

Nonequilibrium Green's Functions

Lecture notes: contour formalism, diagrams, Keldysh space, and quantum transport

E. Arrigoni

Institute of Theoretical and Computational Physics, TU Graz ¹

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Keldysh '64, Kadanoff–Baym '62; following Rammer–Smith (1986) and Haug–Jauho (1998)

¹Printed version of the notes and slides produced with the help of AI, based on original handwritten notes

Outline

- 1 Suggested literature
- 2 Motivation: why nonequilibrium Green's functions?
- 3 The nonequilibrium problem and the Keldysh contour
- 4 Perturbation expansion and Feynman diagrams
- 5 Keldysh space
- 6 Noninteracting Green's functions
- 7 A single-particle potential: the exactly solvable case
- 8 A quench in a closed system: why dissipation matters
- 9 Coupling to a bath: the resonant level model
- 10 Two baths: steady-state transport
- 11 Electron–electron interaction: Anderson model and Hubbard-I
- 12 Time dependence: relaxation after a quantum quench
- 13 Interaction vertices: electron–phonon and the contact electron–electron vertex
- 14 Derivation of the quantum Boltzmann equation

Equilibrium Green's functions

- Lecture notes on many-body theory and Green's functions in equilibrium (E. Arrigoni)
<https://itp.tugraz.at/~arrigoni/vorlesungen/korrelations1/public/green.html>
(credentials: see teach center)
- We take for granted the equilibrium contour-ordered formalism, Wick's theorem, and Dyson's equation developed there; this course extends them to the nonequilibrium (Keldysh) case
- See also the literature quoted therein for the equilibrium case

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What equilibrium theory cannot do

- equilibrium many-body theory: linear response around a thermal state $\rho(h) = Z^{-1}e^{-\beta h}$ — conductivity, susceptibilities, spectral functions ...
- but many situations of interest are **not** small perturbations of an equilibrium state:
 - a finite bias voltage driving a steady current through a nanojunction (not $\rightarrow 0$)
 - strong, possibly ultrafast, laser or THz driving (pump-probe spectroscopy)
 - a sudden change (“quench”) of a system parameter, and the ensuing relaxation
 - a system that never reaches equilibrium at all: two leads at different chemical potential or temperature held *so forever*
- common feature: we need $\langle O(t) \rangle = \text{Tr}[\rho(h)O_H(t)]$ for a state (density matrix) $\rho(h)$ whose time evolution is described by a **different** Hamiltonian $H(t) \neq h$

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Examples

- **Quantum transport:** current through a quantum dot, molecule, or nanowire under finite bias – Landauer-type formulas, Coulomb blockade, Kondo physics out of equilibrium
- **Open quantum systems:** a system coupled to one or more baths (leads, phonon reservoirs) that keep driving it away from its own equilibrium
- **Ultrafast / pump–probe experiments:** a strong pulse prepares a far-from-equilibrium state; time-resolved ARPES, transient optical spectra
- **Quantum quenches:** sudden switch of a coupling or potential in an isolated system — thermalization, prethermalization
- **Cold-atom simulators:** essentially isolated, well-controlled many-body systems, ideal testbeds for quench dynamics

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What we need, and what we will build

- a perturbative / diagrammatic framework that does **not** assume the system returns to (or stays near) a known equilibrium state
- $\Rightarrow$ the Keldysh closed-time contour (Sec. 3) replaces the single time axis of equilibrium theory
- $\Rightarrow$ one needs **one more** Green's function than in equilibrium: not just spectral information (G^r, G^a) but also the actual, possibly unknown, **occupation** of the states (G^K , Sec. 5)
- in equilibrium the two are tied together by the fluctuation–dissipation theorem; out of equilibrium they are **independent** – this is the whole added difficulty, and the whole added richness, of the subject
- the good news: essentially all diagrammatic technology (Wick's theorem, Feynman rules, Dyson's equation, self-energies) carries over almost unchanged, once time runs on the contour

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The nonequilibrium problem

- Hamiltonian

$$H(t) = \textcolor{red}{h} + H'(t), \quad h = H_0 + V$$

- H_0 : noninteracting (quadratic), V : interaction
- $H'(t)$: arbitrary perturbation, switched on at t_0 : $H'(t < t_0) = 0$
- for $t < t_0$: equilibrium, $\rho(h) = \frac{1}{Z} e^{-\beta h}$
- want: expectation values for $t > t_0$

$$\langle O(t) \rangle = \text{Tr}[\rho(h) O_H(t)], \quad \frac{dO_H}{dt} = i[H_H, O_H]$$

- **careful**: H depends on time $\Rightarrow O_H(t) \neq e^{iHt} O e^{-iHt}$

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Interaction representation (w.r.t. h)

- unperturbed: h ; perturbation: $H'(t)$

$$O_h(t) = e^{iht} O e^{-iht} \quad (= \text{“interaction picture”} = \text{Heisenberg picture w.r.to } h)$$

- time evolution of states: S -matrix

$$|\psi_h(t)\rangle = S_h(t, t') |\psi_h(t')\rangle, \quad i \partial_t S_h(t, t') = H'_h(t) S_h(t, t')$$

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$$S_h(t, t_0) = T \exp\left(-i \int_{t_0}^t dt_1 H'_h(t_1)\right), \quad S_h(t_0, t) = S_h(t, t_0)^{-1} = S_h(t, t_0)^\dagger$$

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$$O_h(t) = e^{iht} O e^{-iht} \quad (= \text{“interaction picture”} = \text{Heisenberg picture w.r.to } h)$$

- time evolution of states: S -matrix

$$|\psi_h(t)\rangle = S_h(t, t') |\psi_h(t')\rangle, \quad i \partial_t S_h(t, t') = H'_h(t) S_h(t, t')$$

•

$$S_h(t, t_0) = T \exp\left(-i \int_{t_0}^t dt_1 H'_h(t_1)\right), \quad S_h(t_0, t) = S_h(t, t_0)^{-1} = S_h(t, t_0)^\dagger$$

- Heisenberg (w.r.to H) $\leftrightarrow$ interaction picture (they coincide at t_0):

$$O_H(t) = S_h(t_0, t) O_h(t) S_h(t, t_0)$$

Why the equilibrium trick fails

Correlation functions ($T = 0$, $|\Phi_0\rangle$ ground state of h):

$$\langle \Phi_0 | T A(t_1) B(t_2) \cdots | \Phi_0 \rangle$$

insert the S -matrices:

$$= \langle \Phi_0 | S_h(t_0, \infty) T [S_h(\infty, t_0) A_h(t_1) B_h(t_2) \cdots] | \Phi_0 \rangle$$

- **equilibrium:** $t_0 = -\infty$, $H' = e^{-\theta^+ |d| V}$: Gell-Mann-Low $\Rightarrow S_h(\infty, -\infty) |\Phi_0\rangle = e^{i\varphi} |\Phi_0\rangle$ (phase cancels)
- **out of equilibrium:** $H'(t)$ arbitrary $\Rightarrow$ final state $\neq$ phase $\times |\Phi_0\rangle$
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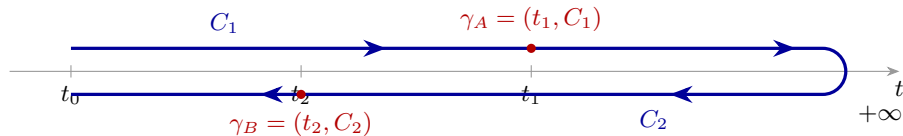
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The Keldysh contour



- contour time = time *and* branch: $\gamma = (t, C)$, $C \in \{C_1, C_2\}$

- ordering along the contour: $\gamma_A >_c \gamma_B$ iff

- $C_A = C_2, C_B = C_1$

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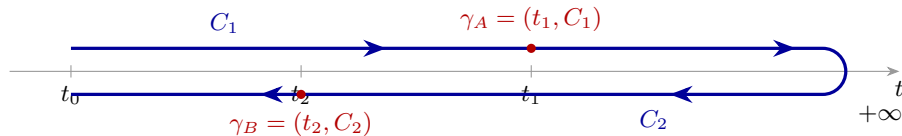
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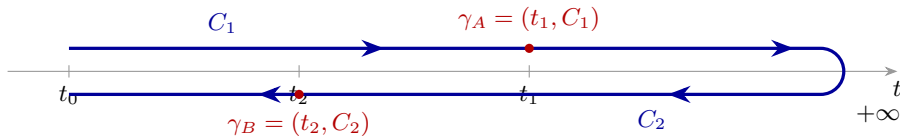
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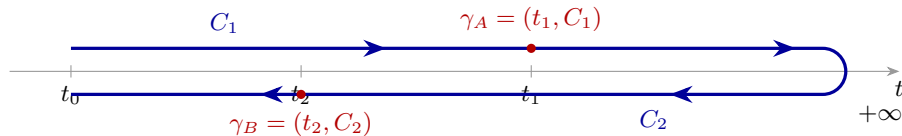
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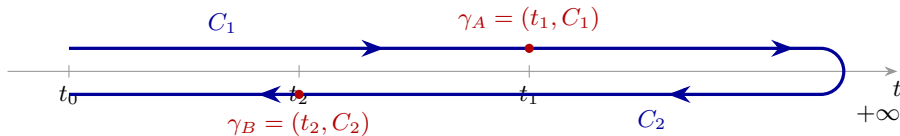
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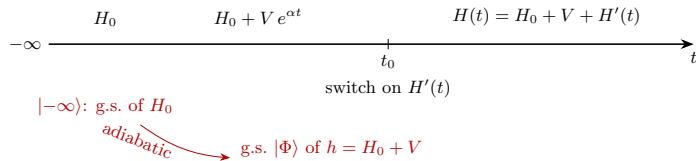
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A quadratic reference: adiabatic switching of V

Wick's theorem needs a **quadratic** unperturbed Hamiltonian — but $h = H_0 + V$ is not.



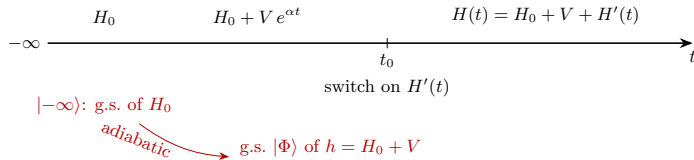
$$H(t) = H_0 + V e^{\alpha t} + H'(t), \quad \alpha \rightarrow 0^+, \quad t_0 \rightarrow -\infty$$

replace everywhere:

$$h \rightarrow H_0, \quad H'(t) \rightarrow W(t) = V e^{\alpha t} + H'(t), \quad |\Phi_0\rangle \rightarrow |\!-\!\infty\rangle \text{ (g.s. of } H_0\text{)}$$

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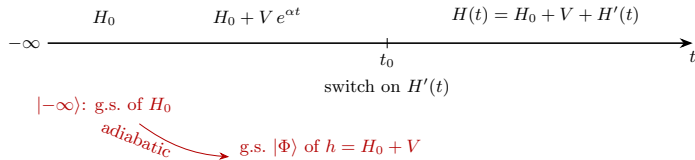
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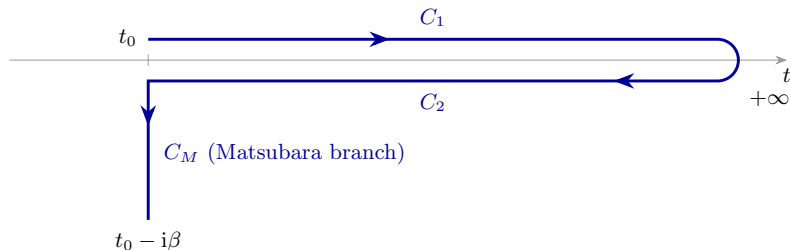
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Outlook: initial correlations

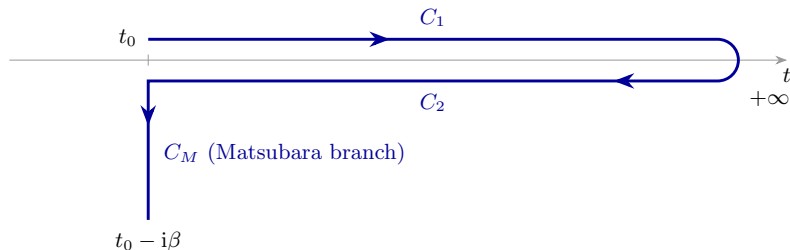
Arbitrary correlated initial state ρ at finite $t_0 \Rightarrow$ additional **imaginary-time branch**:



- negligible for $t_0 \rightarrow -\infty$ at $T = 0$ (adiabatic switching, as above)
- finite- T initial states can also be prepared by coupling to heat baths
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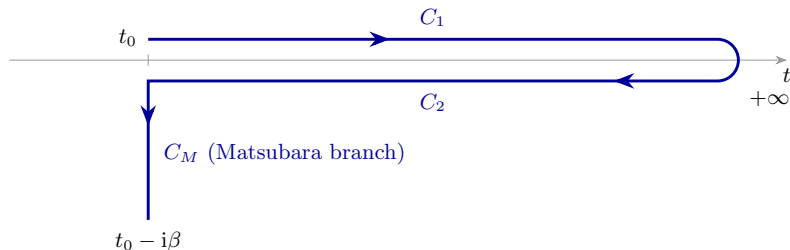
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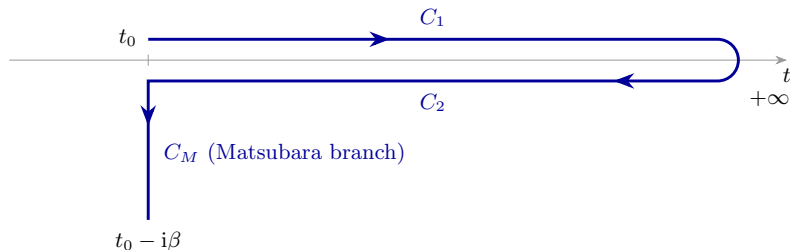
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Everything now refers to the quadratic H_0 : $S \equiv S_{H_0}(-\infty C_2, -\infty C_1) = T_C \exp\left(-i \int_C W_0(\gamma) d\gamma\right)$

$$S = T_C \left(1 - i \int_C W_0(\gamma) d\gamma - \frac{1}{2} \iint_C W_0(\gamma_1) W_0(\gamma_2) d\gamma_1 d\gamma_2 + \dots \right)$$

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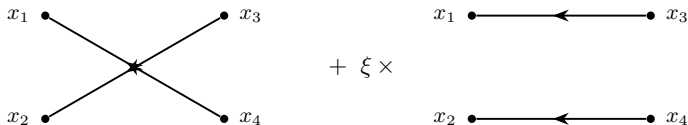
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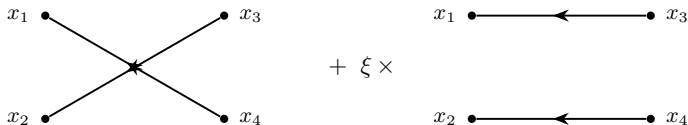


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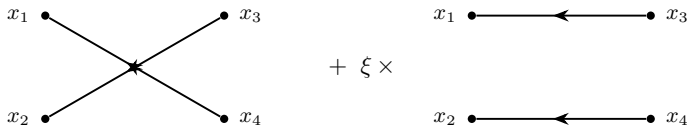


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$$\begin{aligned} & \langle T_C c_0(x_1) c_0(x_2) c_0^\dagger(x_3) c_0^\dagger(x_4) \rangle_0 = \\ & + \xi \langle T_C c_0(x_1) c_0^\dagger(x_4) \rangle_0 \langle T_C c_0(x_2) c_0^\dagger(x_3) \rangle_0 \\ & - \xi \langle T_C c_0(x_1) c_0^\dagger(x_3) \rangle_0 \langle T_C c_0(x_2) c_0^\dagger(x_4) \rangle_0 \end{aligned}$$

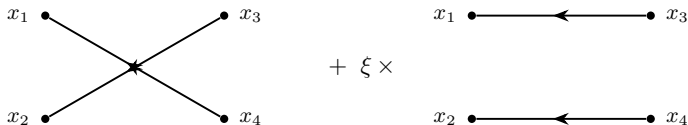


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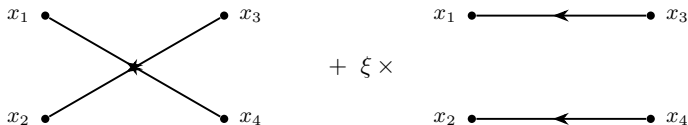


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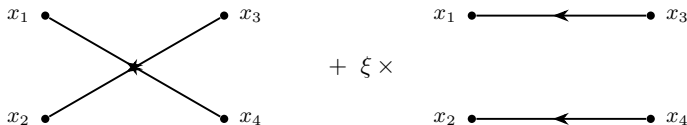


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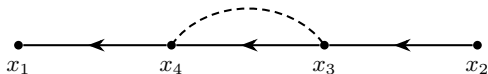


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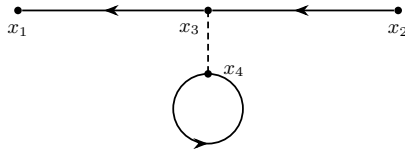
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exchange (Fock) $\equiv F(x_1, x_2)$



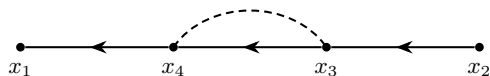
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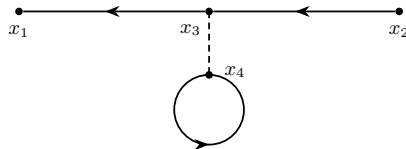
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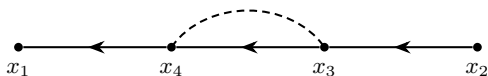
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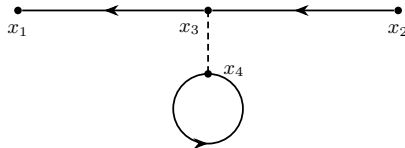
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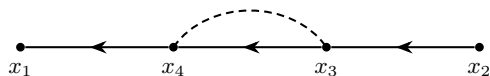
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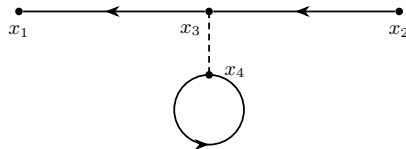
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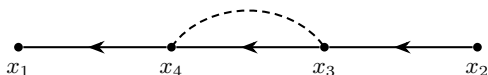
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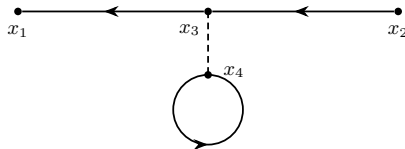
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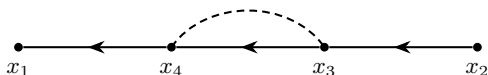
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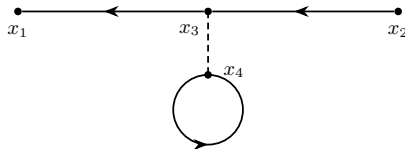
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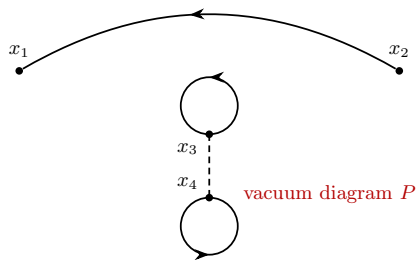
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Disconnected diagrams and the linked-cluster theorem



$$P = \int dx_3 dx_4 \propto G_0(x_1, x_2) \cdot P$$

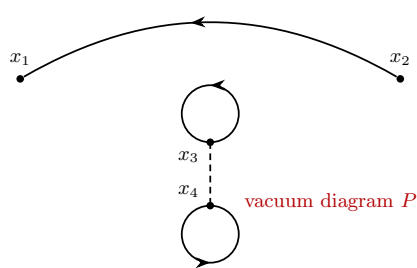
(vacuum diagram)

- disconnected pieces factorize into products of lower-order diagrams and vacuum diagrams
- the denominator $\langle T_C S \rangle_0$ contains *exactly* the vacuum diagrams

Linked-cluster theorem

In $-i \langle T_C S c_0(x_1) c_0^\dagger(x_2) \rangle_0 / \langle T_C S \rangle_0$ the denominator cancels all disconnected contributions: **keep connected diagrams only.**

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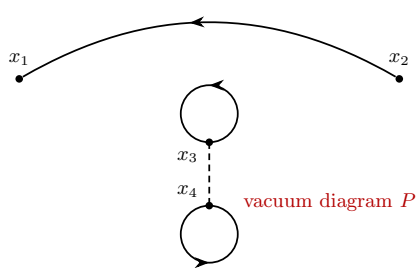
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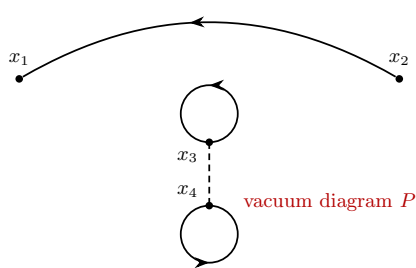
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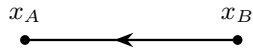
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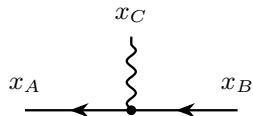
Feynman rules: diagrammatic elements



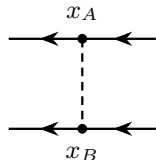
$$= G_0(x_A, x_B) \quad \text{electron propagator}$$



$$= D_0(x_A, x_B) \quad \text{phonon propagator}$$



$$= g(x_A, x_B, x_C) \quad \text{electron-phonon vertex}$$



$$= V(x_A - x_B) \quad \text{electron-electron interaction}$$

x_A x_B

Feynman rules: the recipe (real space and contour time)

Contribution with m interaction vertices to $G(x_A, x_B)$:

- 1 draw all **topologically inequivalent, connected** diagrams starting at x_B and ending at x_A , with m vertices
- 2 assign the values of the elements
- 3 multiply by $(-1)^F$ (F = number of closed fermion loops) and by $i^{m/2}$ (one factor i per interaction line; no factor for a single-particle-potential cross)
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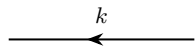
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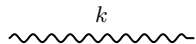
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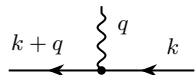
Feynman rules in momentum / frequency space



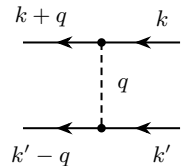
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$$= D_0(k)$$



$$= g(k, q)$$

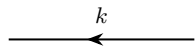


$$= V(q) = V(-q)$$

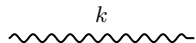
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- mixed representations possible: time+momentum, frequency+position

momentum (and/or frequency) conservation at all vertices

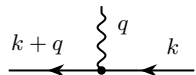
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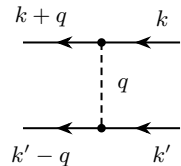
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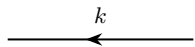


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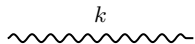
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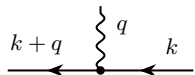
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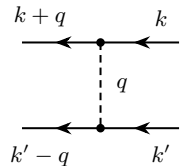
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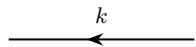


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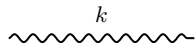
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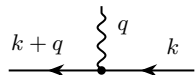
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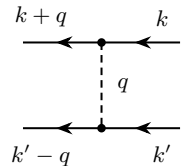
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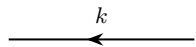


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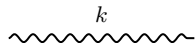
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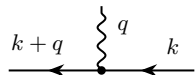
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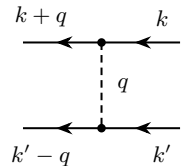
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Self-energy

- classify diagrams for G : **single-particle irreducible** (1PI) = cannot be cut in two by removing one G_0 line
- Σ = sum of all 1PI diagrams with the two external legs amputated:

$$\Sigma = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \text{[diagram 4]} + \dots$$

The equation shows the sum of single-particle irreducible (1PI) diagrams for the self-energy Σ . The diagrams are:

- Diagram 1: A solid line with two external legs (one at the bottom, one at the top) connected by a loop (a circle with an arrow).
- Diagram 2: A solid line with two external legs connected by a dashed arc (a semi-circle).
- Diagram 3: A solid line with two external legs connected by a dashed arc (a semi-circle).
- Diagram 4: A solid line with two external legs connected by two dashed arcs (two semi-circles).

The diagrams are separated by plus signs, and the sequence ends with an ellipsis. A blue 'X' is placed between the second and third diagrams.

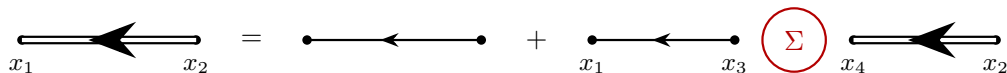
Self-energy

- classify diagrams for G : **single-particle irreducible** (1PI) = cannot be cut in two by removing one G_0 line
- Σ = sum of all 1PI diagrams with the two external legs amputated:

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

The diagram shows the sum of single-particle irreducible (1PI) self-energy diagrams. The first diagram is a self-energy loop (a circle with an arrow) attached to a dashed line. The second diagram is a self-energy loop (a dashed arc) attached to a solid line with an arrow. The third diagram is a crossed-out diagram (a blue 'X'). The fourth diagram is a self-energy loop (a dashed arc) attached to a solid line with an arrow, and a second dashed arc attached to the middle of the solid line. The series continues with an ellipsis.

Dyson's equation



$$G(x_1, x_2) = G_0(x_1, x_2) + \int dx_3 dx_4 G_0(x_1, x_3) \Sigma(x_3, x_4) G(x_4, x_2)$$

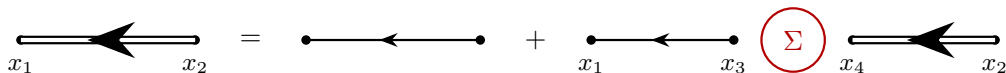
• compact form: $G = G_0 + G_0 * \Sigma * G = G_0 + G * \Sigma * G_0$ (*: convolution + internal sums)

• formally, with $\int A^{-1}(x_1, \bar{x}) A(\bar{x}, x_2) d\bar{x} = \delta(x_1, x_2)$:

$$G^{-1} = G_0^{-1} - \Sigma \quad \Longleftrightarrow \quad G = (G_0^{-1} - \Sigma)^{-1}$$

• in frequency space (steady state) this becomes an algebraic matrix relation — but of course Σ is the hard part

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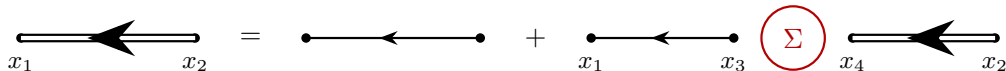
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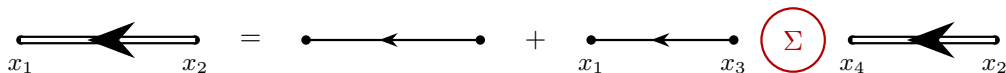
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From the contour to a matrix structure

Replace the double contour by a 2×2 **matrix** structure ($\gamma_A = (t_A, C_A)$, $\gamma_B = (t_B, C_B)$):

$$G(\gamma_A, \gamma_B) \longrightarrow \hat{G}(t_A, t_B) = \begin{pmatrix} G^T(t_A, t_B) & G^<(t_A, t_B) \\ G^>(t_A, t_B) & G^{\bar{T}}(t_A, t_B) \end{pmatrix} \quad (\text{row/column} = \text{branch of 1st/2nd argument})$$

- $G^T(t_A, t_B) = -i \langle T c(t_A) c^\dagger(t_B) \rangle$ (both on C_1 : time-ordered)
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($\xi = +1$ bosons, -1 fermions; the same construction applies to any two-point function)

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Contour convolutions

$$(A * B)(\gamma_A, \gamma_B) = \int_C d\gamma A(\gamma_A, \gamma) B(\gamma, \gamma_B)$$

split into the two branches:

$$= \int_{-\infty}^{+\infty} dt A(t_A C_A, t C_1) B(t C_1, t_B C_B) - \int_{-\infty}^{+\infty} dt A(t_A C_A, t C_2) B(t C_2, t_B C_B)$$

(the **minus**: C_2 runs backward)

In matrix form

$$\hat{C}(t_A, t_B) = \int_{-\infty}^{+\infty} dt \hat{A}(t_A, t) \tau_3 \hat{B}(t, t_B), \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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Keldysh rotation: the RAK representation

- the four functions are **linearly dependent**: $G^T + G^{\bar{T}} = G^> + G^<$
- rotate to eliminate the redundancy *and* the τ_3 :

$$\underline{G} = L \tau_3 \hat{G} L^\dagger, \quad L = \frac{1}{\sqrt{2}} (\tau_0 - i\tau_2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

- result: **upper triangular** (RAK) structure

$$\underline{G} = \begin{pmatrix} G^r & G^K \\ 0 & G^a \end{pmatrix}$$

retarded / advanced / Keldysh

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Algebra of triangular (RAK) matrices

For matrices with RAK structure (entries may themselves be matrices):

$$\underline{B} = \begin{pmatrix} b_r & b_K \\ 0 & b_a \end{pmatrix}, \quad \underline{B} \underline{F} = \begin{pmatrix} b_r f_r & b_r f_K + b_K f_a \\ 0 & b_a f_a \end{pmatrix} \quad (\text{structure preserved!})$$

Inverse ($\underline{F} = \underline{B}^{-1}$ from $\underline{B} \underline{F} = \mathbb{1}$)

$$f_r = b_r^{-1}, \quad f_a = b_a^{-1}$$

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these relations (related to the Langreth rules) will be used over and over

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“Building blocks” of perturbation theory. Diagonal quadratic Hamiltonian:

$$H_0 = \sum_p \varepsilon_p c_p^\dagger c_p$$

- p : complete set of quantum numbers (free particles: momentum, spin; crystal: crystal momentum, band, spin)
- free (interaction-picture) evolution:

$$\frac{dc_p^\dagger}{dt} = i[H_0, c_p^\dagger] = i\varepsilon_p c_p^\dagger \implies c_p^\dagger(t) = e^{i\varepsilon_p t} c_p^\dagger, \quad c_p(t) = e^{-i\varepsilon_p t} c_p$$

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Retarded and advanced components

$$G_0^r(p; t) = -i\theta(t) \langle [c_p(t), c_p^\dagger(0)]_{-\xi} \rangle = -i\theta(t) e^{-i\varepsilon_p t} \underbrace{\langle [c_p, c_p^\dagger]_{-\xi} \rangle}_{=1}$$

- independent of the occupation / distribution!
- Fourier transform (convergence factor $\delta \rightarrow 0^+$):

$$G_0^r(p, \omega) = \frac{1}{\omega - \varepsilon_p + i\delta}$$

$$G_0^a(p, \omega) = \frac{1}{\omega - \varepsilon_p - i\delta} = G_0^r(p, \omega)^*$$

- general quadratic $H_0 = \sum h_{pp'} c_p^\dagger c_{p'}$:

$$\underline{G}_0^r(\omega) = [(\omega + i\delta)\mathbb{1} - h]^{-1}, \quad G_0^a(\omega) = G_0^r(\omega)^\dagger$$

Retarded and advanced components

$$G_0^r(p; t) = -i\theta(t) \langle [c_p(t), c_p^\dagger(0)]_{-\xi} \rangle = -i\theta(t) e^{-i\varepsilon_p t} \underbrace{\langle [c_p, c_p^\dagger]_{-\xi} \rangle}_{=1}$$

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- occupations: $m_p = (e^{\beta(\varepsilon_p - \mu)} - \xi)^{-1}$ (Bose/Fermi), $\bar{m}_p = 1 + \xi m_p$
- Fourier transform: sharp δ -peaks at $\omega = \varepsilon_p$, weighted by the occupations

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$$G_0^K(p; t) = G_0^> + G_0^< = -i e^{-i\varepsilon_p t} (\bar{m}_p + \xi m_p) = -i e^{-i\varepsilon_p t} (1 + 2\xi m_p)$$

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Single-particle (time-dependent) potential

Noninteracting system + one-body perturbation:

$$W_u(t) = \int d\vec{r}_A d\vec{r}_B u(\vec{r}_A, \vec{r}_B, t) c^\dagger(\vec{r}_A) c(\vec{r}_B)$$

on the contour: one vertex with one incoming and one outgoing line (the cross), with

$$u(x_A, x_B) = \delta(\gamma_A, \gamma_B) u(\vec{r}_A, \vec{r}_B, t_A)$$

The contour δ -function

defined by $\int_C d\gamma \delta(\gamma, \gamma_A) f(\gamma) = f(\gamma_A)$:

$$\delta(\gamma, \gamma_A) = \delta_{CC_A}(\tau_3)_{C_A C_A} \delta(t - t_A) \quad (-1 \text{ on } C_2: \text{compensates the backward orientation})$$

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The cross in Keldysh space

branch (hat) representation:

$$\hat{u}(t_A, t_B) = u(\vec{r}_A, \vec{r}_B, t_A) \delta(t_A - t_B) \tau_3$$

RAK representation:

$$\underline{u} = L \tau_3 \hat{u} L^\dagger = u(\vec{r}_A, \vec{r}_B, t_A) \delta(t_A - t_B) L \tau_3 \tau_3 L^\dagger = u \delta(t_A - t_B) \mathbb{1}_{2 \times 2}$$

- the cross is diagonal (proportional to the identity) in RAK space — but only there, not in the hat representation!

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Diagrams with the cross: exact Dyson equation

$$\text{Diagram with double line and arrow} = \text{Diagram with single line and arrow} + \text{Diagram with single line, arrow, cross, arrow, single line} + \text{Diagram with single line, arrow, cross, arrow, cross, arrow, single line} + \dots$$

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$$\Sigma = \text{cross} \quad \text{exact!}$$

- the only 1PI diagram is the single cross: $\Sigma = u$ **exactly** — the perturbative series can be summed
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$$\underline{G} = \underline{G}_0 + \underline{G}_0 * u * \underline{G}$$

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Diagrams with the cross: exact Dyson equation

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

Diagram 1: A double line with an arrow pointing left, ending in a black arrowhead.

Diagram 2: A single line with an arrow pointing left.

Diagram 3: A single line with an arrow pointing left, followed by a blue 'X' (cross), followed by another single line with an arrow pointing left.

Diagram 4: A single line with an arrow pointing left, followed by a blue 'X' (cross), followed by another single line with an arrow pointing left, followed by a blue 'X' (cross), followed by another single line with an arrow pointing left.

$$\text{Diagram 1} = \text{Diagram 2} + \text{Diagram 5}$$

Diagram 5: A single line with an arrow pointing left, followed by a blue 'X' (cross), followed by a double line with an arrow pointing left, ending in a black arrowhead.

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Summary and outlook

- nonequilibrium: same diagrams as equilibrium, times on the **Keldysh contour**
- branch structure $\Rightarrow 2 \times 2$ matrices; RAK rotation $\Rightarrow$ triangular algebra with G^r, G^a, G^K
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The simplest “nonequilibrium” problem

Sudden (diagonal) shift of all levels at t_0 :

$$H_0 = \sum_p \varepsilon_p c_p^\dagger c_p, \quad \hat{V} = \theta(t - t_0) \sum_p v_p c_p^\dagger c_p$$

- assume a steady state at $t - t_0$ large $\Rightarrow$ Fourier transform, RAK Dyson equation with $\underline{\Sigma}_p = v_p \mathbb{1}$:

$$G_p^r = (\omega - \varepsilon_p - v_p + i\delta)^{-1}, \quad G_p^K = (G_p^r - G_p^a) s(\omega), \quad s(\omega) = 1 - 2f(\omega - \mu)$$

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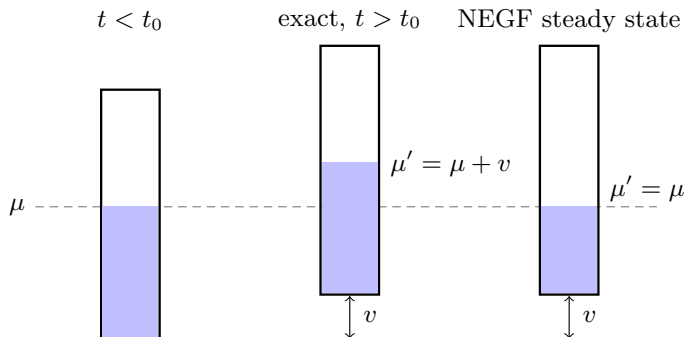
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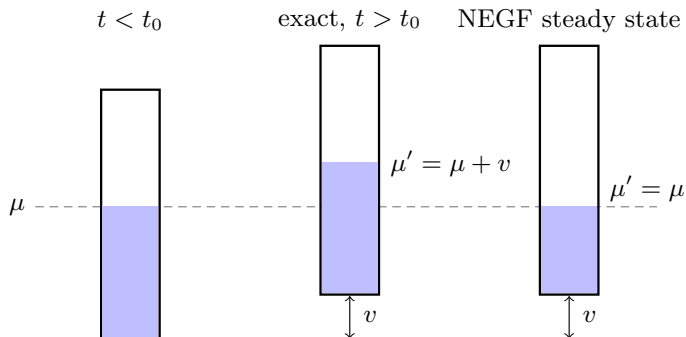
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Resolution: order of limits and (infinitesimal) dissipation

- without dissipation there simply is **no steady state** in a closed system
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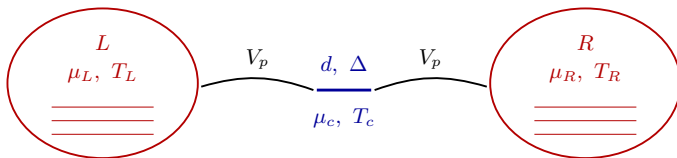
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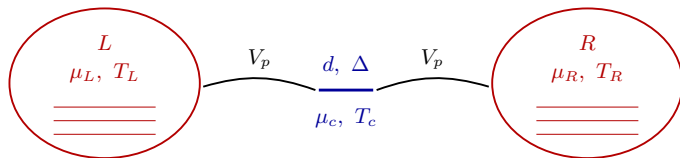
The (noninteracting) resonant level model



$$H_0 = \sum_p \varepsilon_p c_p^\dagger c_p + \Delta d^\dagger d, \quad V = \sum_p V_p (c_p^\dagger d + d^\dagger c_p)$$

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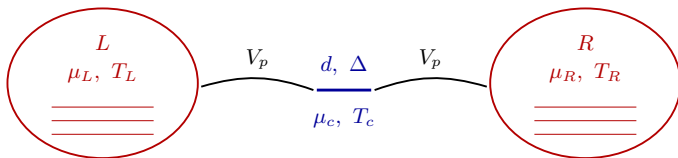
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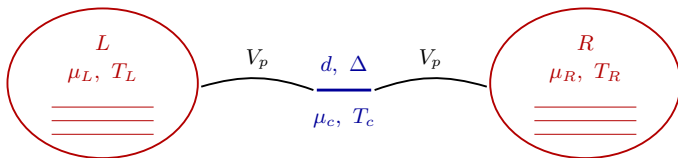
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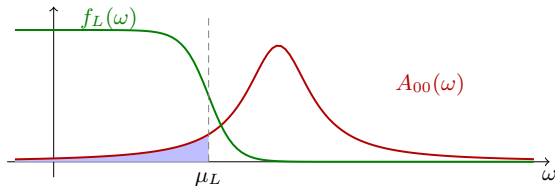
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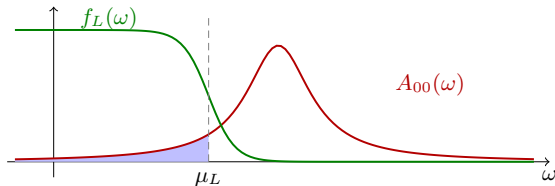


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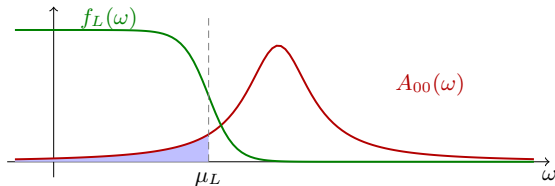


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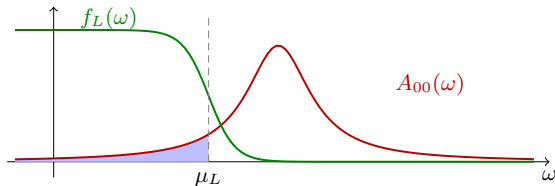


- wide-band limit ($\Gamma_L = \Gamma$, $E = \Delta$ constants), $T = 0$:

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Do we ever get true steady-state nonequilibrium?

- one bath: the central region simply **equilibrates** with it (μ_L, T_L) — an equilibrium problem in disguise
- **yes**: with *two or more infinite reservoirs* at different μ, T a current flows forever
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$$\tilde{\underline{\Sigma}} = \tilde{\underline{\Sigma}}_L + \tilde{\underline{\Sigma}}_R, \quad \tilde{\underline{\Sigma}}_\alpha = \sum_{p \in \alpha} V_{0p} \underline{g}_{pp} V_{p0}$$

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Keldysh component: a distribution that is none

$$G_{00}^K = |G_{00}^r|^2 \sum_{\alpha=L,R} (-2i \Gamma_{\alpha}(\omega) s_{\alpha}(\omega)), \quad s_{\alpha}(\omega) = 1 - 2f(\omega, \mu_{\alpha}, T_{\alpha})$$

can be recast in pseudo-equilibrium form:

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Current through the level

current leaving bath L : $\hat{I}_L = -e \dot{\hat{N}}_L = -ie \sum_{p<0} V_p (c_0^\dagger c_p - c_p^\dagger c_0)$

$$I_L = e \sum_{p<0} V_p \operatorname{Re} G_{0p}^K(t=0) = e \int \frac{d\omega}{2\pi} \sum_{p<0} V_p \operatorname{Re} G_{0p}^K(\omega)$$

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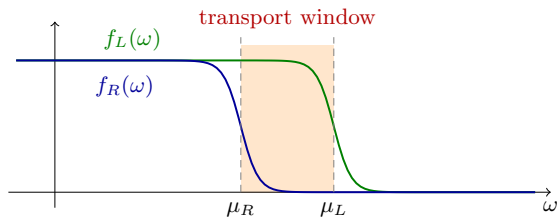
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using $s_L - s_{av} = \frac{\Gamma_R}{\Gamma}(s_L - s_R)$, $s_\alpha = 1 - 2f_\alpha$, $\text{Im } G_{00}^r = -\Gamma |G_{00}^r|^2$:

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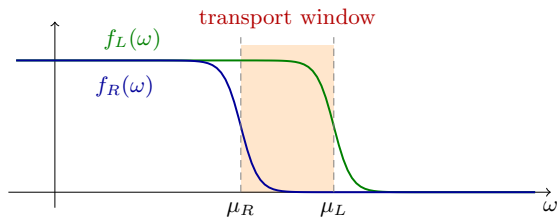
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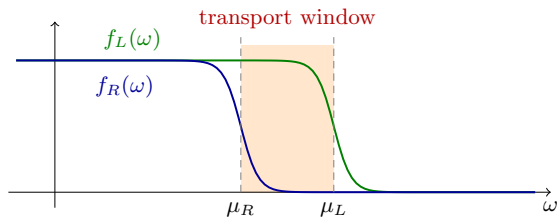
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Interacting dot: single-impurity Anderson model

central region with e-e interaction U (quantum dot), spinful:

$$H_0 = \sum_{p,\sigma} \varepsilon_p c_{p\sigma}^\dagger c_{p\sigma} + \varepsilon_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma}, \quad \varepsilon_d = \Delta - \frac{U}{2},$$

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- diagrams: U attaches only to d ; V_p only connects c with $d \Rightarrow$ distinguish d - and c -lines

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Hubbard-I / cluster-perturbation idea

d - d self-energy $\tilde{\underline{\Sigma}}$ = diagrams that cannot be cut at a d -line:

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Atomic Green's function: two Hubbard poles

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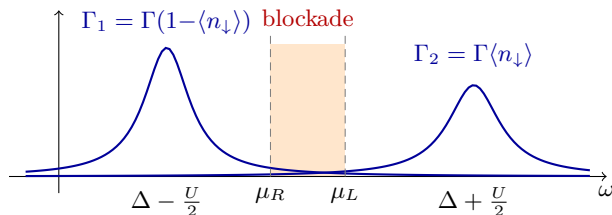
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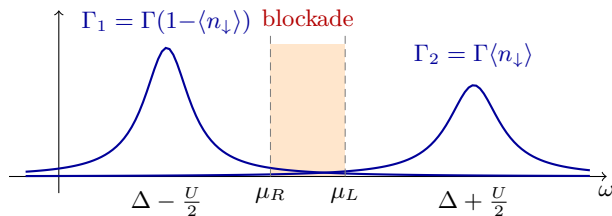


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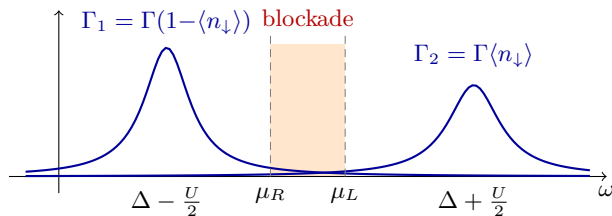


Coupling to the leads: split and broadened peaks

$$\underline{G}_{dd} = \left(\underline{g}_{dd}^{-1} - \tilde{\Sigma}(V=0) - \tilde{\Sigma}(U=0) \right)^{-1} \implies G_{dd}^r = \left(g_{\text{at}}^r(\omega)^{-1} - R(\omega) + i\Gamma(\omega) \right)^{-1}$$

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Current and Coulomb blockade

Keldysh component and current: as in the noninteracting case (the dot contribution to Σ^K is infinitesimal; only the leads enter):

$$G_{dd}^K = (G_{dd}^r - G_{dd}^a) s_{\text{av}}(\omega), \quad I \propto \int_{\mu_R}^{\mu_L} d\omega A_{dd}(\omega) \frac{\rho_L^0 \rho_R^0}{\rho_L^0 + \rho_R^0} \quad (T = 0)$$

- all interaction effects enter through $A_{dd} = -\frac{1}{\pi} \text{Im } G_{dd}^r$
- tunneling regime (Γ small): current flows only when a Hubbard peak $\Delta \mp \frac{U}{2}$ lies inside the transport window — otherwise Coulomb blockade (ϵ_d = gate voltage sweeps the peaks through)
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Beyond the steady state: quantum quench

Central region (N levels, $H = c^\dagger \varepsilon c$, $c = (c_1, \dots, c_N)^T$) suddenly coupled to baths at $t = 0$:
 $V(t) = V \theta(t)$

- no time-translation invariance: work in the **time domain**

$$(A \circ B)(t_1, t_2) = \int dt A(t_1, t) B(t, t_2), \quad I(t_1, t_2) = \delta(t_1 - t_2), \quad A \circ A^{-1} = I$$

- Dyson (left and right), retarded component:

$$G = g + g \circ \tilde{\Sigma} \circ G = g + G \circ \tilde{\Sigma} \circ g, \quad g_r^{-1} \circ G_r = I + \tilde{\Sigma}_r \circ G_r$$

- $\tilde{\Sigma}$ = embedding (hybridization) self-energy of the baths, *no interactions here*

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Unperturbed retarded Green's function

$$g_r(t_1, t_2) = -i \theta(t_1 - t_2) \langle \{c(t_1), c^\dagger(t_2)\} \rangle; \quad \text{equation of motion } (\dot{c} = i[H, c] = -i\varepsilon(t) c):$$

$$\begin{aligned} \partial_{t_1} g_r &= -i \delta(t_1 - t_2) + \theta(t_1 - t_2) \langle \{[H(t_1), c(t_1)], c^\dagger(t_2)\} \rangle \\ &= -i \delta(t_1 - t_2) - i \varepsilon(t_1) g_r(t_1, t_2) \end{aligned}$$

$$\boxed{(i\partial_{t_1} - \varepsilon(t_1)) g_r(t_1, t_2) = \delta(t_1 - t_2)} \quad \Rightarrow \quad g_r^{-1}(t_1, t_2) = (i\partial_{t_1} - \varepsilon(t_1)) \delta(t_1 - t_2)$$

solution (initial condition $g_r(t_1^+, t_1) = -i$):

$$g_r(t_1, t_2) = -i \theta(t_1 - t_2) T \exp\left(-i \int_{t_2}^{t_1} \varepsilon(t) dt\right) \xrightarrow{\varepsilon=\text{const}} -i \theta(t_1 - t_2) e^{-i\varepsilon(t_1 - t_2)}$$

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Retarded G_r after the quench: piecewise

Bath self-energy switched on at 0: $\tilde{\Sigma}(t_1, t_2) = \theta(t_1)\theta(t_2)\tilde{\Sigma}(t_1 - t_2)$

- both $t_1, t_2 \geq 0$: everything time-translation invariant $\Rightarrow$ Fourier/Laplace ($z = \omega + i0^+$)

$$\bar{G}_r(z) = (g_r(z)^{-1} - \tilde{\Sigma}_r(z))^{-1} = (z - \varepsilon - \tilde{\Sigma}_r(z))^{-1}$$

- both $t_1, t_2 \leq 0$: $G_r = g_r$ (bath still off)
- mixed $t_1 > 0 \geq t_2$: integro-differential equation $\Rightarrow$ composition rule

$$G_r(t_1, t_2) = i G_r(t_1, 0) g_r(0, t_2), \quad G_r(t_1, t_3) = i G_r(t_1, t_2) G_r(t_2, t_3) \quad (t_1 \geq t_2 \geq t_3)$$

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Ex. 9.1: time-dependent G_r for a bath with a Lorentzian DOS.

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Ex. 9.1: time-dependent G_r for a bath with a Lorentzian DOS.

Keldysh component: propagating the first time

Keldysh components of the two Dyson equations (neglecting g_k^{-1}):

$$G_r^{-1} \circ G_k = \tilde{\Sigma}_k \circ G_a, \quad G_k \circ G_a^{-1} = G_r \circ \tilde{\Sigma}_k$$

first one at $t_1 > 0$, $t_2 = 0$: the r.h.s. $\int dt_3 \tilde{\Sigma}_k(t_1, t_3) G_a(t_3, 0)$ **vanishes** ($G_a \Rightarrow t_3 < 0$, but then $\tilde{\Sigma}_k = 0$), leaving a homogeneous equation

$$(i\partial_{t_1} - \varepsilon) G_k(t_1, 0) - \int_0^\infty dt_3 \tilde{\Sigma}_r(t_1, t_3) G_k(t_3, 0) = 0$$

$$G_k(t, 0) = i G_r(t, 0) g_k(0, 0) = G_r(t, 0) (1 - 2n_0), \quad g_k(0, 0) = -i(1 - 2n_0)$$

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Keldysh component: propagating the second time

Propagate the second argument via the second Dyson equation (take h.c. and use $G_a^\dagger = G_r$):

$$(i\partial_{t_1} - \varepsilon) G_k^\dagger(t_1, t_2) - \int_0^\infty dt_3 \tilde{\Sigma}_r(t_1, t_3) G_k^\dagger(t_3, t_2) = \underbrace{\int_0^{t_2} dt_3 \tilde{\Sigma}_k^\dagger(t_1, t_3) G_a(t_3, t_2)}_{h(t_1, t_2)}$$

now inhomogeneous ($t_1 > t_2 > 0$: the r.h.s. survives); solving and combining with $G_k(t, 0)$:

$$G_k(t_1, t_2) = -i G_r(t_1, 0) (1 - 2n_0) G_r(t_2, 0)^\dagger + \int_0^{t_2} dt_3 \int_0^{t_1} dt_4 G_r(t_1 - t_4) \tilde{\Sigma}_k(t_4 - t_3) G_r(t_2 - t_3)^\dagger$$

- first term: memory of the initial state; double integral: fed by the baths

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Wide-band limit and the relaxing occupation

$$\text{WBL: } \tilde{\tilde{\Sigma}}_r(z) = -i\Gamma, \quad \Gamma = \sum_{\alpha} \Gamma_{\alpha}; \quad \tilde{\tilde{\Sigma}}_{k\alpha}(\omega) = -2i\Gamma_{\alpha} \text{sign}(\omega - \mu_{\alpha}) \quad (T = 0)$$

$$\bar{G}_r(t) = -i\theta(t)e^{-i\varepsilon t - \Gamma t}, \quad \tilde{\tilde{\Sigma}}_{k\alpha}(t) = -\frac{2\Gamma_{\alpha}}{\pi} \frac{e^{-i\mu_{\alpha} t}}{t}$$

Ex. 9.2, Ex. 9.3: verify these two Fourier transforms.

Time-dependent occupation $(-i(1 - 2n(t)) = G_k(t, t))$

$$G_k(t, t) = \underbrace{-i e^{-2\Gamma t} (1 - 2n_0)}_{\text{initial occupation, decays as } e^{-2\Gamma t}} + e^{-2\Gamma t} \int_0^t dt_3 \int_0^t dt_4 e^{\Gamma(t_3+t_4)} e^{i\varepsilon(t_4-t_3)} \sum_{\alpha} \tilde{\tilde{\Sigma}}_{k\alpha}(t_4 - t_3)$$

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Wide-band limit and the relaxing occupation

$$\text{WBL: } \tilde{\tilde{\Sigma}}_r(z) = -i\Gamma, \quad \Gamma = \sum_{\alpha} \Gamma_{\alpha}; \quad \tilde{\tilde{\Sigma}}_{k\alpha}(\omega) = -2i\Gamma_{\alpha} \text{sign}(\omega - \mu_{\alpha}) \quad (T = 0)$$

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Ex. 9.2, Ex. 9.3: verify these two Fourier transforms.

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Further reading

Foundations Schwinger (1961); Keldysh (1964); Kadanoff & Baym, *Quantum Statistical Mechanics* (1962); Martin & Schwinger (1959).

Reviews / textbooks Rammer & Smith, Rev. Mod. Phys. **58**, 323 (1986); Haug & Jauho, *Quantum Kinetics*... (Springer, 2008); Rammer, *QFT of Non-equilibrium States* (2007); Stefanucci & van Leeuwen, *Nonequilibrium Many-Body Theory* (2013).

Equilibrium diagrammatics Wick (1950); Dyson (1949); Fetter & Walecka (1971); Mahan (2000); Langreth (1976).

Quantum transport Caroli *et al.* (1971); Meir & Wingreen, PRL **68**, 2512 (1992); Jauho, Wingreen & Meir, PRB **50**, 5528 (1994).

Interacting dot / quench Anderson (1961); Hubbard (1963); Meir, Wingreen & Lee (1991); Balzer & Potthoff (2011); Stefanucci & Almbladh (2004); Cini (1980).

(full citations in the lecture-notes bibliography)

Beyond the single-particle potential: genuine vertices

- so far: the cross u – one incoming, one outgoing leg, $\underline{u} \propto \mathbb{1}$ (Sec. 7)
- now: multi-leg **contact** vertices – electron–phonon (g , 3 legs) and, built from it, an effective contact electron–electron vertex (U , 4 legs)
- goal: their representation in Keldysh (branch) and RAK space – needed for diagrammatic corrections beyond Hartree–Fock / Hubbard-I (Sec. 11), and for the collision integral of the Boltzmann equation (Sec. 14)
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The electron-phonon vertex on the contour

$$W_{ep} = \int d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 c^\dagger(\vec{x}_1) c(\vec{x}_2) \rho(\vec{x}_3) g(\vec{x}_1, \vec{x}_2, \vec{x}_3), \quad \rho \in \{b, b^\dagger\}$$

inserting $S_{ep} = \int_C d\gamma \hat{W}_{ep}(\gamma)$ and forcing all three legs to the same contour time (three contour deltas, as for u in Sec. 7):

$$g(x_1, x_2, x_3) = \delta(\gamma_1 - \gamma_3) \delta(\gamma_2 - \gamma_3) g(\vec{x}_1, \vec{x}_2, \vec{x}_3)$$

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Branch representation: all three legs on the same branch

Splitting $\int_C d\gamma = \sum_{\eta} \eta \int dt$ (Sec. 5) and reading off the branch indices of a diagram built with g :

$$\hat{v}_{\eta_1 \eta_2}^{\eta_3} = \eta_1 \delta_{\eta_1 \eta_2} \delta_{\eta_2 \eta_3}$$

- all three branch indices forced equal, $\eta_1 = \eta_2 = \eta_3 \equiv \eta$
- extra factor $\eta = (\tau_3)_{\eta\eta} = \pm 1$ from the measure – exactly the same mechanism as the single τ_3 of the contour delta function, Sec. 7

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RAK representation: a selection rule

Rotating each leg with L (as for $\underline{G} = L\tau_3\hat{G}L^\dagger$) and summing over the shared branch index η explicitly (a finite 2×2 computation, done in the notes):

$$\tilde{v}_{ABC} = \frac{g}{\sqrt{2}} \begin{cases} 1 & \text{an odd number of } A, B, C \text{ equal } 1, \\ 0 & \text{an even number of } A, B, C \text{ equal } 1, \end{cases}$$

with $A, B, C \in \{1, 2\}$ the RAK legs of the two electron lines and the phonon line.

- a **causality/selection rule**: not all combinations of r/a -type ($= 1$) and K -type ($= 2$) legs are allowed at a vertex
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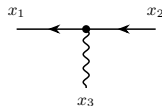
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Contact electron–electron vertex from phonon exchange

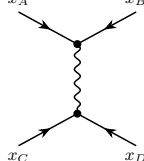
Glue two electron–phonon vertices with a **contact** (frequency independent) phonon line, $\underline{D} = D_0 \mathbb{1}$ (no genuine K component – same structure as $\underline{u}$):

$$U_{B_1 A_2; B'_1 A'_2} = \frac{D_0}{2} \left[\delta_{B_1 A_2} \delta_{B'_1 A'_2} + (1 - \delta_{B_1 A_2})(1 - \delta_{B'_1 A'_2}) \right]$$

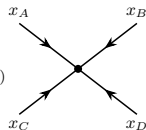
electron–phonon vertex $g(x_1, x_2, x_3)$



contact electron–electron vertex



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($D \rightarrow \text{contact}$)



$U(x_A, x_B, x_C, x_D)$

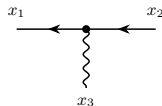
- nonzero only when the two electron pairs are **both** “diagonal” ($B_1=A_2$ and $B'_1=A'_2$) or **both** “off-diagonal”
- the effective, instantaneous (U -type) interaction used in the Hubbard-I treatment of Sec. 11 is a special case of exactly this vertex
- **outlook**: dressing G with this vertex beyond Hartree–Fock/Hubbard-I generates the collision integral of the quantum Boltzmann equation, Sec. 14

Contact electron–electron vertex from phonon exchange

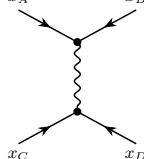
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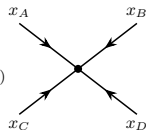
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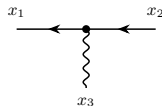
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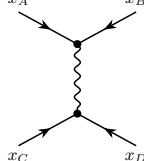
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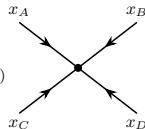
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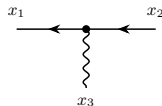
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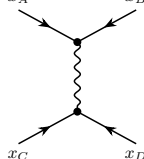
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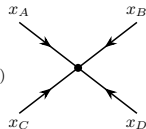
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The classical Boltzmann equation

Distribution function $f(\vec{R}, \vec{p}, t)$: $f d^3R d^3p$ = number of particles in the phase-space volume element at time t

- equilibrium, homogeneous system: $f = f_F(\varepsilon_{\vec{p}})$
- quantum system: $\Delta R, \Delta P$ cannot be infinitesimal, must be coarse-grained, $\Delta R \Delta P \gg \hbar$
- semiclassical equations of motion in a potential $U(\vec{R}, t)$:

$$\dot{\vec{p}} = \vec{F} = -\vec{\nabla}_R U, \quad \dot{\vec{R}} = \vec{v} = \vec{\nabla}_p \varepsilon(\vec{p})$$

- without scattering: $f(\vec{R}, \vec{p}, t) = f(\vec{R} - \vec{v}\Delta t, \vec{p} - \vec{F}\Delta t, t - \Delta t) \Rightarrow$ to linear order,
 $\vec{v} \cdot \vec{\nabla}_R f + \vec{F} \cdot \vec{\nabla}_p f + \partial_t f = 0$
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Strategy: derive it from NEGF

- goal: derive the Boltzmann equation (and its scattering term) from the exact Dyson equation – and see under which conditions, and in which approximation, it holds
- follows Haug and Jauho, *Quantum Kinetics...* (2008) (with minor differences); see also Rammer and Smith (1986)
- route: Dyson equation $\rightarrow$ generalized Kadanoff–Baym equation $\rightarrow$ Wigner transform and gradient expansion $\rightarrow$ quasiparticle approximation $\rightarrow$ Boltzmann equation with an explicit collision integral

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- follows Haug and Jauho, *Quantum Kinetics...* (2008) (with minor differences); see also Rammer and Smith (1986)
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From Dyson's equation to the GKB equation

Split the self-energy into an external potential U and the rest Σ (all products are contour convolutions):

$$G = G_0 + G_0(\Sigma + U)G \implies (G_0^{-1} - U)G = \mathbb{1} + \Sigma G$$

Retarded component: $(G_0^{r-1} - U - \Sigma^r)G^r = \mathbb{1}$. Keldysh component, using $G_0^{K-1} = 0$ (Sec. 6):

$$(G_0^{r-1} - U)G^K + (G_0^{-1} - U)^K G^a = \Sigma^r G^K + \Sigma^K G^a$$

Subtracting the analogous "right" Dyson equation $G = G_0 + G\Sigma G_0$:

$$\boxed{[G_0^{r-1} - U, G^K] = \Sigma^r G^K + \Sigma^K G^a - G^r \Sigma^K - G^K \Sigma^a}$$

the **generalized Kadanoff–Baym (GKB) equation** – exact, not yet restricted to any gradient expansion.

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Wigner coordinates and the Moyal product

Center-of-mass / relative coordinates:

$$X = \frac{1}{2}(x_1 + x_2) = (T, \vec{R}), \quad x = x_1 - x_2 = (t, \vec{r})$$

Fourier transform in the relative coordinate, $P = (\omega, \vec{p})$:

$$C(P, X) = \int d^4x \, e^{iP \cdot x} \, C\left(X + \frac{x}{2}, X - \frac{x}{2}\right)$$

A convolution $C = AB$ becomes, exactly,

$$C(P, X) = A(P, X) \hat{M}(P, X) B(P, X), \quad \hat{M} = \exp\left(\frac{i}{2}(\overleftarrow{\partial}_X \cdot \overrightarrow{\partial}_P - \overleftarrow{\partial}_P \cdot \overrightarrow{\partial}_X)\right)$$

- translation invariant $\Rightarrow \hat{M} \approx 1$: recovers $C(P) = A(P)B(P)$
- **gradient expansion**: fields vary slowly $\Rightarrow$ keep $\hat{M} \approx 1 + \frac{i}{2}(\partial_X \partial_P - \partial_P \partial_X)$

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The transport term

Within the gradient expansion, the GKB commutator acting on a generic $\hat{A}(P, X)$ becomes a first-order differential operator,

$$[G_0^{r-1} - U, \hat{A}] \approx i\hat{\mathcal{L}}\hat{A}, \quad i\hat{\mathcal{L}} = i\left(\partial_T + \vec{v} \cdot \vec{\nabla}_R + \vec{F} \cdot \vec{\nabla}_p + (\partial_T U) \partial_\omega\right)$$

with $\vec{v} = \vec{\nabla}_p \varepsilon(\vec{p})$, $\vec{F} = -\vec{\nabla}_R U$.

- quasiparticle approximation: neglect Σ in $G^{r,a} \Rightarrow A(\vec{p}, X) = \delta(\omega - \varepsilon(\vec{p}) - U)$
- write $G^K = (G^r - G^a)S(\vec{p}, X)$, $S = 1 - 2f$ (fermions) – generalizes the equilibrium fluctuation–dissipation relation of Sec. 6
- $\hat{\mathcal{L}}$ annihilates any function of $G_0^{r-1} - U$ alone (in particular A): $\hat{\mathcal{L}}A = 0$

Applying $\hat{\mathcal{L}}$ to the lhs of the GKB equation with $\Sigma = 0$, integrating over ω , and using $\hat{\mathcal{L}}A = 0$:

$$\left(\partial_T + \vec{v} \cdot \vec{\nabla}_R + \vec{F} \cdot \vec{\nabla}_p\right)f(\vec{p}, X) = \left(\frac{\partial f}{\partial t}\right)_S$$

reproducing the streaming (lhs) side of the Boltzmann equation exactly.

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The collision term: general structure

Split $\Sigma^{r,a} = \Sigma \pm \Sigma_-$ (Hermitian/anti-Hermitian parts, $\Sigma = \text{Re } \Sigma^r$) and define the scattering rate $\Gamma \equiv -\pi^{-1} \text{Im } \Sigma^r$ (so $\Sigma^r - \Sigma^a = -2i\pi\Gamma$). Inserting into the GKB equation, keeping the lowest order in Σ and in gradients, and integrating over ω :

$$\hat{\mathcal{L}}f(\vec{p}, X) = 2\pi \left(A(\vec{p}, X) \Sigma^K(\vec{p}, X) - \Gamma(\vec{p}, X) G^K(\vec{p}, X) \right)$$

- this is $(\partial f / \partial t)_S$: the collision term is fully determined once Σ^K, Σ^r (hence Γ) are known
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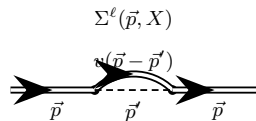
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Application: elastic scattering from impurities

Diluted random impurities, concentration c , potential $V(\vec{R}) = \sum_m v(\vec{R} - \vec{y}_m)$; impurity average (linked-cluster argument: only fully connected impurity lines survive):

$$\overline{V(\vec{q}_1)V(\vec{q}_2)} = c v(\vec{q}_1)v(\vec{q}_2) \delta_D(\vec{q}_1 + \vec{q}_2) + \dots$$

Self-consistent Born approximation (SCBA) for the self-energy:

$$\Sigma^\ell(\vec{p}, X) = c \int d_3p' |v(\vec{p} - \vec{p}')|^2 G^\ell(\vec{p}', X)$$


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Inserting into the collision term above gives the familiar **Fermi's-golden-rule** collision integral:

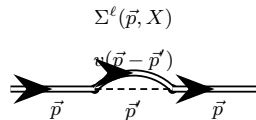
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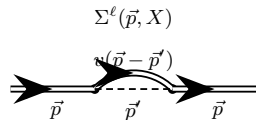
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Validity of the gradient expansion

- impurity-averaged quantities are coarse-grained on a volume ΔV containing many impurities: $\Delta V \gg d^3 \gg k_F^{-3}$ (d = mean interimpurity distance)
- consistency of the gradient expansion in $\overline{v^2}$ and G (wavelength λ of the impurity potential):

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Relaxation-time approximation

Linearize around local equilibrium, $f = f_F(\varepsilon(\vec{p})) + f_1(\vec{p}, X)$, and take the anisotropic part sourced by a uniform force $\vec{F}$: $f_1(\vec{p}, X) \simeq \hat{\vec{p}} \cdot \hat{\vec{F}} \alpha(p_F)$. Evaluating the impurity collision integral on the Fermi surface (spherical average over the angle between $\hat{p}$ and $\hat{p}'$):

$$\left(\frac{\partial f}{\partial t} \right)_S = - \frac{f(\vec{p}, X) - f_F(\varepsilon(\vec{p}))}{\tau_1}, \quad \frac{1}{\tau_1} = \pi c N(\varepsilon_F) \int d(\cos \theta') |v(\cos \theta')|^2 (1 - \cos \theta')$$

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