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**Advanced Workshop on Energy Transport in Low-Dimensional Systems:
Achievements and Mysteries**

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**Nonequilibrium Green's function (NEGF) method in thermal transport and some
applications**

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Nonequilibrium Green's function (NEGF) method in thermal transport and some applications

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Outline of the talk

- **Introduction**
- **Method of nonequilibrium Green's functions**
- **Applications**
 - **Thermal currents in 1D chain and nanotubes**
 - **Transient problems**
 - **Full counting statistics**

Fourier's law for heat conduction



$$\mathbf{J} = -\kappa \nabla T$$

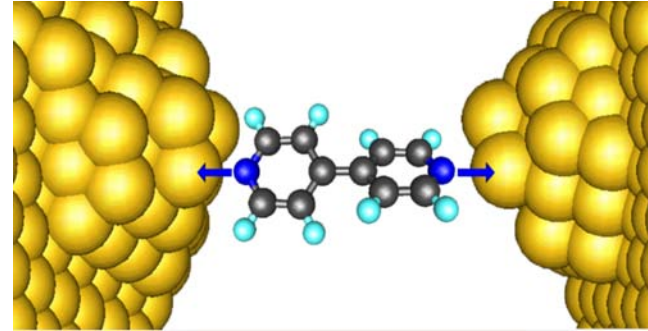
$$\tilde{f}[\omega] = \int_{-\infty}^{+\infty} f(t) e^{i\omega t} dt$$

Fourier, Jean Baptiste Joseph, Baron
(1768-1830)

Thermal conductance

$$I = (T_L - T_R)\sigma$$

$$\kappa = \sigma \frac{L}{S}, \quad I = SJ$$



where I : thermal current, J : current density

T_L, T_R : temperature of left and right lead

σ : conductance

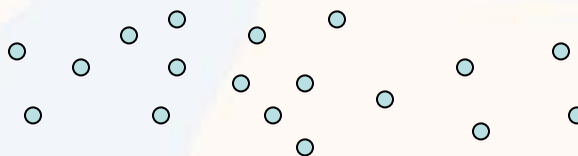
κ : conductivity

S : cross section area

Thermal transport of a junction

Junction

Left
Lead, T_L



Right
Lead, T_R

semi-infinite
leads

Models

$$H = H_L + H_C + H_R + H^{LC} + H^{CR} + H_n$$

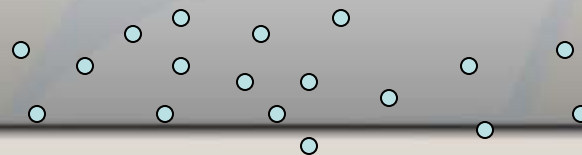
$$H_\alpha = \frac{1}{2} p_\alpha^T p_\alpha + \frac{1}{2} u_\alpha^T K^\alpha u_\alpha, \quad u = \sqrt{m} x, \quad \alpha = L, C, R$$

$$H^{aC} = u_\alpha^T V^{\alpha C} u_C, \quad u_\alpha = \begin{pmatrix} u_j^\alpha \end{pmatrix}$$

$$H_n = \frac{1}{3} \sum_{ijk} T_{ijk} u_i^C u_j^C u_k^C + \frac{1}{4} \sum_{ijkl} T_{ijkl} u_i^C u_j^C u_k^C u_l^C$$

Junction

Left
Lead, T_L



Right
Lead, T_R

Force constant matrix

$$\left[\begin{array}{ccc|cc}
 \cdot & \cdot & k_{01}^L & 0 & & \\
 \cdot & \cdot & k_{00}^L & k_{01}^L & V^{LC} & 0 \\
 0 & & k_{10}^L & k_{11}^L & & \\
 \hline
 & & V^{CL} & & K^C & V^{CR} \\
 \hline
 & & 0 & & V^{RC} & \left. \begin{array}{ccc}
 k_{00}^R & k_{01}^R & 0 \\
 k_{10}^R & k_{11}^R & k_{01}^R \\
 0 & k_{10}^R & k_{11}^R
 \end{array} \right\} K^R
 \end{array} \right]$$

Definitions of Green's functions

- **Greater/lesser Green's function**

$$G_{jk}^>(t, t') = -\frac{i}{\hbar} \langle u_j(t) u_k(t') \rangle = G_{kj}^<(t', t)$$

- **Time-ordered/anti-time ordered Green's function**

$$G^t(t, t') = \theta(t - t') G^>(t, t') + \theta(t' - t) G^<(t, t'),$$

$$G^{\bar{t}}(t, t') = \theta(t' - t) G^>(t, t') + \theta(t - t') G^<(t, t')$$

- **Retarded/advanced Green's function**

$$G^r(t, t') = \theta(t - t') (G^> - G^<),$$

$$G^a(t, t') = -\theta(t' - t) (G^> - G^<)$$

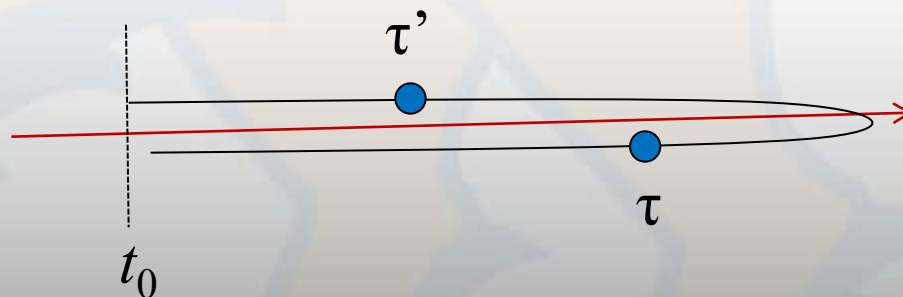
See text books, e.g.,
H. Haug and A.-P.
Jauho, or J.
Rammer, or S.
Datta, or Di Ventura

Contour-ordered Green's function

$$G_{jk}(\tau, \tau') = -\frac{i}{\hbar} \left\langle T_C u_j(\tau) u_k(\tau') \right\rangle$$

$$= \text{Tr} \left[\rho(t_0) T_C u_{j,\tau} u_{k,\tau'} e^{-\frac{i}{\hbar} \int_C H(\tau) d\tau} \right]$$

Contour order: the operators earlier on the contour are to the right.



Relation to the real-time Green's functions

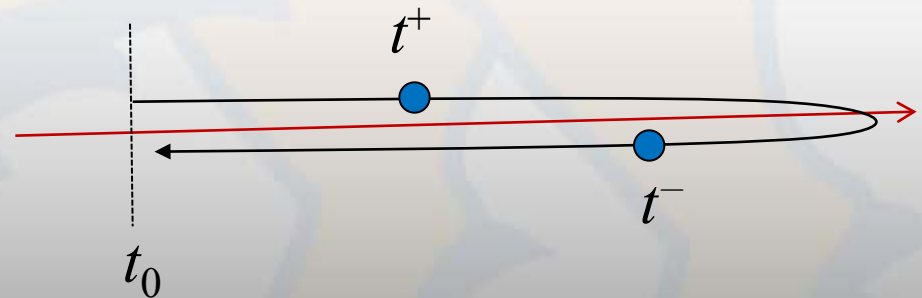
$$\tau \rightarrow (t, \sigma), \quad \text{or} \quad \tau = t^\sigma, \quad \sigma = \pm$$

$$G(\tau, \tau') \rightarrow G^{\sigma\sigma'}(t, t') \quad \text{or} \quad \begin{bmatrix} G^{++} & G^{+-} \\ G^{-+} & G^{--} \end{bmatrix}$$

$$G^{++} = G^t, \quad G^{+-} = G^<$$

$$G^{-+} = G^>, \quad G^{--} = G^{\bar{t}}$$

$$G^> + G^< = G^t + G^{\bar{t}}$$



Equations for Green's functions (in ballistic systems)

$$\frac{\partial^2}{\partial \tau^2} G(\tau, \tau') + K G(\tau, \tau') = -\delta(\tau, \tau') I$$

↓

$$\frac{\partial^2}{\partial t^2} G^{\sigma\sigma'}(t, t') + K G^{\sigma\sigma'}(t, t') = -\sigma \delta_{\sigma\sigma'} \delta(t - t') I$$

↓

$$\frac{\partial^2}{\partial t^2} G^{r,a,t}(t, t') + K G^{r,a,t}(t, t') = -\delta(t - t') I$$

$$\frac{\partial^2}{\partial t^2} G^{\bar{t}}(t, t') + K G^{\bar{t}}(t, t') = \delta(t - t') I$$

$$\frac{\partial^2}{\partial t^2} G^{>,<}(t, t') + K G^{>,<}(t, t') = 0$$

Solution for Green's functions

$$\frac{\partial^2}{\partial t^2} G^{r,a,t}(t, t') + K G^{r,a,t}(t, t') = -\delta(t - t') I$$

using Fourier transform:

$$-\omega^2 G^{r,a,t}[\omega] + K G^{r,a,t}[\omega] = -I$$

$$G^{r,a,t}[\omega] = \left(\omega^2 I - K\right)^{-1} + c \delta(\omega - \sqrt{K}) + d \delta(\omega + \sqrt{K})$$

$$G^r[\omega] = G^a[\omega]^+ = \left((\omega + i\eta)^2 I - K\right)^{-1}, \quad \eta \rightarrow 0^+$$

$$G^< = f(G^r - G^a), \quad G^> = e^{\beta\hbar\omega} G^<$$

$$G^t = G^r + G^<$$

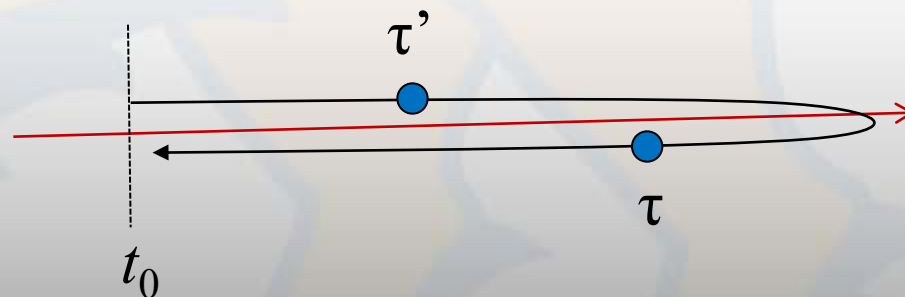
c and *d* can be fixed by initial/boundary condition.

Transform to interaction picture

$$G_{jk}(\tau, \tau') = -\frac{i}{\hbar} \langle u_j(\tau) u_k(\tau') \rangle$$

$$= \text{Tr} \left[\rho(t_0) T_C u_{j,\tau} u_{k,\tau'} e^{-\frac{i}{\hbar} \int_C H(\tau'') d\tau''} \right]$$

$$= \text{Tr} \left[\rho_I T_C u_j^I(\tau) u_k^I(\tau') e^{-\frac{i}{\hbar} \int_C H_n^I(\tau'') d\tau''} \right]$$

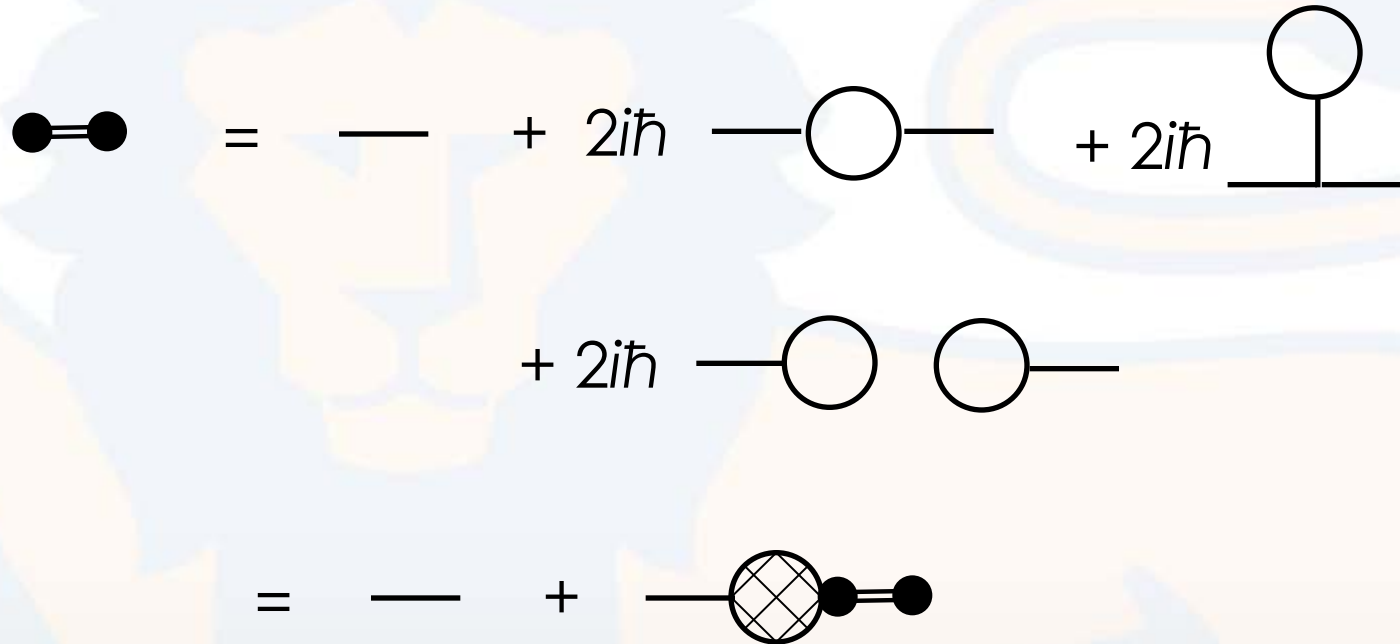


Perturbative expansion of contour ordered Green's function

$$\begin{aligned}
 G_{jk}(\tau, \tau') &= -\frac{i}{\hbar} \left\langle T_C u_j(\tau) u_k(\tau') e^{-\frac{i}{\hbar} \int H_n(\tau'') d\tau''} \right\rangle \\
 &= -\frac{i}{\hbar} \left\langle T_C u_j(\tau) u_k(\tau') \left\{ 1 - \frac{i}{\hbar} \int H_n(\tau_1) d\tau_1 + \frac{1}{2!} \left(-\frac{i}{\hbar} \right)^2 \int H_n(\tau_1) d\tau_1 \int H_n(\tau_2) d\tau_2 \right\} + \dots \right\rangle \\
 &= -\frac{i}{\hbar} \langle T_C u_j(\tau) u_k(\tau') \rangle + \frac{1}{2} \left(-\frac{i}{\hbar} \right)^3 \left\langle T_C u_j(\tau) u_k(\tau') \iiint \frac{1}{3} \sum_{lmn} T_{lmn}(\tau_1, \tau_2, \tau_3) u_l(\tau_1) u_m(\tau_2) u_n(\tau_3) d\tau_1 d\tau_2 d\tau_3 \right. \\
 &\quad \left. \times \iiint \frac{1}{3} \sum_{opq} T_{opq}(\tau_4, \tau_5, \tau_6) u_o(\tau_4) u_p(\tau_5) u_q(\tau_6) d\tau_4 d\tau_5 d\tau_6 \right\rangle \\
 &= G_{jk}^0(\tau, \tau') + \dots \left\langle T_C u_j(\tau) u_k(\tau') u_l(\tau_1) u_m(\tau_2) u_n(\tau_3) u_o(\tau_4) u_p(\tau_5) u_q(\tau_6) \right\rangle + \dots \\
 &\quad \downarrow \text{(Wick's theorem)} \\
 &\quad \left\langle T_C u_j(\tau) u_l(\tau_1) \right\rangle \left\langle T_C u_m(\tau_2) u_p(\tau_5) \right\rangle \left\langle T_C u_n(\tau_3) u_q(\tau_6) \right\rangle \left\langle T_C u_o(\tau_4) u_k(\tau') \right\rangle
 \end{aligned}$$

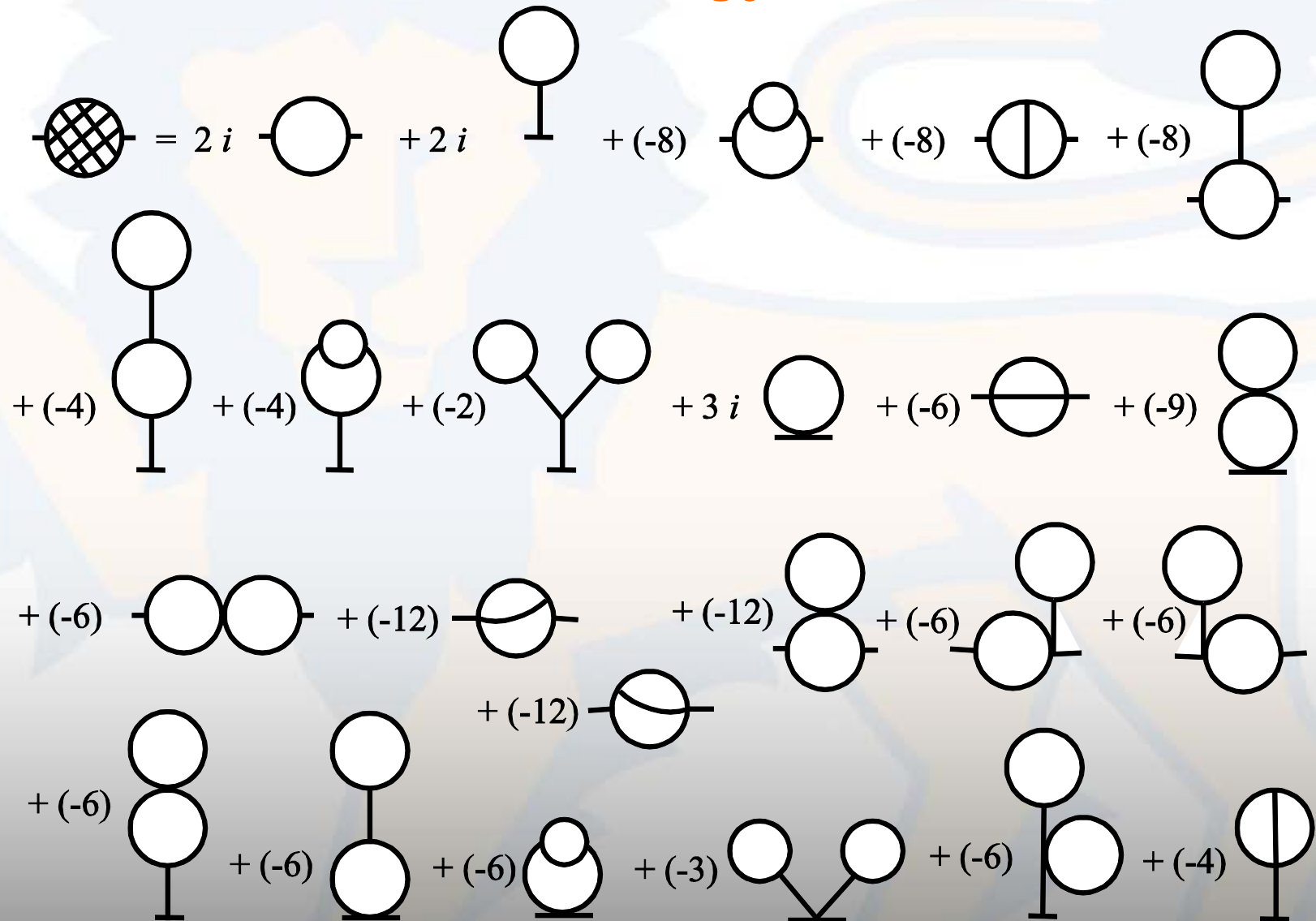
See, e.g., A. L. Fetter & J. D. Walecka.

Diagrammatic representation of the expansion



$$G_{conn}(\tau, \tau') = G_0(\tau, \tau') + \int \int G_0(\tau, \tau_1) \Sigma_n(\tau_1, \tau_2) G_{conn}(\tau_2, \tau') d\tau_1 d\tau_2$$

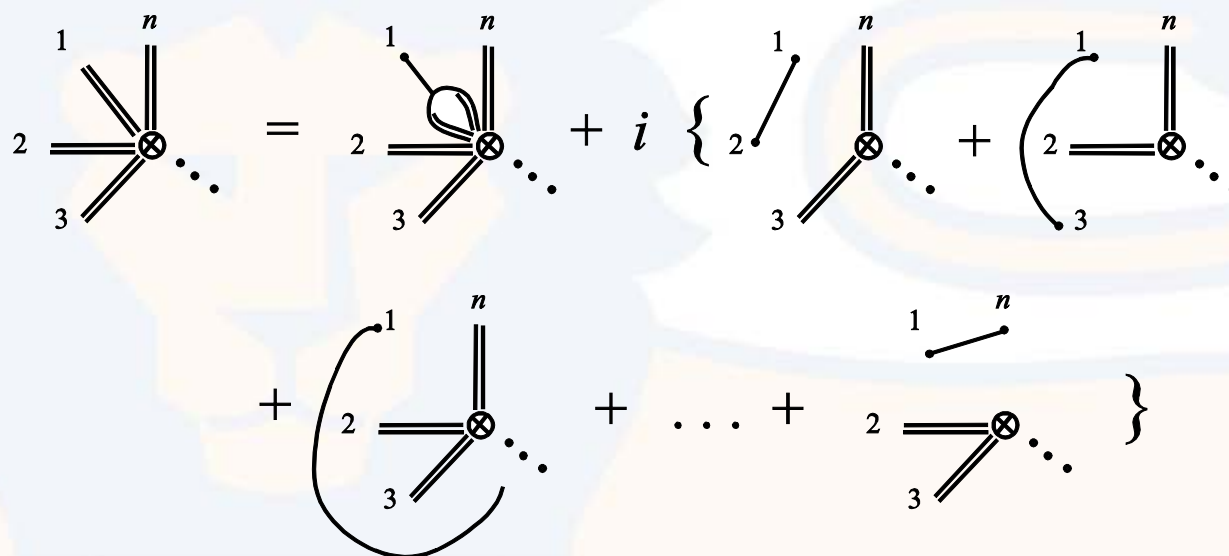
Diagrammatic representation of the nonlinear self-energy



Explicit expression for self-energy

$$\begin{aligned}
 \Sigma_{n,jk}^{\sigma\sigma'}[\omega] &= 2i \sum_{lmrs} T_{jlm} T_{rsk} \int_{-\infty}^{+\infty} G_{0,lr}^{\sigma\sigma'}[\omega'] G_{0,ms}^{\sigma\sigma'}[\omega - \omega'] \frac{d\omega'}{2\pi} \quad \text{---} \bigcirc \text{---} \\
 &+ 2i\sigma \delta_{\sigma,\sigma'} \sum_{lmrs,\sigma''} \sigma'' T_{jkl} T_{mrs} \int_{-\infty}^{+\infty} G_{0,lm}^{\sigma\sigma''}[0] G_{0,rs}^{\sigma''\sigma''}[\omega'] \frac{d\omega'}{2\pi} \quad \bigcirc \text{---} \\
 &+ O(T_{ijk}^4)
 \end{aligned}$$

General expansion rule



Single line

$$G_0(\tau, \tau')$$

3-line vertex

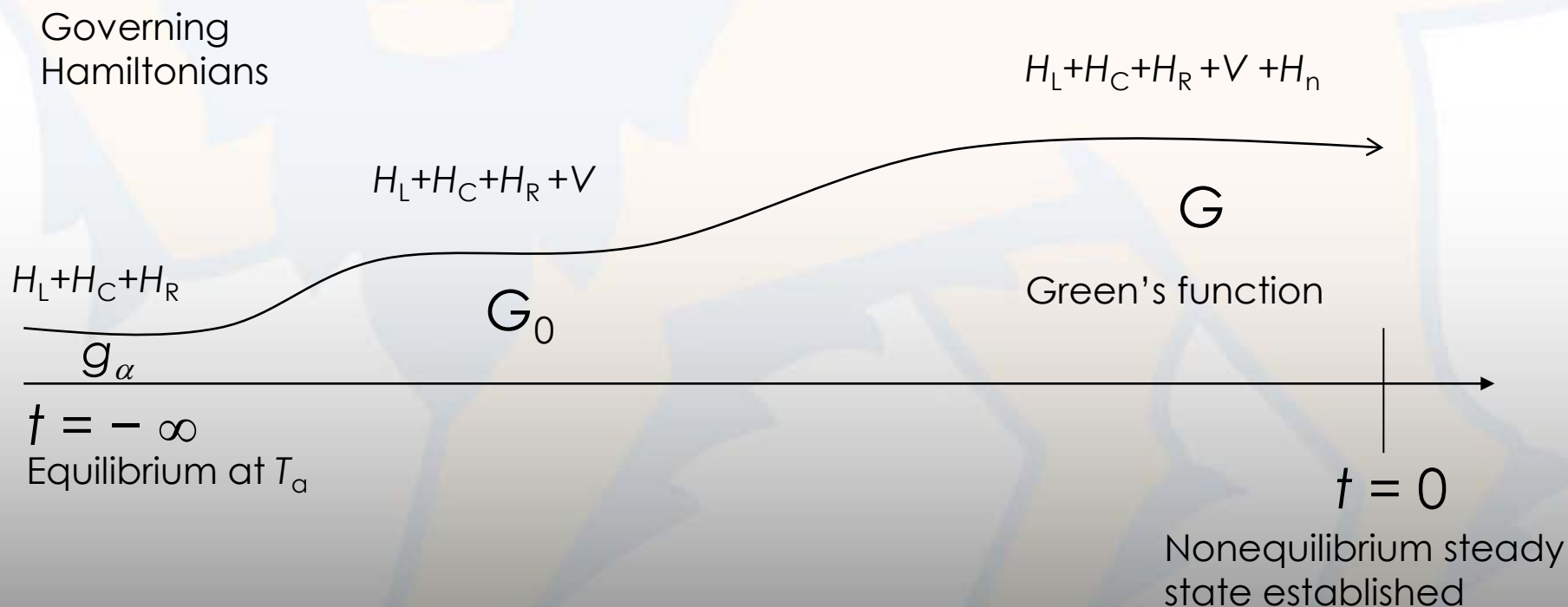
$$T_{ijk}(\tau_i, \tau_j, \tau_k)$$

n -double line
vertex

$$G_{j_1 j_2 \dots j_n}(\tau_1, \tau_2, \dots, \tau_n) = -\frac{i}{\hbar} \left\langle T_C u_{j_1}(\tau_1) u_{j_2}(\tau_2) \dots u_{j_n}(\tau_n) \right\rangle$$

Junction systems

- Three types of Green's functions:
 - g for isolated systems when leads and centre are decoupled
 - G_0 for ballistic system
 - G for full nonlinear system



Three regions

$$u = \begin{pmatrix} u_L \\ u_C \\ u_R \end{pmatrix}, \quad u_L = \begin{pmatrix} u_L^1 \\ u_L^2 \\ \dots \end{pmatrix}, \quad u_C = \dots$$

$$G_{\alpha\beta}(\tau, \tau') = -\frac{i}{\hbar} \langle T_C u_\alpha(\tau) u_\beta(\tau')^T \rangle, \quad \alpha, \beta = L, C, R$$

Dyson equations and solutions

$$G_0 = g_C + g_C \Sigma G_0, \quad \Sigma = V^{CL} g_L V^{LC} + V^{CR} g_R V^{RC}$$

$$G = G_0 + G_0 \Sigma_n G$$

$$G_0^r = \left((\omega + i\eta)^2 I - K^C - \Sigma^r \right)^{-1}, \quad \eta \rightarrow 0^+$$

$$G_0^< = G_0^r \Sigma^< G_0^a \quad (\text{Keldysh equation})$$

$$G^r = \left((G_0^r)^{-1} - \Sigma_n^r \right)^{-1},$$

$$\begin{aligned} G^< &= G^r \Sigma_n^< G^a + (I + G^r \Sigma_n^r) G_0^< (I + \Sigma_n^a G^a) \\ &= G^r (\Sigma^< + \Sigma_n^<) G^a \end{aligned}$$

Energy current (Meir-Wingreen)

$$\begin{aligned}
 I_L &= - \left\langle \frac{dH_L}{dt} \right\rangle = \left\langle \dot{u}_L^T V^{LC} u_C \right\rangle \\
 &= - \frac{1}{2\pi} \int_{-\infty}^{+\infty} \text{Tr} \left(V^{LC} G_{CL}^<[\omega] \right) \hbar \omega d\omega \\
 &= - \frac{1}{2\pi} \int_{-\infty}^{+\infty} \text{Tr} \left(G^r[\omega] \Sigma_L^<[\omega] + G^<[\omega] \Sigma_L^a[\omega] \right) \hbar \omega d\omega
 \end{aligned}$$

Landauer/Caroli formula

$$I_L = - \left\langle \frac{dH_L}{dt} \right\rangle = \int_0^{+\infty} \hbar \omega \text{Tr} \left(G_{CC}^r \Gamma_L G_{CC}^a \Gamma_R \right) (f_L - f_R) \frac{d\omega}{2\pi}$$

$$\Gamma_\alpha = i \left(\Sigma_\alpha^r - \Sigma_\alpha^a \right)$$

$$I_L \rightarrow \frac{I_L - I_R}{2},$$

$$G^< = G^r \Sigma^< G^a, \quad i\Sigma^< = f_L \Gamma_L + f_R \Gamma_R$$

$$G^a - G^r = iG^r (\Gamma_L + \Gamma_R) G^a$$

Ballistic transport in a 1D chain

- Force constant matrix

$$K = \begin{bmatrix} \dots & -k & 0 & & \dots \\ -k & 2k + k_0 & -k & 0 & \\ & -k & 2k + k_0 & -k & \\ & 0 & -k & 2k + k_0 & \\ \dots & 0 & 0 & -k & \dots \end{bmatrix}$$

- Equation of motion

$$m\ddot{u}_j = ku_{j-1} - (2k + k_0)u_j + ku_{j+1}, \quad j = \dots, -1, 0, 1, 2, \dots$$

Solution of g

- Surface Green's function

$$\left((\omega + i\eta)^2 - K^R \right) g_R = I, \quad \eta \rightarrow 0^+$$

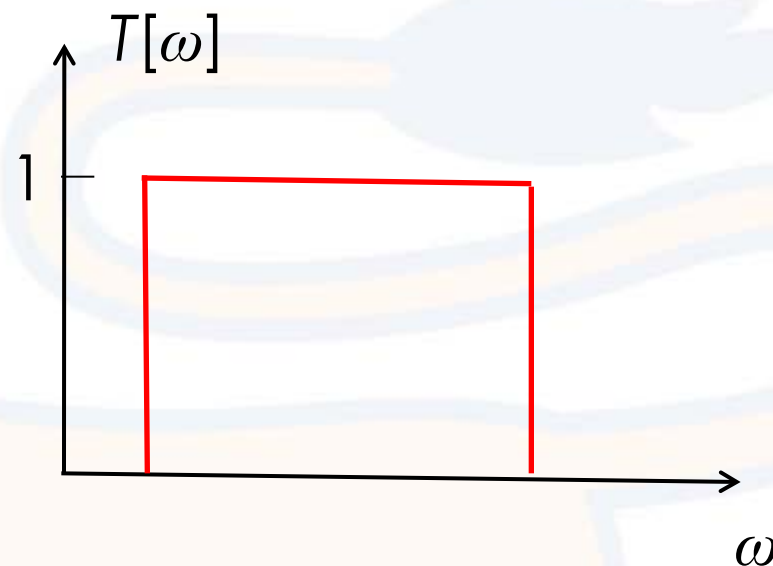
$$K^R = \begin{bmatrix} 2k + k_0 & -k & 0 & \dots \\ -k & 2k + k_0 & -k & 0 \\ 0 & -k & 2k + k_0 & -k \\ 0 & 0 & -k & \dots \end{bmatrix}$$

$$g_{j0}^R = -\frac{\lambda^j}{k}, \quad j = 0, 1, 2, \dots,$$

$$\lambda^{-1} + ((\omega + i\eta)^2 - 2k - k_0) / k + \lambda = 0, \quad |\lambda| < 1$$

Lead self energy and transmission

$$\Sigma_L = \begin{bmatrix} -k\lambda & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ \dots & 0 & 0 & 0 \end{bmatrix}$$



$$G^r = (\omega^2 - K^C - \Sigma_L - \Sigma_R)^{-1},$$

$$G_{jk}^r = \frac{\lambda^{|j-k|}}{k(\lambda - \lambda^{-1})}$$

$$T[\omega] = \text{Tr}(G^r \Gamma_L G^a \Gamma_R) = \begin{cases} 1, & k_0 < \omega^2 < 4k + k_0 \\ 0, & \text{otherwise} \end{cases}$$

Heat current and “universal” thermal conductance

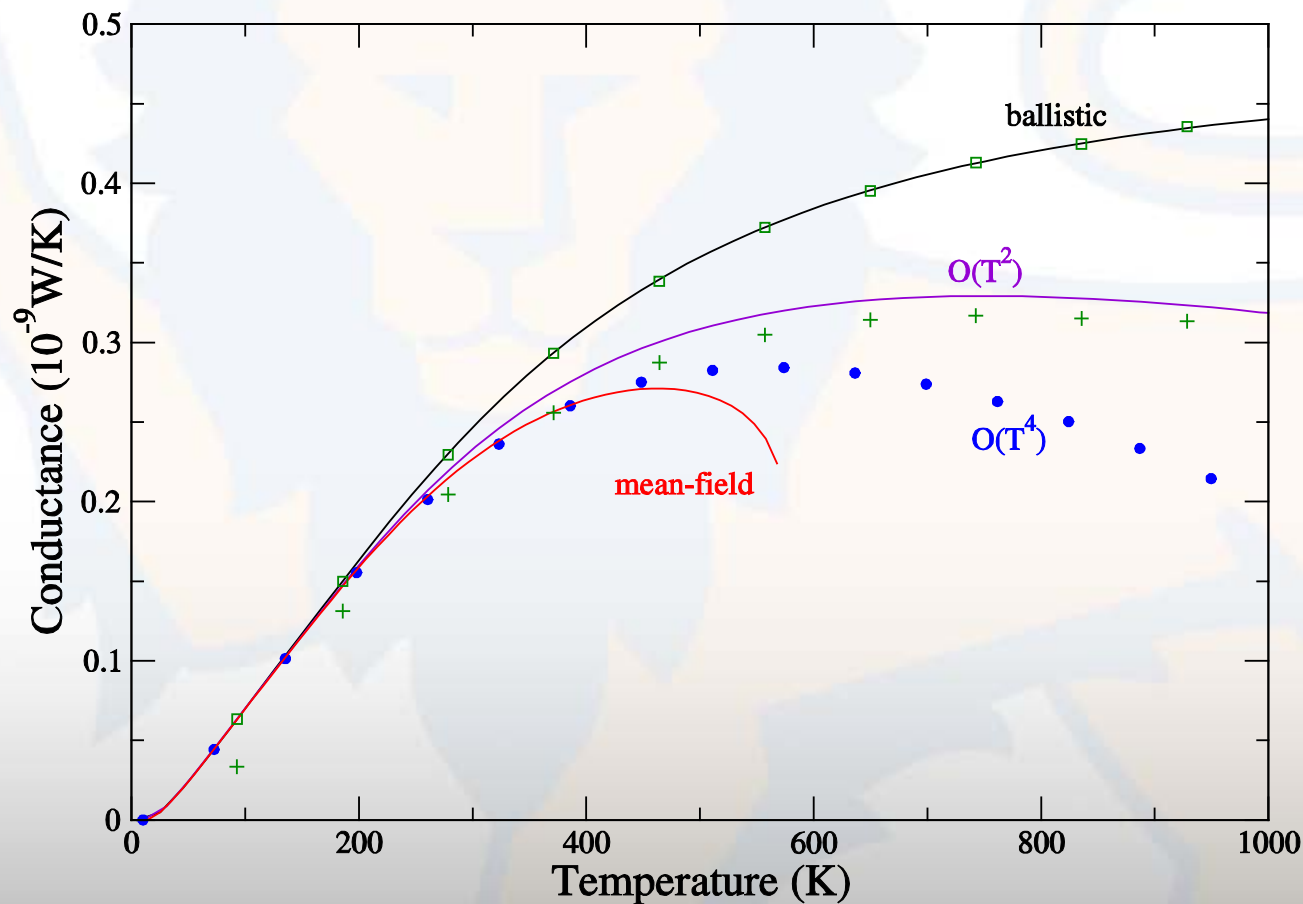
$$I_L = \int_0^{+\infty} \hbar \omega T[\omega] (f_L - f_R) \frac{d\omega}{2\pi}$$

$$\sigma = \lim_{T_L \rightarrow T_R} \frac{I_L}{T_L - T_R} = \int_{\omega_{\min}}^{\omega_{\max}} \hbar \omega \frac{\partial f}{\partial T} \frac{d\omega}{2\pi}, \quad f = \frac{1}{e^{\beta \hbar \omega} - 1}$$

$$\sigma \approx \frac{\pi^2 k_B^2 T}{3h}, \quad k_0 = 0, T \rightarrow 0$$

Rego and
Kirczenow, 1998.

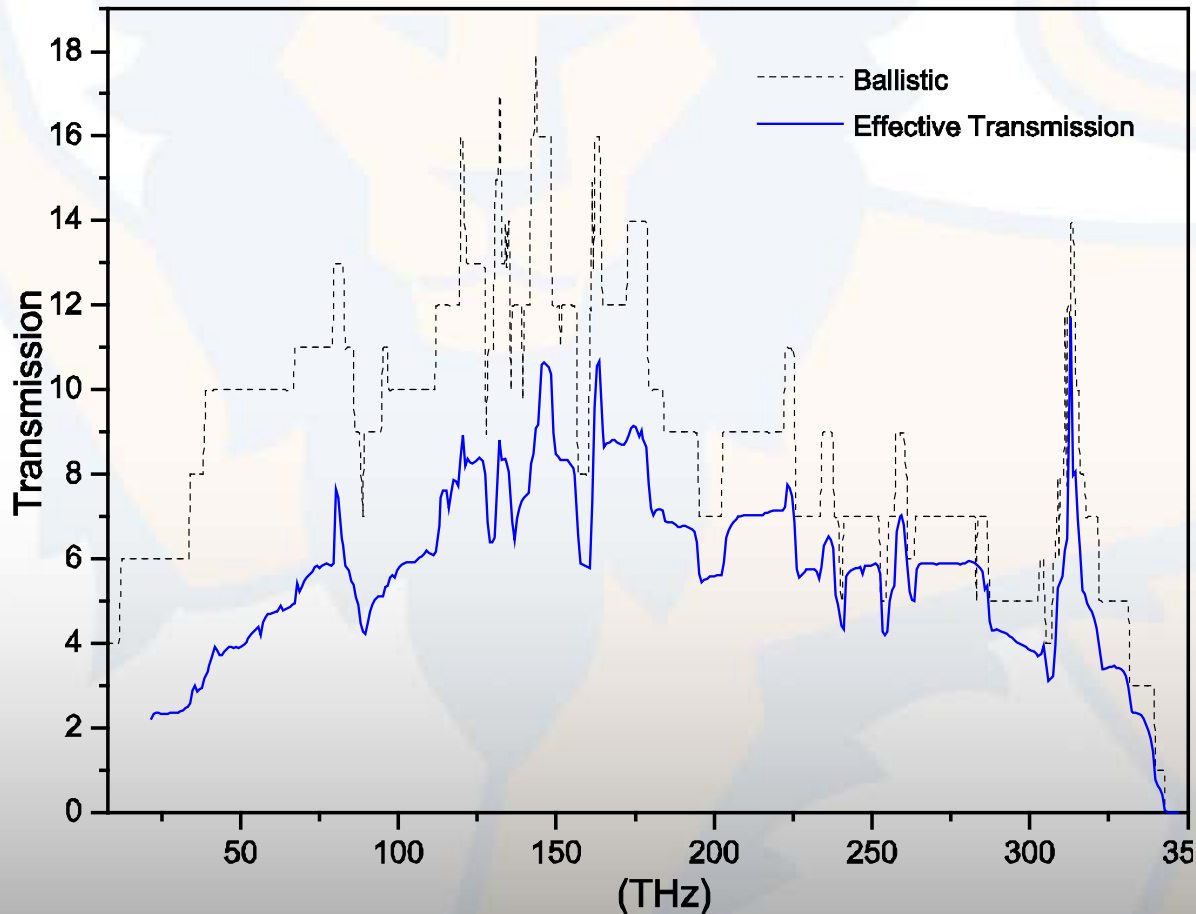
1D nonlinear model



Three-atom junction with cubic nonlinearity (FPU- α). From JSW, Wang, Zeng, PRB 74, 033408 (2006). Cross + from QMD: JSW, Wang, Lü, Eur. Phys. J. B, 62, 381 (2008).

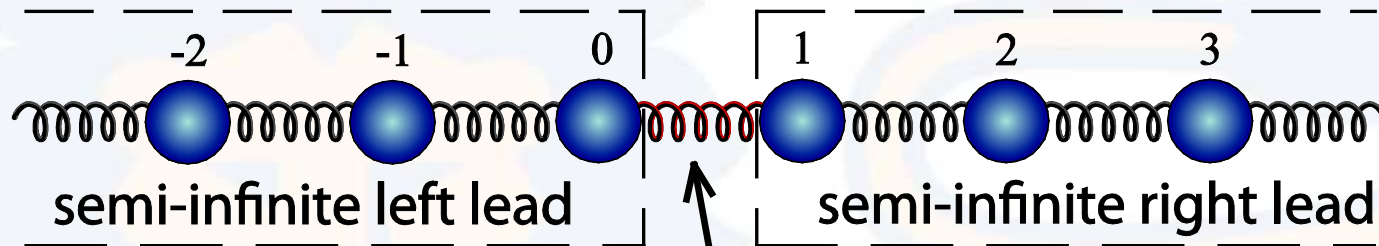


Carbon nanotube, nonlinear effect



The transmissions in a one-unit-cell carbon nanotube junction of (8,0) at 300K. From J-S Wang, J Wang, N Zeng, Phys. Rev. B 74, 033408 (2006).

Transient problems



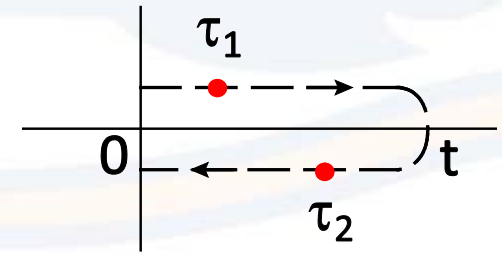
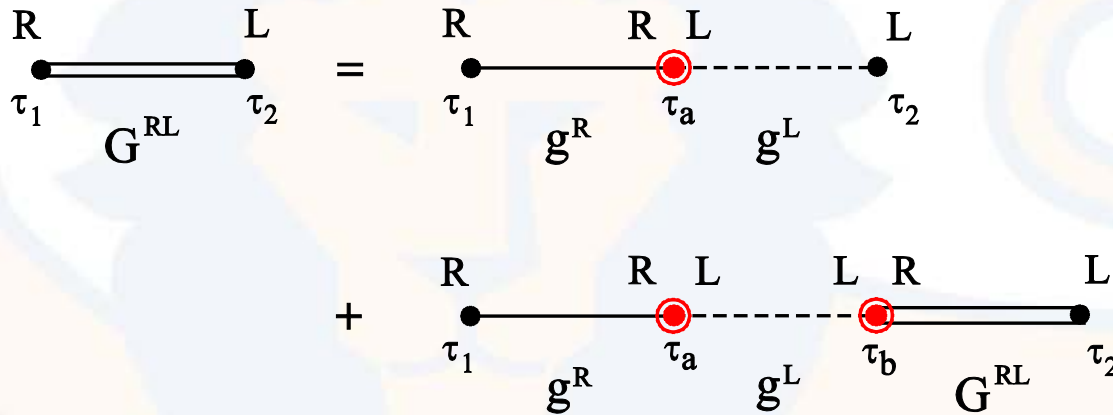
coupling is switched on at $t=0$

$$H_0 = H_L + H_R$$

$$H(t) = \begin{cases} H_0, & t \leq 0 \\ H_0 + u_L^T V^{LR} u_R, & t > 0 \end{cases}$$

$$I_L(t) = \hbar k \operatorname{Im} \left[\frac{\partial G^{RL, <}(t_1, t_2)}{\partial t_2} \right]_{t_1=t_2=t}$$

Dyson equation on contour from 0 to t

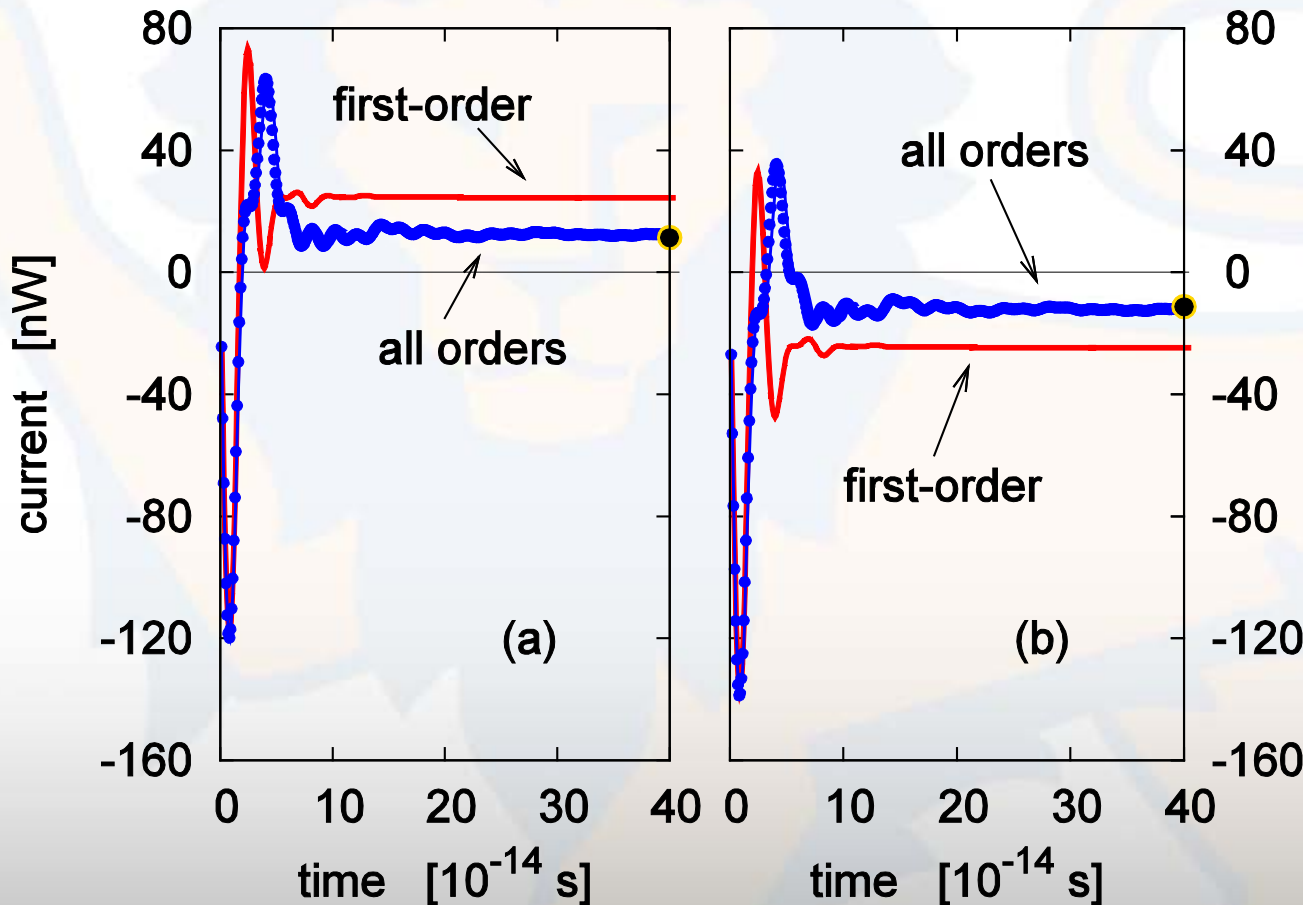


Contour C

$$G^{RL}(\tau, \tau') = \int_C d\tau_1 g^R(\tau - \tau_1) V^{RL} g^L(\tau_1 - \tau')$$

$$+ \int_C d\tau_1 \int_C d\tau_2 g^R(\tau - \tau_1) V^{RL} g^L(\tau_1 - \tau_2) V^{LR} G^{RL}(\tau_2, \tau')$$

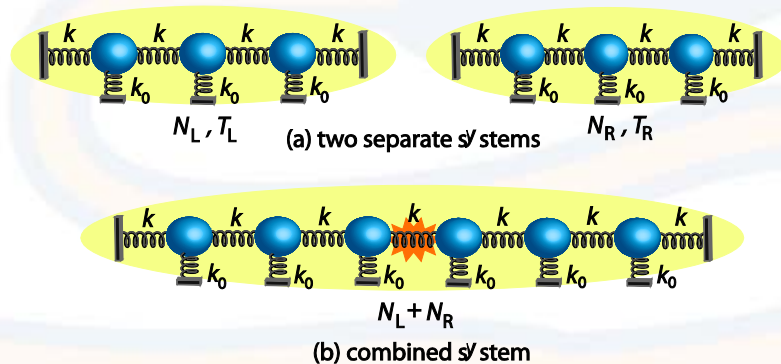
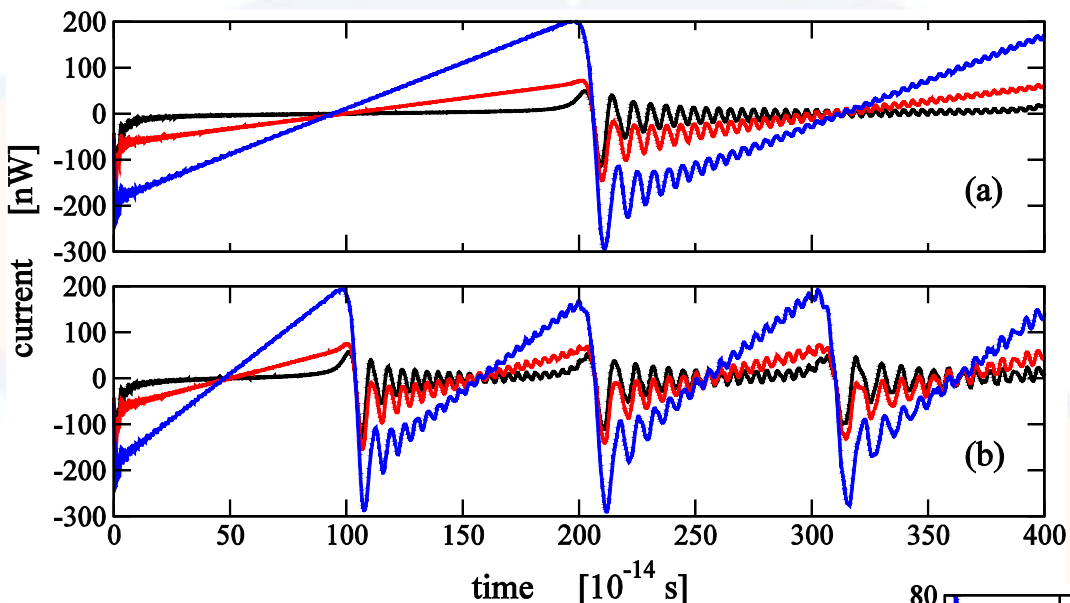
Transient thermal current



The time-dependent current when the coupling is suddenly switched on. (a) Current flow out of left lead, (b) out of right lead. Dots are what predicted from Landauer formula.

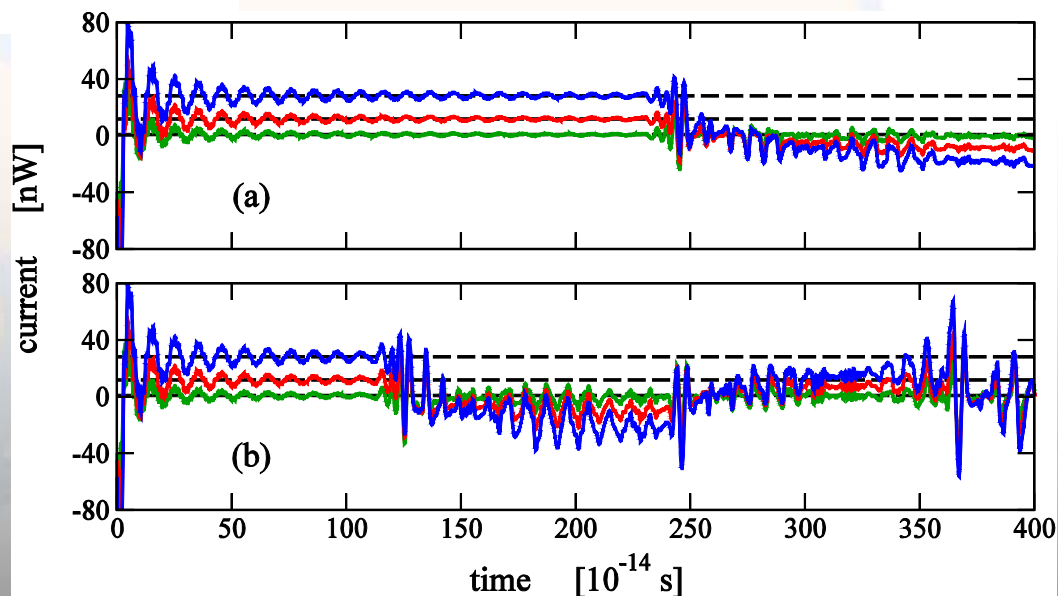
$T=300\text{K}$, $k=0.625$ eV/ $(\text{\AA}^2\text{u})$ with a small onsite $k_0=0.1k$. From E. C. Cuansing and J.-S. Wang, Phys. Rev. B 81, 052302 (2010). See also PRE 82, 021116 (2010).

Finite lead problem



Top $\hat{1}$: no onsite ($k_0=0$), (a) $N_L = N_R = 100$, (b) $N_L = N_R = 50$, temperature $T=10, 100, 300$ K (black, red, blue). $T_L=1.1T$, $T_R = 0.97T$.

Right \mapsto : with onsite $k_0=0.1k$ and similarly for other parameters. From E. C. Cuansing, H. Li, and J.-S. Wang, Phys. Rev. E 86, 031132 (2012).



Full counting statistics (FCS)

- What is the amount of energy (heat) Q transferred in a given time t ?
- This is not a fixed number but given by a probability distribution $P(Q)$
- Generating function

$$Z(\xi) = \int e^{i\xi Q} P(Q) dQ$$

- All moments of Q can be computed from the derivatives of Z .
- The objective of full counting statistics is to compute $Z(\xi)$.

A brief history on full counting statistics

- L. S. Levitov and G. B. Lesovik proposed the concept for electrons in 1993; rederived for noninteracting electron problems by I. Klich, K. Schönhammer, and others
- K. Saito and A. Dhar obtained the first result for phonon transport in 2007
- J.-S. Wang, B. K. Agarwalla, and H. Li, PRB 2011; B. K. Agarwalla, B. Li, and J.-S. Wang, PRE 2012.

Definition of generating function based on two-time measurement

$$Z = \text{Tr} \left[\rho' e^{i\xi H_L} e^{-i\xi H_L(t)} \right]$$

$$\rho' = \sum_a P_a \rho P_a$$

$$P_a^2 = P_a = |a\rangle\langle a|$$

$$H_L |a\rangle = a |a\rangle$$

$$H_L(t) = U(0,t) H_L U(t,0)$$

$$\text{e.g., } U(t,0) = e^{-iHt/\hbar}$$

Consistent history quantum mechanics (R. Griffiths).

Approaches to compute Z

- Express Z as expectation value of some effective evolution operator over a contour
- Evaluate the expression using
 - Feynman path integral/influence functional
 - Feynman diagrammatic expansion

Product initial state

$$\rho \propto \prod_{\alpha=L,C,R} e^{-\beta_\alpha H_\alpha}, \quad [P_L, H_L] = 0, \quad \rho' = \rho$$

$$Z = \text{Tr} \left[\rho e^{i\xi H_L} e^{-i\xi H_L(t)} \right]$$

$$= \text{Tr} \left[\rho e^{i\xi H_L} U(0,t) e^{-i\xi H_L} U(t,0) \right]$$

$$= \text{Tr} \left[\rho e^{i\xi H_L/2} U(0,t) e^{-i\xi H_L} U(t,0) e^{i\xi H_L/2} \right]$$

$$= \text{Tr} \left[\rho U_{\xi/2}(0,t) U_{-\xi/2}(t,0) \right]$$

$$U_x(t,t') = e^{ixH_L} U(t,t') e^{-ixH_L}$$

$$\begin{aligned}
 U_x(t, t') &= e^{ixH_L} T e^{-\frac{i}{\hbar} \int_{t'}^t H(t) dt} e^{-ixH_L} \\
 &= T e^{-\frac{i}{\hbar} \int_{t'}^t H_x(t) dt}, \quad t \geq t'
 \end{aligned}$$

$$\begin{aligned}
 H_x(t) &= e^{ixH_L} H(t) e^{-ixH_L} \\
 &= e^{ixH_L} (H_L + H_C + H_R + H^{LC} + H^{RC}) e^{-ixH_L} \\
 &= H_L + H_C + H_R + H^{RC} + e^{ixH_L} H^{LC} e^{-ixH_L} \\
 &= H_0 + H^{RC} + (u_x^L)^T V^{LC} u^C = H_0 + H_I^x
 \end{aligned}$$

$$u_x^L = e^{ixH_L} u^L e^{-ixH_L} = u^L(\hbar x)$$

Schrödinger, Heisenberg, and interaction pictures

Schrödinger picture

$$|\Psi(t)\rangle = U(t, t') |\Psi(t')\rangle \quad \rho = \sum w_i |i\rangle\langle i|$$
$$i\hbar \frac{\partial U(t, t')}{\partial t} = H(t)U(t, t')$$

Heisenberg picture

$$A_H(t) = U(0, t) A U(t, 0), \quad |\Psi_H\rangle = |\Psi(0)\rangle$$
$$i\hbar \frac{\partial A_H(t)}{\partial t} = [A_H(t), H_H(t)]$$

Interaction picture

$$H = H_0 + H_I$$
$$|\Psi_I(t)\rangle = e^{\frac{i}{\hbar} H_0 t} |\Psi(t)\rangle = S(t, t') |\Psi_I(t')\rangle$$
$$i\hbar \frac{\partial S(t, t')}{\partial t} = H_I(t) S(t, t'), \quad S(t, t') = T e^{-\frac{i}{\hbar} \int_{t'}^t H_I(t'') dt''}, \quad t > t'$$
$$A_I(t) = e^{\frac{i}{\hbar} H_0 t} A e^{-\frac{i}{\hbar} H_0 t}$$

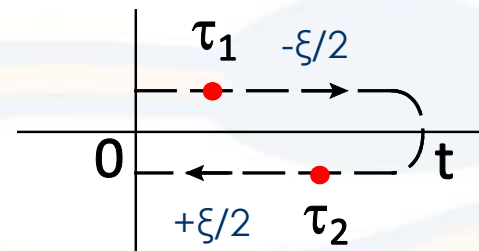
Compute Z in interaction picture

$$Z = \text{Tr}[\rho U_{\xi/2}(0,t)U_{-\xi/2}(t,0)]$$

$$= \text{Tr}[\rho T_C e^{-\frac{i}{\hbar} \int_C H_I^x(\tau) d\tau}]$$

$$= \text{Tr} \left[\rho T_C \left\{ 1 - \frac{i}{\hbar} \int_C H_I^x(\tau) d\tau + \frac{1}{2} \left(-\frac{i}{\hbar} \right)^2 \int_C \int_C H_I^x(\tau) H_I^x(\tau') d\tau d\tau' + \dots \right\} \right]$$

$$= 1 + \frac{1}{2} \text{Tr}[g_C V^{CL} g_L^x V^{LC}] + \dots$$



$$\ln Z = -\frac{1}{2} \text{Tr} \ln[1 - g_C (\Sigma_L^x + \Sigma_R)] = -\frac{1}{2} \ln \det[(1 - g_C \Sigma)(1 - G_0 \Sigma_L^A)]$$

$$= -\frac{1}{2} \text{Tr} \ln[(1 - G_0 \Sigma_L^A)]$$

$$G_0 = g_C + g_C \Sigma G_0, \quad \Sigma = \Sigma_L + \Sigma_R, \quad \Sigma_L^A = \Sigma_L^x - \Sigma_L$$

Important result

$$\ln Z = -\frac{1}{2} \text{Tr} \left[\ln(1 - G_0 \Sigma_L^A) \right]$$

$$G_0 = g_C + g_C \Sigma G_0, \quad \Sigma = \Sigma_L + \Sigma_R, \quad \Sigma_L^A = \Sigma_L^x - \Sigma_L$$

$$\Sigma_L^A(\tau, \tau') = \Sigma_L(\tau + \hbar x(\tau), \tau' + \hbar x(\tau')) - \Sigma_L(\tau, \tau')$$

$$x(\tau) \rightarrow x^+(t) = -\xi/2 \text{ if } 0 < t < t_M$$

$$x^-(t) = +\xi/2 \text{ if } 0 < t < t_M$$

0 otherwise

Long-time result, Levitov-Lesovik formula

$$\begin{aligned}
 \ln Z &= -\frac{1}{2} \text{Tr} \left[\ln(1 - G_0 \Sigma_L^A) \right] \\
 &= -\frac{1}{2} \text{Tr} \left[\ln \left\{ 1 - \begin{pmatrix} G_0^r & G^K \\ 0 & G_0^a \end{pmatrix} \begin{pmatrix} \frac{a-b}{2} & \frac{a+b}{2} \\ -\frac{a+b}{2} & -\frac{a-b}{2} \end{pmatrix} \right\} \right] \\
 &\approx -t_M \int_{-\infty}^{+\infty} \frac{d\omega}{4\pi} \ln \det \left\{ I - G_0^r \Gamma_L G_0^a \Gamma_R \left[(e^{i\zeta\hbar\omega} - 1) f_L + (e^{-i\zeta\hbar\omega} - 1) f_R + (e^{i\zeta\hbar\omega} + e^{-i\zeta\hbar\omega} - 2) f_L f_R \right] \right\}
 \end{aligned}$$

where

$$a = \Sigma_L^>[\omega](e^{-i\zeta\hbar\omega} - 1), \quad b = \Sigma_L^<[\omega](e^{i\zeta\hbar\omega} - 1)$$

$$\Gamma_\alpha = i(\Sigma_\alpha^r - \Sigma_\alpha^a), \quad \alpha = L, R$$

$$f_\alpha = 1/(e^{\beta_\alpha \hbar\omega} - 1), \quad \beta_\alpha = 1/(k_B T_\alpha)$$

Arbitrary time, transient result

$$\ln Z = -\frac{1}{2} \text{Tr} \ln(1 - G_0 \Sigma_L^A)$$

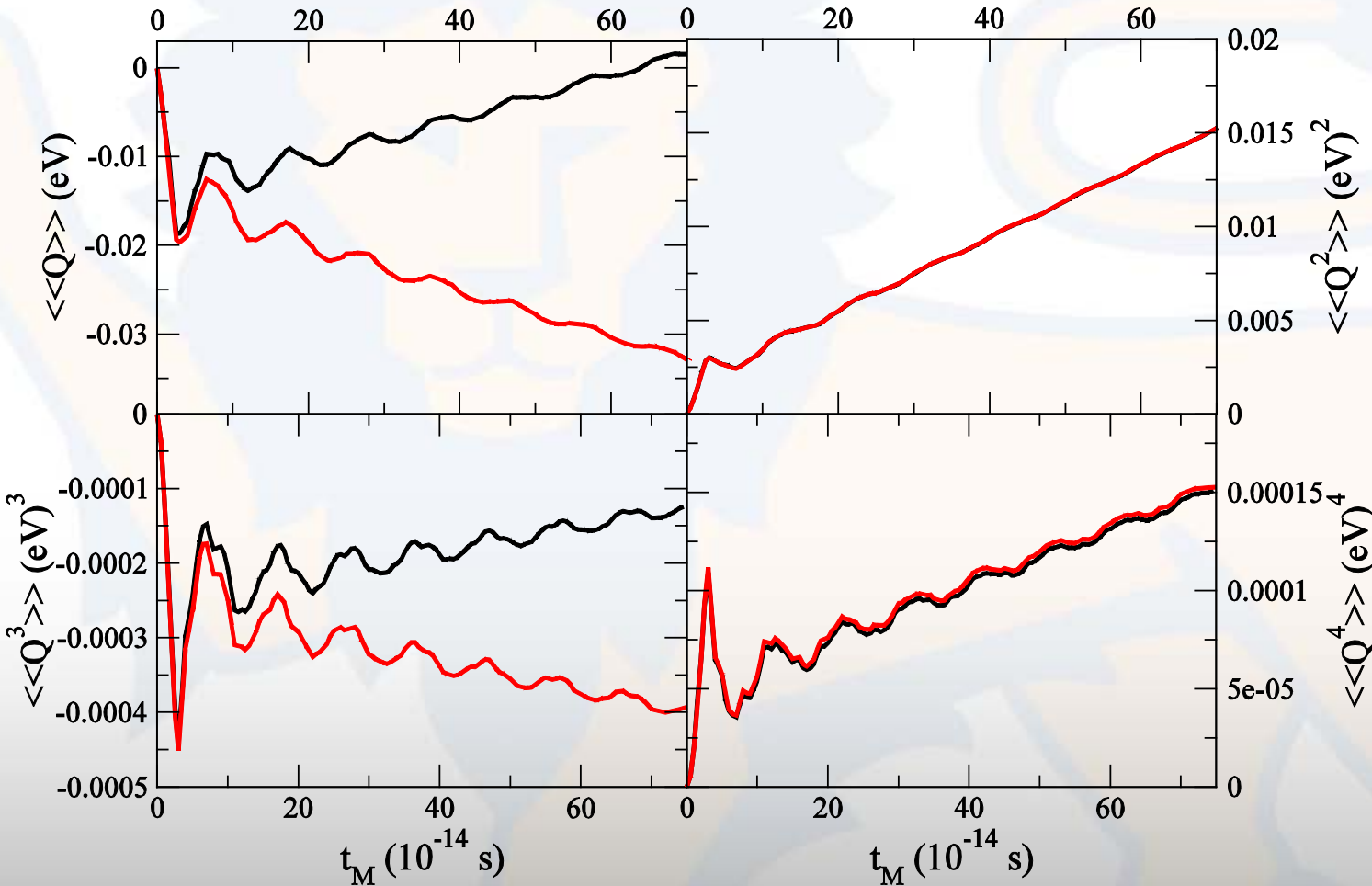
$$\langle\langle Q^n \rangle\rangle = \left. \frac{\partial^n \ln Z}{\partial (i\xi)^n} \right|_{\xi=0}$$

$$\langle\langle Q \rangle\rangle = \langle Q \rangle = \left. \frac{\partial \ln Z}{\partial (i\xi)} \right|_{\xi=0} = \frac{1}{2} \text{Tr} \left[G_0 \frac{\partial \Sigma_L^A}{\partial (i\xi)} \right]$$

$$\langle\langle Q^2 \rangle\rangle = \langle Q^2 \rangle - \langle Q \rangle^2 = \frac{\partial^2 \ln Z}{\partial (i\xi)^2}$$

$$\langle Q \rangle \approx t_M I \quad (\text{in long time})$$

Numerical results, 1D chain



1D chain with a single site as the center.

$$k = 1 \text{ eV}/(u \text{ \AA}^2),$$

$$k_0 = 0.1 k,$$

$$T_L = 310 \text{ K},$$

$$T_C = 300 \text{ K},$$

$$T_R = 290 \text{ K}. \text{ Red}$$

line right lead;

black, left lead.

B. K. Agarwalla,

B. Li, and J.-S.

Wang, PRE 85,

051142, 2012.

FCS for coupled leads

$$K = \begin{bmatrix} K_L & V^{LC} & V^{LR} \\ V^{CL} & K_C & V^{CR} \\ V^{RL} & V^{RC} & K_R \end{bmatrix}, \quad G = g + gVG$$

$$\ln Z = -t_M \int_{-\infty}^{+\infty} \frac{d\omega}{4\pi} \ln \det \left\{ I - \left[(e^{i\xi\hbar\omega} - 1) f_L (1 + f_R) + (e^{-i\xi\hbar\omega} - 1) f_R (1 + f_L) \right] T_g[\omega] \right\}$$

$$T_g[\omega] = \left(G_{LR}^r \tilde{\Gamma}_R G_{RL}^a \tilde{\Gamma}_L \right), \quad \tilde{\Gamma}_\alpha = i \left[\left(g_\alpha^a \right)^{-1} - \left(g_\alpha^r \right)^{-1} \right], \quad \alpha = L, R$$

If center is absent $V^{LC} = V^{RC} = 0$, then

$$T_g[\omega] \rightarrow T_I[\omega] = \left(G_{RR}^r \tilde{\Gamma}_R G_{RR}^a \Gamma_L \right)$$

From H. Li, B. K. Agarwalla, and J.-S. Wang, Phys. Rev. E 86, 011141 (2012); and arXiv:1208.4915

FCS in nonlinear systems

- Can we do nonlinear?
- Yes we can. Formal expression generalizes Meir-Wingreen
- Interaction picture defined on contour
- Some example calculations

Vacuum diagrams, Dyson equation, interaction picture transformation on contour

$$\frac{\partial \ln Z}{\partial (i\xi)} = \frac{1}{2} \text{Tr}_{j,\tau} \left[\tilde{G} \frac{\partial \tilde{\Sigma}_L}{\partial (i\xi)} \right]$$

$$\tilde{G} = G_0 + G_0 \left(\Sigma_L^A + \tilde{\Sigma}_n \right) \tilde{G}$$

$$\tilde{G}(\tau_1, \tau_2) = -\frac{i}{\hbar} \text{Tr} \left[\rho^I T_C u^I(\tau_1) u^I(\tau_2)^T e^{-\frac{i}{\hbar} \int_C H_n^I(\tau) d\tau} \right] \frac{1}{Z_n}$$

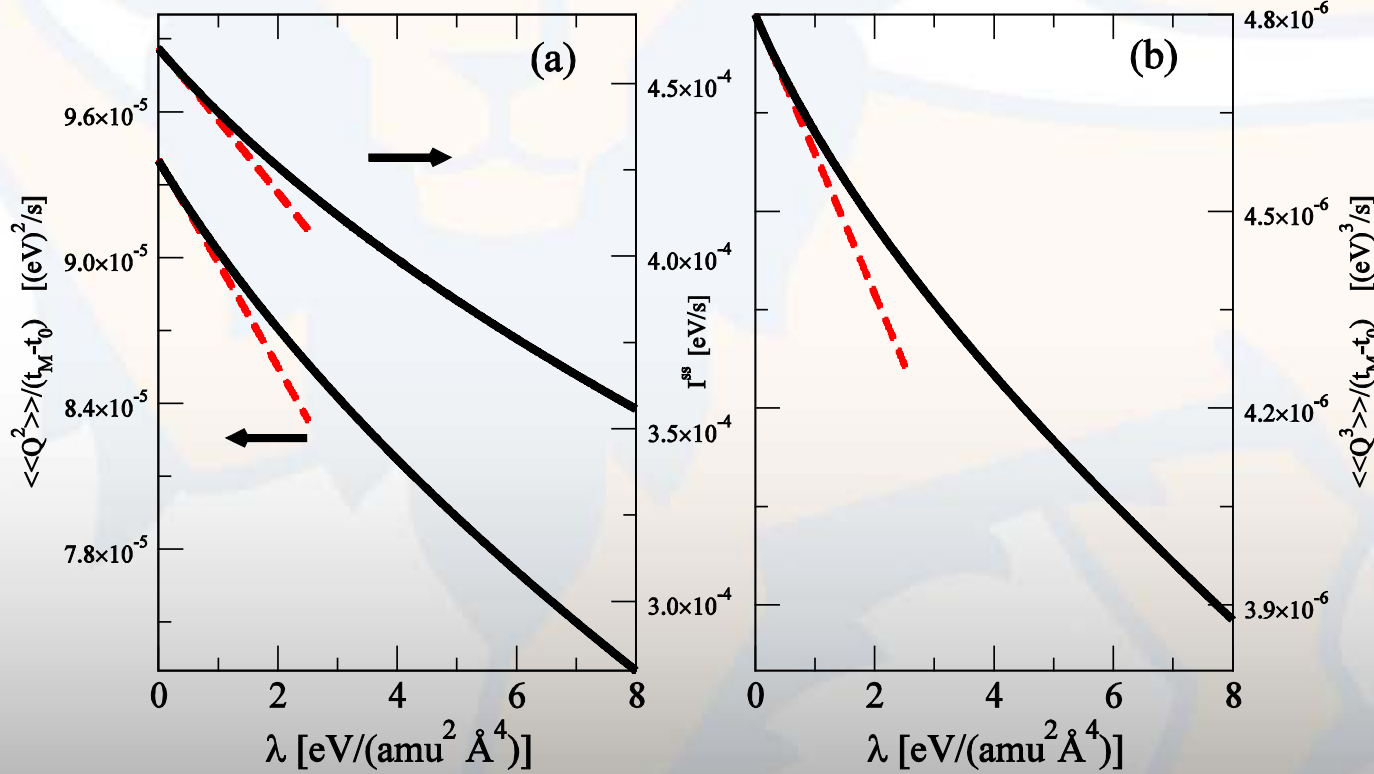
$$Z = Z_0 Z_n, \quad \rho^I = \rho V(0^-, t_M) V(t_M, 0^+) / Z_0$$

$$O^I(\tau) = V(0^+, \tau) O(\tau) V(\tau, 0^+)$$

$$V(\tau, 0^+) = T_C e^{-\frac{i}{\hbar} \int_{C[\tau, 0^+]} (u_L^{x,T} V^{LC} u_C + u_C^T V^{CR} u_R) d\tau}$$

Nonlinear system self-consistent results

$$\tilde{\Sigma}_n(\tau, \tau') = 3i\hbar\lambda\tilde{G}(\tau, \tau')\delta(\tau, \tau')$$



Single-site
(1/4) λu^4 model
cumulants.

$k=1 \text{ eV}/(u\text{\AA}^2)$,
 $k_0=0.1k$,
 $K_C=1.1k$,
 $V_{-1,0}^{LC}=V_{0,1}^{CR}=-$
 $0.25k$, $T_L=660$
K, $T_R=410$ K.

From H. Li, B. K.
Agarwalla, B. Li,
and J.-S. Wang,
arxiv::1210.2798

Other results

- We can also compute the cumulants for the projected steady state ρ'
- Entropy production
- Fluctuation theorem, $Z(\xi) = Z(-\xi + i(\beta_R - \beta_L))$
- The theory is applied equally well to electron number of electron energy transport

Summary remarks

- **NEGF is a powerful tool to handle thermal transport problems in nanostructures**
- **Steady state current is obtained from Landauer and Caroli formula**
- **New results for transient and full counting statistics. A key quantity is the self-energy Σ_L^A**

Group members/acknowledgements



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Thank you

see <http://staff.science.nus.edu.sg/~phywjs/> for
more information