \\ G^> & G^a & G^{\uparrow} \\ \hline G^{\uparrow} & G^{\downarrow} & G^M \end{array} \right)$$

- Need equations for the elements of the Keldysh matrix

$$G^{\lessgtr}(1, \bar{1}), \quad G^M(1, \bar{1}), \quad G^{\uparrow/\downarrow}(1, \bar{1})$$

- Question:** How to evaluate the integrals  $\int_{\mathcal{C}'} d2 \Sigma(1, 2) G(2, \bar{1})$  for the matrix elements of a product or convolution?  $\Rightarrow$  "Langreth rules"

# Langreth rules

Results for Convolution and product of two (Keldysh) functions defined on  $\mathcal{C}'$

quantity <sup>1</sup>	convolution	product
	$c(z, z') = \int_{\mathcal{C}'} d\bar{t} a(t, \bar{t}) b(\bar{t}, t')$	$c(z, z') = a(t, t') b(t', t)$
$c^>(t, t')$	$a^> \circ b^A + a^R \circ b^> + a^{\lceil} \star b^{\lceil}$	$a^> b^<$
$c^<(t, t')$	$a^< \circ b^A + a^R \circ b^< + a^{\lceil} \star b^{\lceil}$	$a^< b^>$
$c^{\lceil}(\tau, t)$	$a^R \circ b^{\lceil} + a^{\lceil} \star b^M$	$a^{\lceil} b^{\lceil}$
$c^{\lceil}(t, \tau)$	$a^{\lceil} \circ b^A + a^M \star b^{\lceil}$	$a^{\lceil} b^{\lceil}$
$c^M(\tau, \tau')$	$a^M \star b^M$	$a^M b^M$
$c^R(t, t')$	$a^R \circ b^R$	$a^R b^{\geq} + a^{\geq} b^A$
$c^A(t, t')$	$a^A \circ b^A$	$a^A b^{\leq} + a^{\leq} b^R$
	$[a \circ b](t, t') = \int_{t_0}^{\infty} d\bar{t} a(t, \bar{t}) b(\bar{t}, t')$ $[a \star b](t, t') = -i \int_{t_0}^{t_0 - i\beta} d\bar{t} a(t, \bar{t}) b(\bar{t}, t')$	$a^{R/A}(t, t') = a^{\geq}(t, t') - a^{\leq}(t, t')$

<sup>1</sup>Space variables are dropped for simplicity

Equation of motion for the correlation functions  $G^{\gtrless}$ Summary:Write  $\partial_t$  instead of  $\frac{\partial}{\partial t}$ 

$$\begin{aligned} \left( i\partial_{t_1} - H^1(\mathbf{1}) \right) G^{\gtrless}(\mathbf{1}, \bar{\mathbf{1}}) &= \int_{t_0}^{t_1} d2 \Sigma^R(\mathbf{1}, 2) G^{\gtrless}(\mathbf{2}, \bar{\mathbf{1}}) + \int_{t_0}^{t_1} d2 \Sigma^{\gtrless}(\mathbf{1}, 2) G^A(\mathbf{2}, \bar{\mathbf{1}}) \\ &\quad - i \int_0^\beta d2 \Sigma^{\lrcorner}(\mathbf{1}, 2) G^{\lrcorner}(\mathbf{2}, \mathbf{1}) \end{aligned}$$

1-p. energy
memory kernel
memory kernel
initial correlations

$$\begin{aligned} \left( -i\partial_{t_1} - H^1(\bar{\mathbf{1}}) \right) G^{\gtrless}(\mathbf{1}, \bar{\mathbf{1}}) &= \int_{t_0}^{t_1} d2 G^R(\mathbf{1}, 2) \Sigma^{\gtrless}(\mathbf{2}, \bar{\mathbf{1}}) + \int_{t_0}^{t_1} d2 G^{\gtrless}(\mathbf{1}, 2) \Sigma^A(\mathbf{2}, \bar{\mathbf{1}}) \\ &\quad - i \int_0^\beta d2 G^{\lrcorner}(\mathbf{1}, 2) \Sigma^{\lrcorner}(\mathbf{2}, \mathbf{1}) \end{aligned}$$

with definitions of retarded ( $R$ ) and advanced ( $A$ ) quantities

$$G^{R/A}(\mathbf{1}, \bar{\mathbf{1}}) = G^{\gtrless}(\mathbf{1}, \bar{\mathbf{1}}) - G^{\lessgtr}(\mathbf{1}, \bar{\mathbf{1}}), \quad \Sigma^{R/A}(\mathbf{1}, \bar{\mathbf{1}}) = \Sigma^{\gtrless}(\mathbf{1}, \bar{\mathbf{1}}) - \Sigma^{\lessgtr}(\mathbf{1}, \bar{\mathbf{1}})$$

Memory kernels: Memory and dissipation, decay of the Green's function. Initial correlations enter via the Matsubara Green's function  $G^M \Rightarrow G^{\gtrless}(\mathbf{r}_1 t_0, \mathbf{r}_{\bar{\mathbf{1}}} t_0)$  and  $G^{\lrcorner}(\mathbf{r}_1 t_0, \mathbf{r}_{\bar{\mathbf{1}}} t_0 - i\tau)$ ,  $G^{\lrcorner}(\mathbf{r}_1 t_0 - i\tau, \mathbf{r}_{\bar{\mathbf{1}}} t_0)$ .

# Derivation of single-time kinetic equations

Single-time kinetic equations can be obtained in the limit of slowly varying disturbances.

Motivation:

- Avoid to deal with two-time quantities, or obtain only statistical information (fully included in the Wigner function—the time-diagonal part of  $G^{<}$ )
- Relevant for studying *simple* transport processes

Basic assumptions:

- Consider the case where the single-particle energy  $H^1(\mathbf{r}_1, t_1)$  is slowly varying in time and space
- Consequence of a scale separation:  $G^{\gtrless}(1, \bar{1})$  are slowly varying functions of the coordinates

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_{\bar{1}}}{2}, \quad \mathbf{T} = \frac{t_1 + t_{\bar{1}}}{2},$$

but are sharply peaked about zero values of

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_{\bar{1}}, \quad \mathbf{t} = t_1 - t_{\bar{1}}.$$

⇒ Consider  $G^{\gtrless}(\mathbf{r}\mathbf{t}, \mathbf{R}\mathbf{T})$  and its Fourier transform in  $\mathbf{r}$  and  $\mathbf{t}$

▶ remind yourself

# Derivation of the Boltzmann equation I

Recipe: [see L.P. Kadanoff, and G. Baym, *Quantum Statistical Mechanics* (Benjamin, Inc., New York, 1962)]

- 1 Subtract adjoint KBE (with time arguments  $t_1$  and  $t_{\bar{1}}$  interchanged) from the KBE for  $G^<(1, \bar{1})$ , and express the space time variables of  $G$  and  $\Sigma$  in terms of relative and center of mass coordinates.
- 2 Neglect the third collision integral on the r.h.s. accounting for initial correlations—instead integrate over  $\int_{-\infty}^{t_1} d\bar{t} \dots$  and  $\int_{-\infty}^{t_{\bar{1}}} d\bar{t} \dots$
- 3 Expand the difference of

$$H^1 \left( \mathbf{r}_1 = \mathbf{R} - \frac{\mathbf{r}}{2}, t_1 = T - \frac{t}{2} \right) - H^1 \left( \mathbf{r}_{\bar{1}} = \mathbf{R} + \frac{\mathbf{r}}{2}, t_{\bar{1}} = T - \frac{t}{2} \right)$$

in powers of  $\mathbf{r}$  and  $t$ , and retain only lowest-order terms ( $\mathbf{r}$  and  $t$  small)

- 4 Similarly, proceed with the relative variables on the r.h.s. (collision integrals) of the KBE—fully neglect the small quantities added to  $\mathbf{R}$  and  $T$ .

**Typical integrals:**

$$\int_{\mathcal{C}'} d^3\bar{r} d\bar{t} G(\bar{\mathbf{r}}\bar{t}; \mathbf{R} T) \Sigma(\mathbf{r} - \bar{\mathbf{r}} t - \bar{t}; \mathbf{R} T)$$

convolution in Fourier space

## Derivation of the Boltzmann equation II

- 5 Fourier transformation with respect to variables  $\mathbf{r}$  and  $t$  lead to approximate equations for  $G^{\lessgtr}(\mathbf{p}\omega, \mathbf{R}T)$

Intermediate result:  $H^1 = \frac{-\nabla^2}{2m} + V(\mathbf{1})$   $\hbar = 1$

$$\begin{aligned} & \left[ \partial_T + \frac{\mathbf{p} \cdot \nabla_{\mathbf{R}}}{m} - \nabla_{\mathbf{R}} V(\mathbf{R}, T) \nabla_{\mathbf{p}} + \partial_T V(\mathbf{R}, T) \partial_{\omega} \right] G^<(\mathbf{p}\omega, \mathbf{R}T) \\ &= -G^<(\mathbf{p}\omega, \mathbf{R}T) \Sigma^>(\mathbf{p}\omega, \mathbf{R}T) \\ & \quad + G^>(\mathbf{p}\omega, \mathbf{R}T) \Sigma^<(\mathbf{p}\omega, \mathbf{R}T) \end{aligned}$$

- 6 Insert second Born expressions for the self-energy  $\Sigma^{\lessgtr}$  (take all second spatial arguments in  $G$  to be  $\mathbf{R}$ —the disturbance varies very little within a distance of the order of the potential range)
- 7 Fourier transform in  $\mathbf{r}, t$ :  $\Sigma^{\lessgtr}(\mathbf{r}t, \mathbf{R}T) \rightarrow \Sigma^{\lessgtr}(\mathbf{p}\omega, \mathbf{R}T)$

# Derivation of the Boltzmann equation III

*Self-energy (second order):*

$$\begin{aligned} \Sigma^{\lessgtr}(\mathbf{p}\omega, \mathbf{R}T) &\approx \frac{1}{2} \int d^3\mathbf{p}' d\omega' d\bar{\mathbf{p}} d\bar{\omega} d^3\bar{\mathbf{p}}' d\omega' \\ &\times \delta(\mathbf{p} + \mathbf{p}' - \bar{\mathbf{p}} - \bar{\mathbf{p}}') \delta(\omega + \omega' - \bar{\omega} - \bar{\omega}') \\ &\times [w(\mathbf{p} - \bar{\mathbf{p}}) \pm w(\mathbf{p} - \bar{\mathbf{p}}')]^2 \\ &\times G^{\lessgtr}(\mathbf{p}'\omega', \mathbf{R}T) G^{\lessgtr}(\bar{\mathbf{p}}\bar{\omega}, \mathbf{R}T) G^{\lessgtr}(\bar{\mathbf{p}}'\bar{\omega}', \mathbf{R}T) \end{aligned}$$

- 8 Reconstruction problem: Assume that the Green's functions can be expressed via the Wigner distribution function  $f(\mathbf{p}, \mathbf{R}, T)$  and the spectral function  $A(\mathbf{p}\omega, \mathbf{R}T) = 2\pi\delta[\omega - E(\mathbf{p}, \mathbf{R}, T)]$

$$G^<(\mathbf{p}\omega, \mathbf{R}T) = A(\mathbf{p}\omega, \mathbf{R}T) f(\mathbf{p}, \mathbf{R}, T)$$

$$G^>(\mathbf{p}\omega, \mathbf{R}T) = A(\mathbf{p}\omega, \mathbf{R}T) [1 \pm f(\mathbf{p}, \mathbf{R}, T)]$$

- 9 Some differential algebra ...



# The Boltzmann (Landau) equation

Result: Boltzmann equation with Born approximation collision cross section:

$$\begin{aligned}
 & \left[ \partial_T + \frac{\mathbf{p} \cdot \nabla_{\mathbf{R}}}{m} - \nabla_{\mathbf{R}} V(\mathbf{R}, T) \nabla_{\mathbf{p}} \right] f(\mathbf{p}, \mathbf{R}, T) = I(\mathbf{p}, \mathbf{R}, T) \\
 & = -\frac{1}{2} \int d^3 \mathbf{p}' d^3 \bar{\mathbf{p}} d^3 \bar{\mathbf{p}}' \delta(\mathbf{p} + \mathbf{p}' - \bar{\mathbf{p}} - \bar{\mathbf{p}}') \delta(E(\mathbf{p}) + E(\mathbf{p}') - E(\bar{\mathbf{p}}) - E(\bar{\mathbf{p}}')) \\
 & \quad \times [w(\mathbf{p} - \bar{\mathbf{p}}) \mp w(\mathbf{p} - \bar{\mathbf{p}}')]^2 \\
 & \quad \times [f f' (1 \pm \bar{f}) (1 \pm \bar{f}') - (1 \pm f) (1 \pm f') \bar{f} \bar{f}']
 \end{aligned}$$

collision integral

- $f(\mathbf{p}, \mathbf{R}, T)$  is the Wigner distribution function,  $E(p) = \frac{p^2}{2m}$  denotes the quasiparticle energy.  $f = f(\mathbf{p}, \mathbf{R}, t)$ ,  $f' = f(\mathbf{p}', \mathbf{R}, t)$ , etc.
- Kinetic energy and momentum are preserved due to the  $\delta$ -functions
- Limited to times larger than the correlation time,  $T \gg \tau_{\text{corr}}$

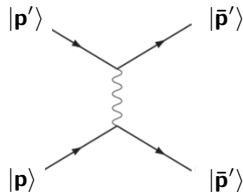


Figure: Feynman diagram

# Conclusion I

## Boltzmann equation

- Single-time equation for the Wigner function  $f(\mathbf{p}, \mathbf{R}, T)$
- **Stationary solutions:** Maxwell, Fermi or Bose distributions
- $I(\mathbf{p}, \mathbf{R}, T) \rightarrow 0$  leads to thermodynamic properties of the *ideal gas*, where correlations are neglected
- **Reason:** local approximation (neglect of memory)  
⇒ Memory is fully contained in the two-time Keldysh/Kadanoff-Baym equations for  $G(1, \bar{1})$

# Conclusion II

- MS hierarchy formally decoupled by introducing the self-energy  $\Sigma[G, W]$   
 $\Rightarrow$  Describe binary interactions as an infinite summation of diagrams
- Conserving approximations allow for a systematic truncation of the hierarchy.  
 Examples: Hartree-Fock, second Born, GW ▶ GW

$$\Sigma = \text{a)} + \text{b)} + \text{c)} + \text{d)}$$

**Figure:** Self-energy diagrams. First order in the interaction  $W(1, \bar{1})$ : a) Hartree, b) Fock. Second order in  $W(1, \bar{1})$ : c) & d) second Born terms.

- Structure/identification and meaning of the appearing terms in the equation:  
 memory kernels                      &                      inclusion of initial correlations

Fin

Thanks for your attention!

Next lecture: (i) Numerical technique solving the KBE  
(ii) Applications to semiconductors (homogeneous systems) as well as quantum dots, atoms and molecules (inhomogeneous systems)

## Structure of the nonequilibrium Green's function [◀ back](#)

**Indeed**, the nonequilibrium Green's function (NEGF) has the structure of a usual (mathematical) Green's function in the following sense:

- (a) When neglecting all collision integrals on the r.h.s. of the KBE  $\rightarrow$  effective single-particle or ideal quantum system described by  $G_0(1, \bar{1})$  which obeys

$$\left[ i \frac{\partial}{\partial t_1} - H^1(1) \right] G_0(1, \bar{1}) = \delta_{\mathcal{C}'}(1 - \bar{1}) \quad (3)$$

Eq. (3) then gives rise to an inverse Green's function

$$G_0^{-1}(1, \bar{1}) = \left[ i \frac{\partial}{\partial t_1} - H^1(1) \right] \delta_{\mathcal{C}'}(1 - \bar{1})$$

with matrix equation  $G_0^{-1} G_0 = 1$ .

- (b) generalization to case with correlations: define

$$G^{-1}(1, \bar{1}) = G_0^{-1}(1, \bar{1}) - \Sigma(1, \bar{1})$$

such that

$$\int_{\mathcal{C}'} d2 G^{-1}(1, 2) G(2, \bar{1}) = \delta_{\mathcal{C}'}(1 - \bar{1})$$

is equivalent to the Kadanoff-Baym equations.

# Lowest-order $\Phi$ -diagrams ◀ back

$$\Phi = -\frac{1}{2} \text{diagram}_1 - \frac{1}{2} \text{diagram}_2 - \frac{1}{4} \text{diagram}_3 - \frac{1}{4} \text{diagram}_4 - \frac{1}{6} \text{diagram}_5 - \frac{1}{6} \text{diagram}_6 - \frac{3}{6} \text{diagram}_7 + \dots$$

**Figure:** Generating  $\Phi$ -diagrams. Prefactor is given by  $n_{\Sigma}/2n$ .

The functional  $\Phi$  can be constructed by summation over irreducible self-energy diagrams closed with an additional Green's function line and multiplied by appropriate numerical factors:

$$\Phi[G] = \sum_{n,k} \frac{1}{2n} \int d1 d2 \Sigma_k^{(n)}(1, \bar{1}) G(\bar{1}, 1^+)$$

- $n$  denotes the number of interaction lines
- $k$  labels  $\Sigma$ -diagrams
- $n_{\Sigma}$  is the number of topologically different  $\Sigma$ -diagrams that can be generated from the  $\Phi$ -diagram

# $G^{\gtrless}$ in relative and center of mass coordinates ◀ back

We recall that

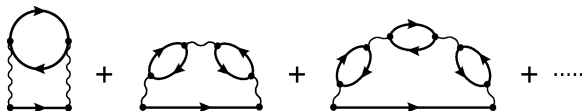
$$G^<(\mathbf{p}\omega, \mathbf{R}T) = \int d^3r dt e^{-i\mathbf{p}\mathbf{r}+i\omega t} [\pm iG^<(\mathbf{r}t, \mathbf{R}T)]$$

$$G^>(\mathbf{p}\omega, \mathbf{R}T) = \int d^3r dt e^{-i\mathbf{p}\mathbf{r}+i\omega t} iG^>(\mathbf{r}t, \mathbf{R}T)$$

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_{\bar{1}}}{2}, \quad \mathbf{T} = \frac{t_1 + t_{\bar{1}}}{2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_{\bar{1}}, \quad t = t_1 - t_{\bar{1}}$$

- $G^<(\mathbf{p}\omega, \mathbf{R}T)$  can be interpreted as the density of particles with momentum  $\mathbf{p}$  and energy  $\omega$  at the space time point  $(\mathbf{R}, t)$
- Correspondingly,  $G^>(\mathbf{p}\omega, \mathbf{R}T)$  denotes the density of states available to a particle that is added to the system at  $(\mathbf{R}, t)$  with momentum  $\mathbf{p}$  and energy  $\omega$

## GW approximation ◀ back



**Figure:** GW self-energy ( $\sim$  dynamical screened potential)—summation of all bubble-like diagrams [A. Stan et al, *Europhys. Lett.* **76**, 298 (2006)]