1 Nonequilibrium Green's functions (Martin and Schwinger '59, Schwinger '61, Konstantinov and Perel '60, Dzyaloshinski (62), <u>Kadanoff-Baym '62</u>, Keldysh '64, ...) Freely taken mainly from Rammer and Smith (1986) and Haug and Jauho (1998) = h + H'(t)h= Hot V noninteracting  $H'(t < t_0) = O$ FOR  $r_{i} < t_{0}$  system is at equilibrium with density matrix C(h)= == ph Expectation values of operators for any t  $T_{\mu}(\mathcal{C}(h) \mathcal{O}_{\mu}(k))$ Heisenber repr. evolved according to H

## Interaction representation

When introducing the interaction representation one should specify with respect to which "perturbation". Now we take as the unperturbed hamiltonian and  $\mathcal{H}'(\mathcal{E})$  as the perturbation  $Q_{I}(t) = e^{iht} O e^{-iht}$ so it is the same as a Heisenberg representation with Hamiltonian 🆌 we therefore denote it as (h) (t) instead of  $O_{t}(t)$ the reason is that later we will consider  $\mathcal{H}_{o}$  as the unperturbed Ham. Similarly we denote the S - matrix as  $S_{l}(t,t')$ Since for  $t \leq t_0$   $O_H(t) = O_h(t)$  $Q_{\mu}(t) = S_{\mu}^{\dagger}(t, t_{o}) Q_{\mu}(t) S_{\mu}(t_{o})$  $S_h(t,t_o) = T exp\left(-i \int dt' H'_h(t')\right)$ to (we can as well consider  $t_{nz} - \infty$  ) NTIL HERE 23.3

3 We need expressions of the form (for simplicity we take zero temperature, and thus we have the ground state of h  $| \oint_{O} 
angle$  , later we can take  $\left( \frac{1}{2} - c \right) = \left( \frac{1}{2} \right) \left( \frac{1}{2} - c \right)$  $\langle \phi \rangle T A(t_1) B(t_2) - - - | \phi \rangle$ By proceeding as for the equilibrium case we get:  $(+\infty | T S_{h}(+\infty, t_{o}) A_{h}(t_{1}) B_{h}(t_{2}) \cdots | F_{o})$ (+ 0) 7 PHASE ( \$ ) The crucial point is that now The reason is that H' is not necessarily switched on adiabatically, neither it is switched off We thus need to "go back" to  $\mathcal{L}_{\mathcal{O}}$  $\Phi_0 | S_R(t_0, +\infty) T S_R(+\infty, t_0) A_R(t_1) B_R(t_2) - - (\Phi)$ I cannot move the time ordering! Notice, instead of CO, we could already "turn back" at max(t1,t2,..)

Trick: introduce contour C along the time axis "Keldysh" contour  $t_1$ to TIME now each operator must specify BOTH its time AND on which side of the contour it lays :  $C_1 \circ R_2$  $B = (t_B, C_B) \quad ETC.$  $T_A = (E_A, C_A)$ with an obvious definition of the ordering  $C_A = C_Z / C_B = C_1$ TAZ TB IF EITHER CA=(B=C1, EA)EB CAEGEC, EAKEB  $-\mathcal{A}(\gamma_{A})\mathcal{B}(\gamma_{B}) (\gamma_{A},\gamma_{C})$  $-\mathcal{E}\mathcal{B}(\gamma_{B})\mathcal{A}(\gamma_{A}) (\gamma_{B},\gamma_{A})$ Introduce contour ordering operator  $(\gamma_A) \mathcal{B}(\gamma_B)$ 

 $\langle \overline{\Phi}_{0} | S_{R}(t_{0,+}) T S_{h}(t_{0},t_{0}) A_{h}(t_{1}) B_{h}(t_{2}) \cdots \langle \overline{\Phi}_{0} \rangle$  $= \langle \overline{\varphi}_{0} | \overline{f}_{c} S_{h}(t_{0}(z_{1} + \infty) S_{h}(t_{0}, t_{0}(z_{1})) A_{h}(t_{1}(z_{1})) B_{h}(t_{2}(z_{1})) \cdots | \overline{\varphi} \rangle$ notice that  $+ \infty$  is the turning point, so we do not need to specify on which part of the contour it is.  $\langle \overline{\mathcal{F}}_{0} | \overline{\mathcal{T}}_{c} S_{h}(t_{0}C_{2}, t_{0}C_{1}) A_{h}(t_{1}C_{1}) B_{h}(t_{2}C_{1}) \cdots | \overline{\mathcal{F}}_{0} \rangle$ of course the operators A, B need not to be restricted to C1 so we can generalize the expression for a generic Green's function (which in the end we will need for perturbation theory)  $\left\langle f_{0} \right\rangle T_{C} A(\gamma_{1}) B(\gamma_{2}) - - - \left\langle f_{0} \right\rangle =$ =  $\langle \Phi_0 | T_c S_h(t_0(z, t_0(1)) A_h(T_1) B_h(T_2) - | t_0 \rangle$ where  $S_R(t_0C_2,t_0C_1) = T_C l^{-i} H_R'(\gamma) d\gamma$ 

We still cannot apply Wick's theorem, because his not quadratic. What to do ? For zero temperature T=0 we only have the ground state we can again think of switching on adiabatically the interaction)at  $E = -\infty$ V/(E)Thus we can write (E) +& O(t-to dt  $\left( \mathcal{L} \rightarrow \mathcal{Q} \right)$  adiabatic to = - a we can now take Ho  $\rightarrow H'(t) + V(t) = VV(t)$ and apply formally the same results as above. The difference is now that the Interaction representation evolution and the initial state refer to a noninteracting (quadratic) hamiltonian and thus Wick's theorem applies ! Notice, by adiabatically switching on V , I guarantee that at the time in which I switch on H' (nonadiabatically) my state has evolved to the ground state of

7 FURTHER OPTIONS/155VES WHICH WE ARE NOT GOING TO TREAT FOR THE TOMENT START AT E= to WITH AN ARBITRARY PRÉPARED STATE DÉFINED BY A CORRELATED PENSITY MATRIX =) PATH ALONG IMAGINARY TIME JO TREAT INITIAL CORRELATIONS 1(1ko TIME to-iB C 0 → → → ∞ and T=0 It can be neglected when Besides, also an initial state with finite T at some t\_0 can be produced with the help of a heat bath

8 Perturbation expansion The nice point is that now perturbation expansion in  $\mathcal{M}(\mathcal{E}) \neq \mathcal{M}(\mathcal{E})$ works very similarly to ordinary perturbation theory Diagrammatic rules are the same except that now all time integrals have to be carried out on the Keldysh contour C1+C2 Again the central object is the S Matrix elp(-r) W<sub>Ho</sub>(E  $-\infty(j)$ : | interaction repr w.r. H\_0. Again one expands the exponential example:  $-\frac{1}{2}T_{c}$   $\partial\gamma_{1}\partial\gamma_{2}$  $\mu_0(\gamma_2)$ 

We need an expansion for objects of the form  $\sum_{c} A(t_1) B(t_2) - - - |$  $\langle -\infty | \overline{t} S | - \infty \rangle$ The denominator is actually not necessary, because it is 1 However, one should use it for the linked-cluster theorem. i.e. to cancel disconnected diagrams in the numerator Each term of the expansion will contain expectation values in the noninteracting ground state  $\left| - \infty \right\rangle$  of Tc ordered products of single-particle operators (i.e. creation and annihilation operators) time evolved according to H, Wick's theorem tells us that this can be decomposed into expectation values of time ordered pairs of products, i. e. Green's functions  $(N_{\nu}, other quantum numbers such as position, spin, orbital, etc.$ 



Example evaluation of a Green's function  $(X_1, X_2) = -\lambda \quad \langle T_c \quad (X_1) \quad (X_1, X_2) = -\lambda \quad \langle T_c \quad (X_1) \quad (X_1) \quad (X_1) \quad (X_2) \quad (X_2) \quad (X_1) \quad (X_2) \quad (X_2) \quad (X_1) \quad (X_2) \quad (X_2) \quad (X_2) \quad (X_2) \quad (X_1) \quad (X_2) \quad$  $(\lambda_2)$  $\int \left( \left( X_1 \right) \left( \left( X_2 \right) \right) \right)$ Consider first numerator  $\times_1, \times_2$  External points  $\frac{\zeta^{(0)}}{\zeta^{-}}$ 0th order  $G_{0}(X_{1}, X_{2}) = -\lambda \left( T_{C} C_{0}(X_{1}) C_{0}^{\dagger}(X_{2}) \right)$ 

1st order (example, e. e. interaction)

 $\int_{0}^{(1)} \alpha - \frac{i}{2} \int_{0}^{+} \left( \chi_{3} \right) \left( \frac{i}{2} \left( \chi_{4} \right) \left( \chi_{4} \right) \left( \chi_{3} \right) \left( \chi_{3} - \chi_{4} \right) d\chi_{3} d\chi_{4} d\chi_{4}$ X3, X4 ARE DIFFERENT BUT HAVE THE SAME TIME) Represented by vertex  $X_3$ Wick's theorem: ) "all lines have to be paired in all possible ways" 12  $\int dX_3 \, dX_4 \, G_0(X_1, X_3) \, G_0(X_3, X_2) \, G_0(X_4, X_4) \, \mathcal{N}(X_3 \cdot X_4)$ 

13 All internal variables  $X_{3_1} X_4$  are integrated or summed over times are integrated over contour  $\chi_{1,\chi_2}$  being external variables are fixed 12  $\times_1$ topologically equivalent to the former, just cancels factor 1/2  $\times$  $\times_1$ + a topolgically equivalent one  $\int dX_3 dX_4 G_0(X_1, X_4) G_0(X_4, X_3) G_0(X_3, X_2) N(X_3 - X_4)$ X 



15	
Exa dis	mple of second order connected diagram
$\sim$	$F(X_1, X_2)$
Can	be written as a product of lower-order diagrams !
	Denominator $\overline{CS}_{0}$ only has vacuum diagrams such as
	Linked cluster theorem
	When evaluating numerator / denominator $ \frac{-\lambda \langle I_C \rangle (\lambda^{1}) \langle \lambda^{2} \rangle}{\langle I_C \rangle \rangle} = \frac{-\lambda \langle I_C \rangle (\lambda^{1}) \langle \lambda^{2} \rangle}{\langle I_C \rangle \rangle} $
r D	The effect of the denominator is simply to cancel out all disconnected diagram contributions !
I	In the end one can restrict in evaluating CONNECTED diagrams

16 FEYNMAN DIAGRAMS RULES DIAGRAMMATIC ELEMENTS  $X_{B} = G_{O}(X_{A}, X_{B})$  ELECTRON G.F.  $\mathcal{N}_{B} = \mathcal{D}_{O}(X_{A}, X_{B})$  PHONON Xa G.F.  $X_{A} = Y(X_{A}, X_{B}, X_{C}) = ELECTR. - PHONON$ IN TERACTION INTERACTION XA-ELECTRON-ELECTRON  $= \mathcal{N}\left(X_{A} - X_{B}\right)$ INTERACTION  $= \mathcal{M}\left(X_{A_{j}}X_{B}\right)$ SINGLE-PARTICLE POTENTIAL

QIAGRAMMATIC RULES (SEE E.G. (REAL SPACE AND TIME) (SEE E.G. MAHAN, 17 FOR EXAMPLE FOR GREEN'S FUNCTION  $G(X_A, X_B) = -i \langle T_C C(X_A) C^{\dagger}(X_B) \rangle$ Contibution at a certain order  $1) \qquad \begin{array}{c} X_{\mathcal{A}} \\ \downarrow \end{array} \\ \downarrow \end{array} \qquad \begin{array}{c} X_{\mathcal{B}} \\ \downarrow \end{array} \\ \downarrow \end{array}$ PRAK ALL TOPOLOGICALLY NEQUIVALENT CONNECTED (LINKED (LUSTER!) DIAGRAMS STARTING AT XB AND ENDING AT XA with m vertices 2) ASSIGN THEIR VALUES ACCORDING TO ELEMENTE )  $\mathcal{M}\mathcal{VLTIPLY}$   $\mathcal{B}\mathcal{Y}$   $(-1)^F$   $\mathcal{F} = \mathcal{N}$ .  $\mathcal{OF} = \mathcal{FERMON} \mathcal{K}$  LOOPS  $\mathcal{B}\mathcal{Y}$   $(\mathcal{N})$   $\mathcal{M}_{\mathcal{I}}$  m = number of vertices3) SUM PR INTEGRATE OVER ALL INTERNAL VARIABLES TIME HAS TO BE IN TEGRATED OVER KELDYSH CONTOUR

BOMMOMENTUM SPACE MAY BÉ MORE CONVENIENT IN CASE OF TRANSLATION INVARIANCE FREQUENCY SPACE FOR TIME INDEPENDENCE (EQUILIBRIUM OR STEADY STATE)  $\frac{K_{A}}{M} = G_{o}(K_{A})$  $\sim \sim \sim = D_o(K_A)$ 39 KAVKEP = J(K, J) MONENTUM CONSERVATION  $\frac{1}{1} = N(9)$   $\frac{1}{1} = N(9)$   $\frac{1}{1} = 1$   $\frac{1}{1} = 1$ +X IN GENERAL NOT MOMENTUM CONSERVING SOMETIMES MIXED REPRESENTATION TIME + MOMENTUM OR FREQUENCY + POSITION

19 DYSON EQUATION  $(X_1, X_2)$  $\langle \neg$ \_\_\_\_ SINGLE-PARTICLE REPUGIBLE DIAGRAMS -<del>X-X--</del>  $\mathbf{N}$ +Define self-energy  $\geq$  = sum of single-particle irreducible diagrams i. e. diagrams that cannot be taken apart by cutting a single line + my Ĵ A

20  $G(X_1, X_2) \equiv X_1 \equiv$  $=X_{2}$ - - L ^ ٤ (2)-7\_  $X_{\chi}$ + +  $\times_1$   $\times_2$  $\frac{1}{\chi}$ - $= G_0(X_1, X_2) +$  $X_{1/}$  $[X_3, X_4]$  $X_{\mu} \quad G_{o} \left( X_{1}, X_{3} \right)$  $\mathcal{S}$ q TEGRAL EQUATION FOR Also "left" Dyson's equation 4 Go+6\*5 \*60 Ť convolution, sum over internal indices

21 IN FREQUENCY SPACE (EQUILIBRIUM) BECOMES EASY 5(w) = 6o(w) + 6o(w) = 6(w)CANBESEEN AS A MATRIX EXPRÉSSION IN OTHER INTERNAL NDIGES, POSITION/MORENTUM, SPIN, BAND, ETC. (EVEN IN TIME)  $G = \left(G^{-1} - \overline{Z}\right)^{-1}$ BUT, OF COURSE, Z IS PIFFICULT

22 KELDYSH SPACE IT IS CONVENIENT TO REPLACE THE DOUBLE REPLACE (SUTILARLY FOR OTHER TWO-POINT FUNCTIONS)  $G(\gamma_A,\gamma_B) = G(t_ACA,t_BCB)$  with  $G(t_A, t_B) G(t_A, t_B)$  $G(t_A, t_B) = G(t_A, t_B) = G(t_A, t_B) = G(t_A, t_B)$ (A22)  $G^{C}(t_{A}, t_{B}) \equiv -i \langle T C(t_{A}) (t_{B}) \rangle$  $G^{\overline{c}}(t_{A},t_{B}) = -i\langle \overline{T}(t_{A})(t_{B})\rangle$  $(f_A, f_B) = -i \int (f_A) (f_A)$  "Lesser" GF  $\begin{pmatrix} M = 1 & FERHIONS \\ T = +1 & BOSONS \end{pmatrix}$  $(f(t_A, t_B) = \Lambda (C(t_A)C(t_B))$  "Greater" GF

CONVOLUTIONS OVER INTERNAL TIMES BECAME  $\begin{array}{c}
\left(\left(\begin{array}{c}
\gamma \\ A, \end{array}\right) = \left(\begin{array}{c}
A\left(\begin{array}{c}
\gamma \\ A, \end{array}\right) B\left(\begin{array}{c}
\gamma \\ B\end{array}\right) d\gamma = \\
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+  $= \int_{A}^{+\infty} (t_A(A, t_2) B(t_2, t_B(B)) dt$ FOR THE CORRÉSPONDING MATRICES THIS GIVES:  $\begin{array}{c}
 & t \otimes & & & \\
 & f \otimes & & & \\
 & f \otimes & & \\
 & f \otimes$ PAULI MATRIX

24 THE 4 GREEN'S FUNCTIONS ARE LINEARLY DEPENDENT G'+G'=G'+G'SQ ONLY THREE ARE LINEARLY INDEPENDENT THERE ARE SEVERAL CONVENTIONS, WE USE THE MATRIX  $G = L C_3 G L$  (A24) WHERE  $L = \frac{1}{\sqrt{2}} \left( \frac{\gamma_0 - i \gamma_2}{\sqrt{2}} \right) = \frac{1}{\sqrt{2}} \left( \frac{1 - 1}{1} \right)$ N = PAULI MATRICES Yo > I ~r ? (A242)

WHERE WE HAVE USED THE RELATIONS  $G^{T} = G = G^{T} = G^{T} = G^{T}$  $G^{a} = G^{c} - G^{c} = G^{c} - G^{c}$  $G^{K} = G^{2} + G^{2} = G^{2} + G^{2}$ (A25) Consider now the convolution  $\frac{1}{(t_A, t_B)} = \left( dt A(t_A, t), \gamma_3, B(t, t_B) \right)$ multiply by  $L\gamma_3 - - - - 1$ for example: LY3 CL= C

26 we obtain 1) +00  $\frac{1}{2}$ + Q ß (A26) + 00  $(t, t_B)$  (A261) (EA dt A E)  $\sim \infty$ 1/3 any more ! no

Noninteracting Green's functions "building blocks" of perturbation theory Z Ep Cp Cp can in general be a quantum number labeling an eigenstate of the single-particle Hamiltonian For free particles p=(momentum, spin) for electrons in a crystal:(crystal momentum, band, spin) etc. Evolution according to  $H_{0}$  (interaction representation) - x Ep t

 $G_0^n(\mathbf{r}, \mathbf{t}) = -i \Theta(\mathbf{t}) \langle [C_p(\mathbf{t}), C_p^{(0)}] \rangle$  $= -\overline{\lambda} \Theta(k) l \left( \left( e, \left( p \right) \right) \right)$  $z - \overline{\lambda} \Theta(t) e^{-\overline{\lambda} \xi \rho t}$ Fourier transformation  $G_{0}^{\pi}(P,W) = -\dot{n} \int elt l \qquad (W - Ep + \dot{n}S) t$   $G_{0}(F,W) = -\dot{n} \int elt l \qquad (W - Ep + \dot{n}S) t$ convergence factor  $\delta z$  positive infinitesimal  $W - Ep + \lambda S$ (A1) Similarly  $G_{\alpha}(P,t) = i \Theta(-t) - i e^{-i e t} G_{\alpha}(P,-t)^{*}$  $G_{0}^{\alpha}(P,W) = \frac{1}{W - \epsilon_{P} - i\delta} = G_{0}^{\alpha}(P,W)^{*}$ (A2)

Greater and lesser Green's functions

 $G_{a}^{\prime}(Pt_{A}, P't_{B}) = S_{PP'}G_{a}^{\prime}(P, t_{A} - t_{B})$  $= -i \left( C_{p}(t_{A}) \left( f_{p}(t_{B}) \right) \right)$  $= -\frac{i}{2} \frac{E_P(t_A - t_B)}{\langle C_P C_P \rangle}$  $= -i \ell \frac{\xi_p(t_A - t_B)}{M_p}$  $M_P = 1 + M_P$ distribution function  $M_{P} \ge \begin{pmatrix} \mathcal{B}(\mathcal{E}_{P} - \mathcal{M}) \\ \mathcal{C} & -\mathcal{M} \end{pmatrix}^{-1}$ Fourier transform  $G_{o}(P,W) = \int dt e^{iwt} G_{o}(P,t)$  $-2\pi\lambda\delta(W-E_{P})\tilde{M}_{P}$  (A3)

30  $G'(P,t) = i q \left( C_{p}^{\dagger}(0) C_{p}(t) \right)$ like  $\int$  with  $M_p - M_p$  $= -\pi \ell M M p$  $G_{o}(P,W) = -Z\pi i S(W-E_{P})MM_{P}$ (A4) Keldysh Green's function  $G_{o}(P,t) = G_{P}(t) + G_{P}(t)$  $= -i \ell^{-i} \ell^{-i} \left( \frac{m_{p}}{m_{p}} + \frac{m_{p}}{m_{p}} \right)$  $= -i \ell \left( 1 + 2\eta M_P \right)$  $G_{0}^{K}\left(\mathcal{P},\mathcal{W}\right) = -2\pi i S\left(\mathcal{W}-\mathcal{E}_{\mathcal{P}}\right)\left(1+2\eta \mathcal{M}_{\mathcal{P}}\right) (A5)$ For the case, as here, in which  $\mathcal{M}_{\rho}$  is a function  $\mathcal{M}(\mathcal{E}_{\rho})$  we can exploit the  $\mathcal{S}$  - distribution to write  $G^{K}(P_{\ell}W) = -2\pi i S(W-\epsilon_{P}) J(W)$  $\mathcal{Y}(w) = 1 + 2\eta M(w)$ (A6)

31 By using the property  $= P - \frac{1}{W - \epsilon_{P}} - i T S (W - \epsilon_{P})$ - Ep + 10+ We can write the relation  $W) = \begin{bmatrix} \pi & (P, W) - G & (P, W) \\ G & (P, W) - G & (P, W) \end{bmatrix}$ (A7) Notice that for fermions at T=0  $\mathcal{J}(W) = 1 - 2\Theta(\mu - W) = \operatorname{Nign}(W - \mu)$ 

Time-dependent potential noninteracting case The only vertex term is  $\mathcal{M}(X_{A}, X_{B})$  $X_{i} = \left(\begin{array}{c} X_{i} \\ I_{i} \end{array}\right) \times \left(\begin{array}{c} X_{i} \\ X_{i} \end{array}\right)$ let us sort out time by defining Yi= tit. 11 11 and replace the contour index by the 2x2 matrix representation  $\mathcal{X}(X_{A}, X_{B}) = \mathcal{M}(\overline{X}_{A}, \overline{X}_{B} t_{A}) \mathcal{S}(t_{A} - t_{B}) \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ Identity in Keldysh space (does not hold in the  $^{\eta} \bigwedge$  "repr.) (A8)

33	
	Diagrams
	= - + + - +
	$- \frac{\sqrt{X}}{\sqrt{X}} + \frac{\sqrt{X}}{$
	= - + - + - + - + - + - + - + - + - + -
	I.e. the self-energy (exactly) consists of a single
	diagram, thig is the only single-partials irrdusible
	diagram diagram
	The perturbative sum can be carried out exactly

 $G_{0} + G_{0} * \sum * G$ is a convolution over internal variables and a matrix product in Keldysh space  $\begin{pmatrix} X_{1}, X_{2} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \begin{pmatrix} X_{1}, X_{2} \end{pmatrix}$  $d_{X_{3}ol}X_{4}$   $G_{o}(X_{1}, X_{3}) \ge (X_{3}, X_{4}) G(X_{4}, X_{2})$ A simplifiction can be achieved for the "steady state" If u is switched on at a certain time and then remains time independent, we may expect that the system reaches a stationary, i.e. time-independent state. In this case, Green's function only depend on time difference and one can Fourier transform over time.

## Some useful relations

Suppose we have to matrices in Keldysh space, i. e. of the form ł ĸ 2  $h_{\pi/k}$  to be matrices We allow also the elements (B,F), = BinFKJ Then the product has the same form hrfu thuta hrtr = hafa Now, let us look at the inverse of B  $F = B^{-1} \Rightarrow B \cdot F = I$ If fa = ha $\Rightarrow fr = h_n$ (A9)  $b_n f_n + b_n f_q = 0 \Rightarrow f_h = -b_n b_h b_q$ (A10) (also termed Langreth Rules)