Transient behavior and full counting statistics in thermal transport in nanojunctions

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Outline of the talk

- Introduction
- Method of nonequilibrium Green's functions
- Applications
  - Thermal currents in1D chain and nanotubes
  - Transient problem
  - Full counting statistics

Fourier's law for heat conduction

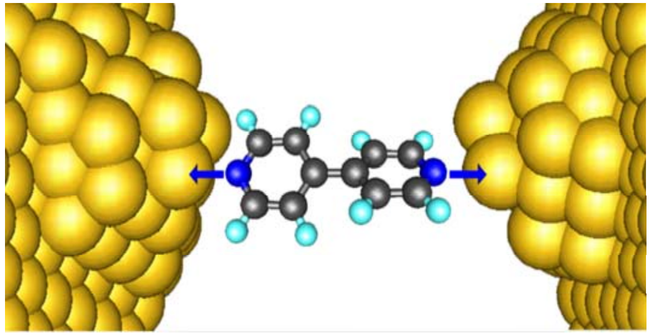
$$\mathbf{J} = -\kappa \nabla T$$

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

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

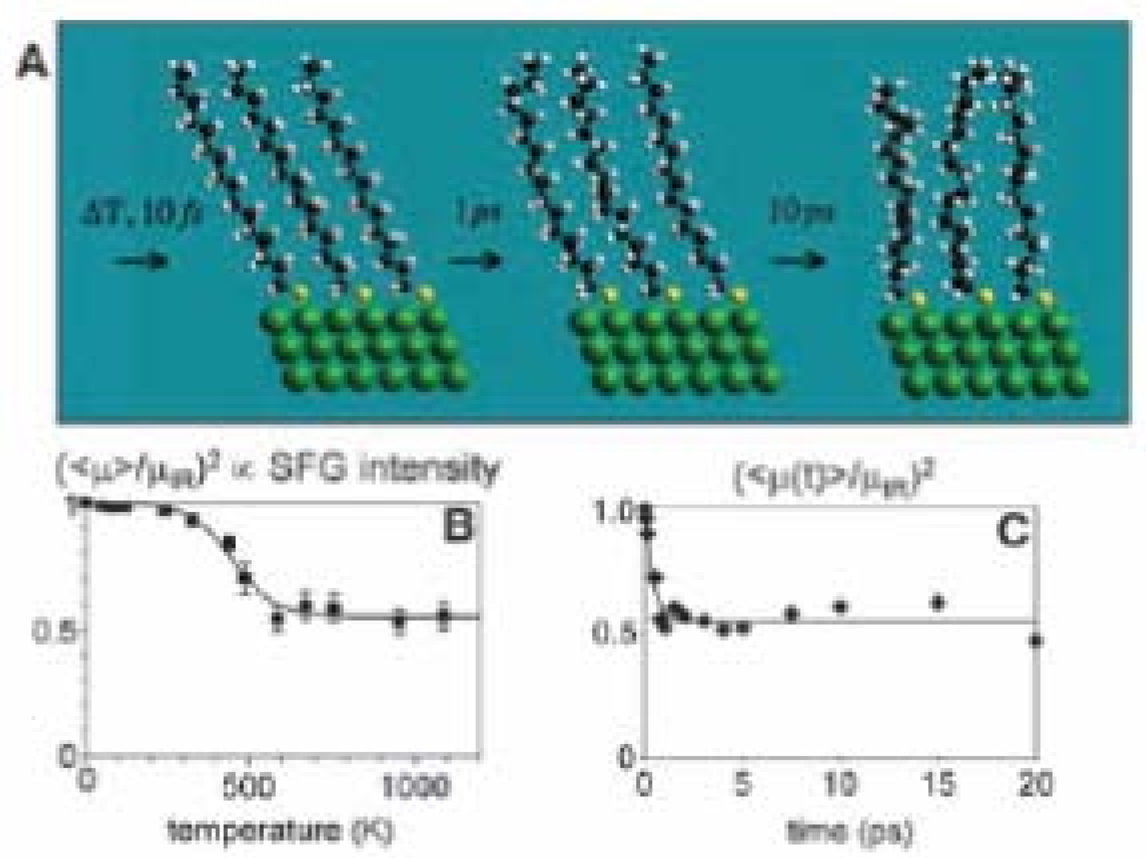
T_L, T_R : temperature of left and right lead

σ : conductance

κ : conductivity

S : cross section area

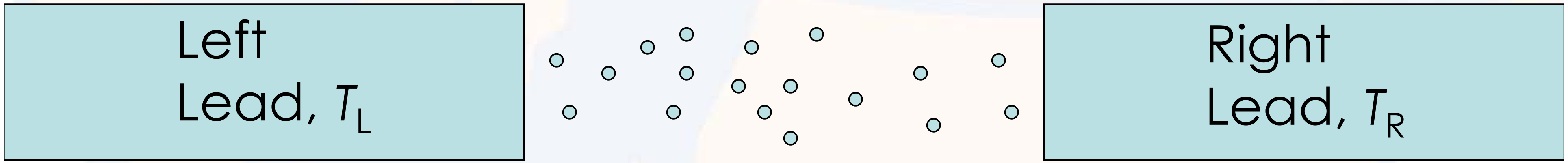
Experimental report of Z Wang et al (2007)



The experimentally measured thermal conductance is 50pW/K for alkane chains at 1000K. From Z Wang et al, Science 317, 787 (2007).

Thermal transport of a junction

Junction



semi-infinite

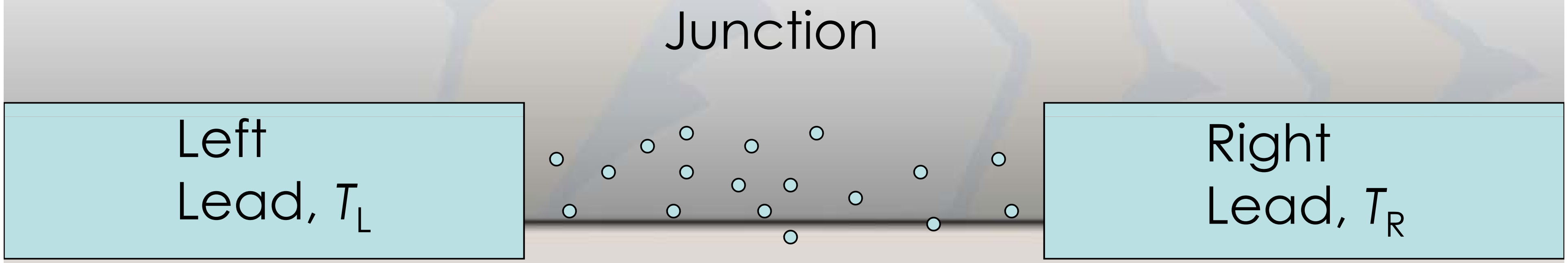
Models

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

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

$$H^{aC} = u_\alpha^T V^{\alpha C} u_C, \qquad u_\alpha = \left(u_j^\alpha\right)$$

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



Force constant matrix

$$
\left[\begin{array}{ccc|c|ccc}
\ddots & k^{L}_{01} & 0 & & & & \\
\ddots & k^{L}_{00} & k^{L}_{01} & V^{LC} & & 0 & \\
0 & k^{L}_{10} & k^{L}_{11} & & & & \\
\hline
 & V^{CL} & & K^{C} & & V^{CR} & \\
\hline
 & & & & k^{R}_{00} & k^{R}_{01} & 0 \\
 & 0 & & V^{RC} & k^{R}_{10} & k^{R}_{11} & k^{R}_{01} \\
 & & & & 0 & k^{R}_{10} & k^{R}_{11}
\end{array}\right]
\qquad K^{R}
$$

Definitions of Green's functions

- Greater/lesser Green's function

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

- 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

$$G^{r}(t,t') = \theta(t-t')\left(G^{>} - G^{<}\right),$$

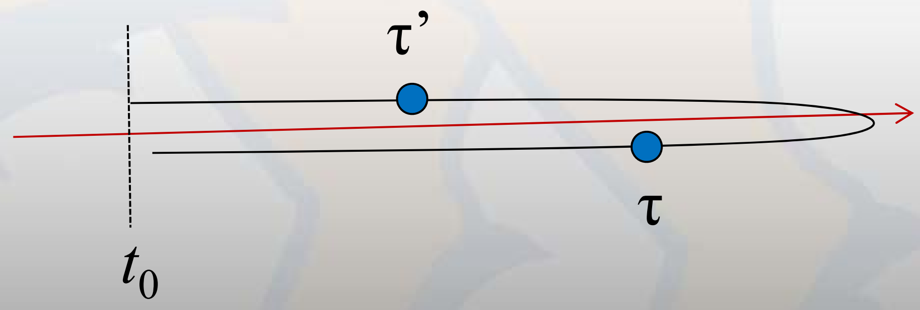
$$G^{a}(t,t') = -\theta(t'-t)\left(G^{>} - G^{<}\right)$$

Contour-ordered Green's function

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

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

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



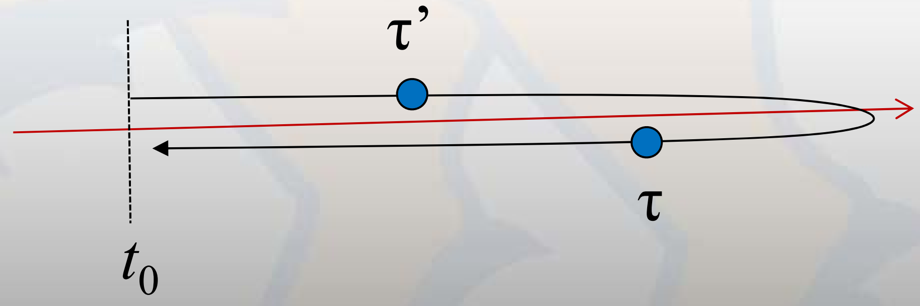
Relation to the real-time Green's functions

$$\tau \to (t,\sigma), \quad \text{or} \quad \tau = t + i\varepsilon\sigma, \quad \sigma = \pm,\ \varepsilon \to 0^{+}$$

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

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

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



Equations for Green's functions

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

$$\downarrow$$

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

$$\downarrow$$

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

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

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

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:

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

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

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

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

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

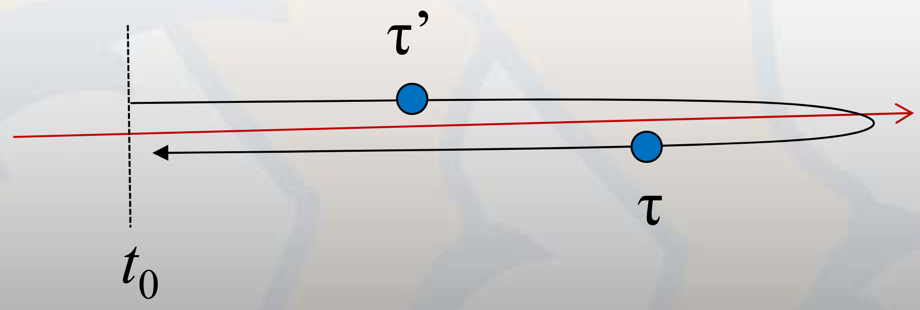
c and *d* can be fixed by initial/boundary condition.

Contour-ordered Green's function

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

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

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



Perturbative expansion of contour ordered Green's function

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

$$= -\frac{i}{\hbar}\left\langle T_C u_j(\tau) u_k(\tau') \left\{ 1 - \frac{i}{\hbar}\int H_n(\tau_1)d\tau_1 + \left(-\frac{i}{\hbar}\right)^2 \int H_n(\tau_1)d\tau_1 \int H_n(\tau_2)d\tau_2 \right\} + \cdots \right\rangle$$

$$= -\frac{i}{\hbar}\left\langle T_C u_j(\tau) u_k(\tau') \right\rangle + \left(-\frac{i}{\hbar}\right)^3 \left\langle T_C u_j(\tau) u_k(\tau') \iiint \frac{1}{3}\sum_{lmn} T_{lmn}(\tau_1,\tau_2,\tau_3) u_l(\tau_1) u_m(\tau_2) u_n(\tau_3) d\tau_1 d\tau_2 d\tau_3 \right.$$

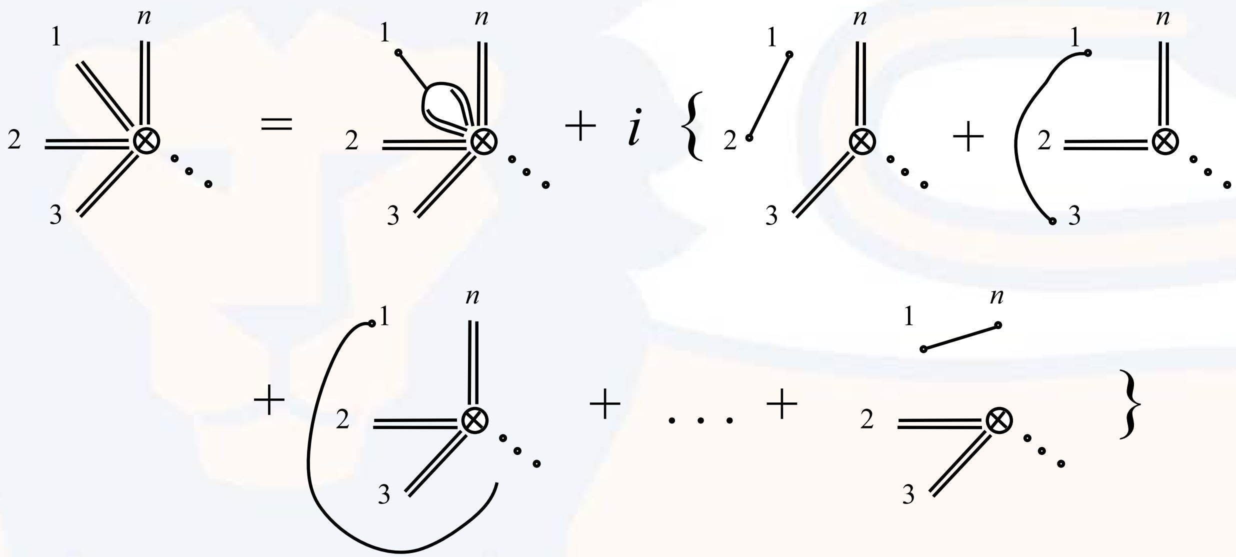
$$\left. \times \iiint \frac{1}{3}\sum_{opq} T_{opq}(\tau_4,\tau_5,\tau_6) u_o(\tau_4) u_p(\tau_5) u_q(\tau_6) d\tau_4 d\tau_5 d\tau_6 \right\rangle$$

$$= G^0_{jk}(\tau,\tau') + \ldots \left\langle T_C u_j(\tau) u_k(\tau') u_l(\tau_1) u_m(\tau_2) u_n(\tau_3) u_o(\tau_4) u_p(\tau_5) u_q(\tau_6) \right\rangle + \cdots$$

$$\downarrow \quad \text{(Wick theorem)}$$

$$\cdots + \cdots \left\langle T_C u_j(\tau) u_l(\tau_1) \right\rangle \left\langle T_C u_m(\tau_2) u_p(\tau_5) \right\rangle \left\langle T_C u_n(\tau_3) u_q(\tau_6) \right\rangle \left\langle T_C u_o(\tau_4) u_k(\tau') \right\rangle + \cdots$$

General expansion rule

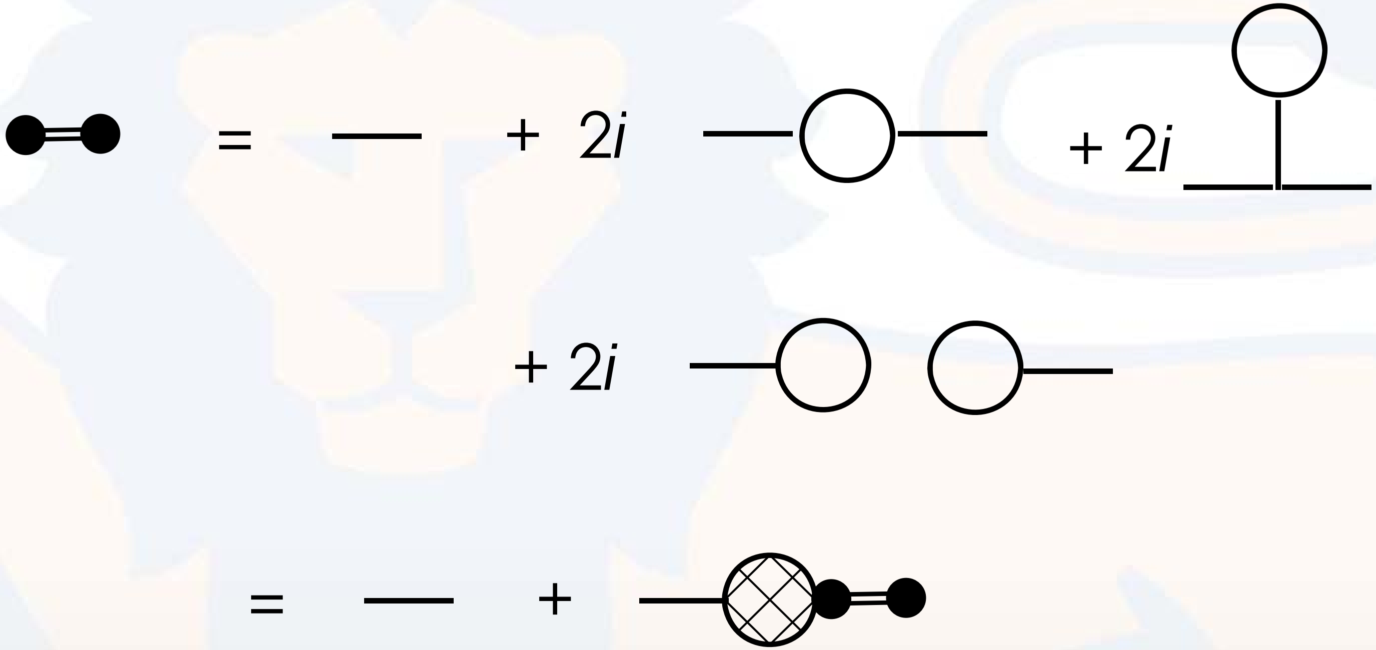


Single line $G_0(\tau, \tau')$

3-line vertex $T_{ijk}(\tau_i, \tau_j, \tau_k)$

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

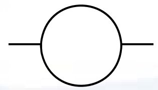
Diagrammatic representation of the expansion



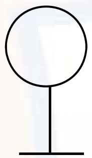
$$G(\tau,\tau') = G_0(\tau,\tau') + \int\int G_0(\tau,\tau_1)\Sigma_n(\tau_1,\tau_2)G(\tau_2,\tau')d\tau_1 d\tau_2$$

Explicit expression for self-energy

$$\Sigma^{\sigma\sigma'}_{n,jk}[\omega] = 2i\sum_{lmrs} T_{jlm}T_{rsk}\int_{-\infty}^{+\infty} G^{\sigma\sigma'}_{0,lr}[\omega']\,G^{\sigma\sigma'}_{0,ms}[\omega-\omega']\frac{d\omega'}{2\pi}$$



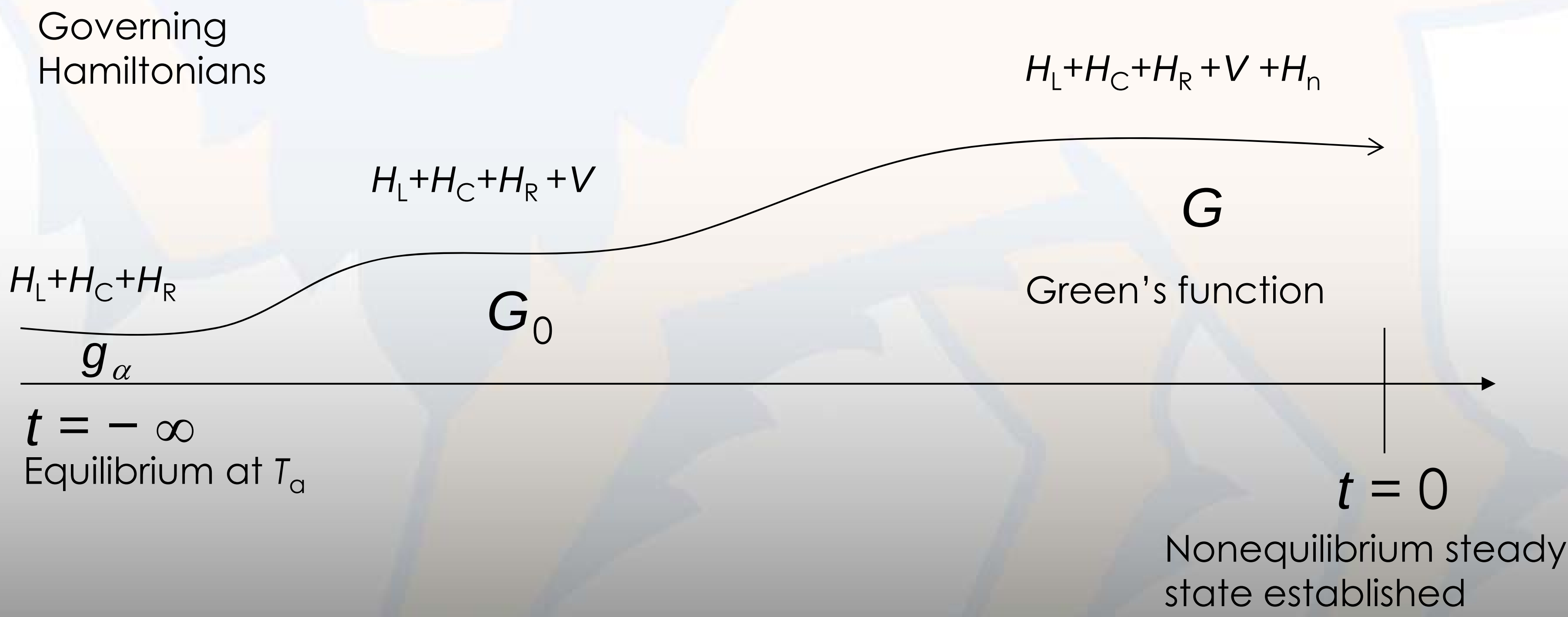
$$+2i\sigma\delta_{\sigma,\sigma'}\sum_{lmrs,\sigma''}\sigma''\, T_{jkl}T_{mrs}\int_{-\infty}^{+\infty} G^{\sigma\sigma''}_{0,lm}[0]\,G^{\sigma''\sigma''}_{0,rs}[\omega']\frac{d\omega'}{2\pi}$$



$$+O(T^{4}_{ijk})$$

Junction system

- 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

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

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

Dyson equations and solutions

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

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

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

$$G_0^< = G_0^r \Sigma^< G_0^a$$

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

$$G^< = G^r \Sigma_n^< G^a + (I + G^r \Sigma_n^r) G_0^< (I + \Sigma_n^a G^a)$$

$$= G^r (\Sigma^< + \Sigma_n^<) G^a$$

Energy current

$$I_L = -\left\langle \frac{dH_L}{dt} \right\rangle = \left\langle \dot{u}_L^T V^{LC} u_C \right\rangle$$

$$= -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{Tr}\left(V^{LC} G_{CL}^{<}[\omega] \right) \hbar \omega \, d\omega$$

$$= -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{Tr}\left(G_{CC}^{r}[\omega] \Sigma_L^{<}[\omega] + G_{CC}^{<}[\omega] \Sigma_L^{a}[\omega] \right) \hbar \omega \, d\omega$$

Caroli formula

$$I_L = -\left\langle \frac{dH_L}{dt} \right\rangle = \frac{1}{2\pi} \int_0^{+\infty} \hbar\omega \mathrm{Tr}\left(G^r_{CC} \Gamma_L G^a_{CC} \Gamma_R \right) \left(f_L - f_R \right) d\omega$$

$$\Gamma_\alpha = i\left(\Sigma^r_\alpha - \Sigma^a_\alpha \right)$$

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

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

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

Ballistic transport in a 1D chain

- Force constants

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

- Equation of motion

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

Solution of *g*

- Surface Green's function

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

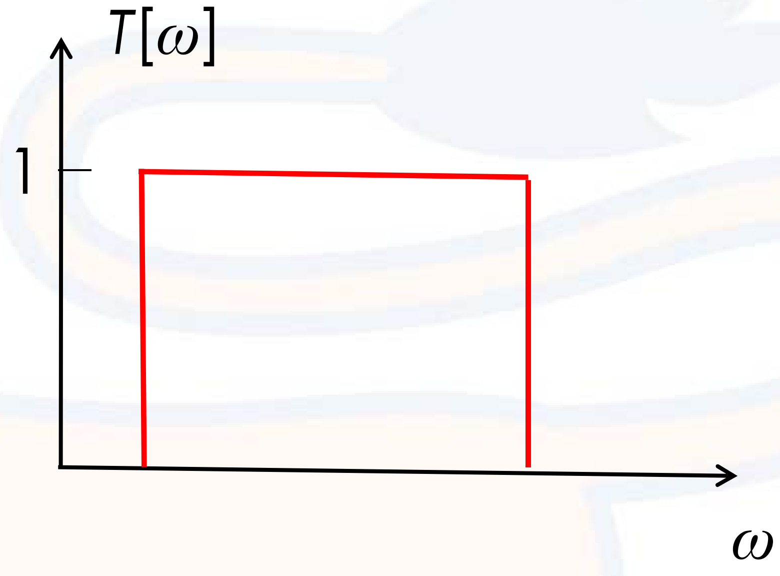
$$K^R = \begin{bmatrix} 2k+k_0 & -k & 0 & \cdots \\ -k & 2k+k_0 & -k & 0 \\ 0 & -k & 2k+k_0 & -k \\ 0 & 0 & -k & \cdots \end{bmatrix}$$

$$g^R_{j0} = -\frac{\lambda^j}{k}, \quad j = 0, 1, 2, \cdots,$$

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

Lead self energy and transmission

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



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

$$G^r_{jk} = \frac{\lambda^{|j-k|}}{k\left(\lambda - \lambda^{-1}\right)}$$

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

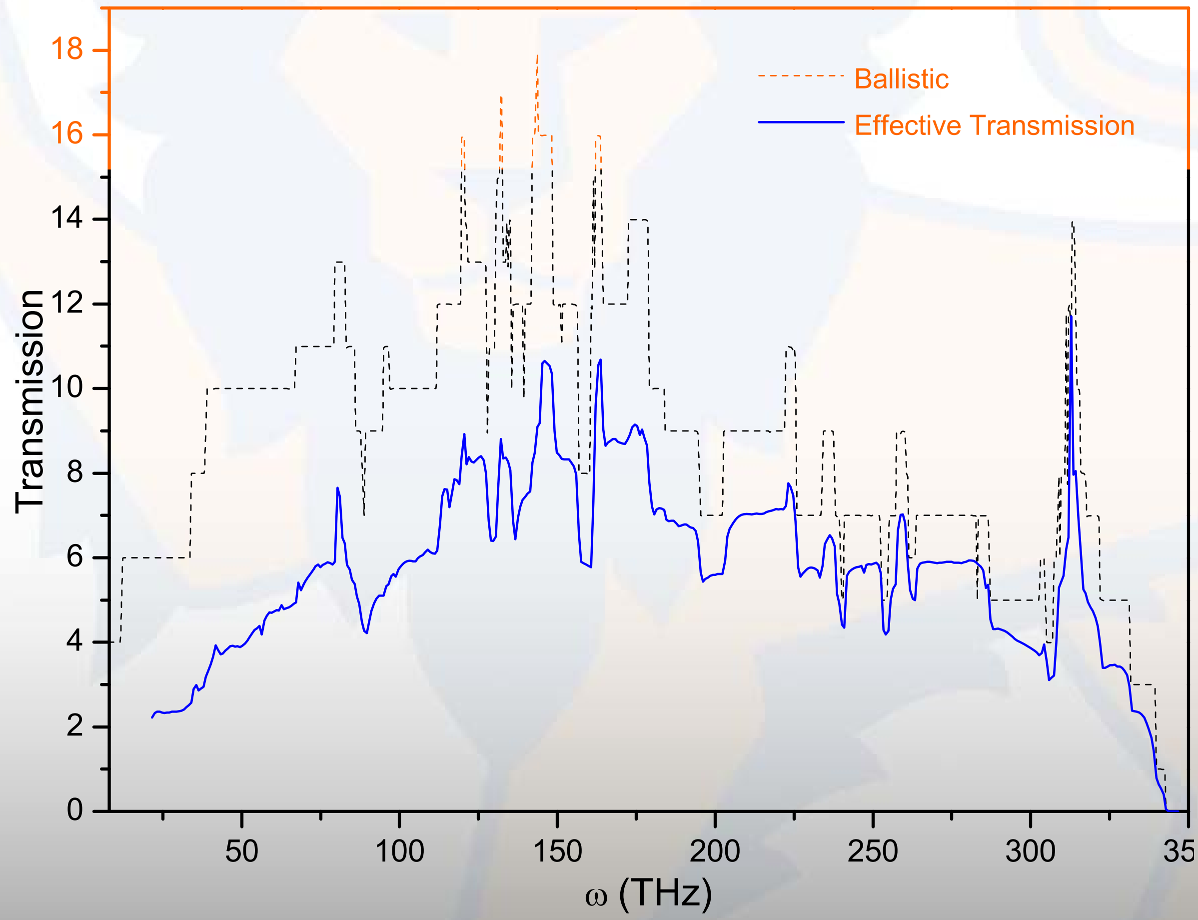
Heat current and conductance, Landauer formula

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

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

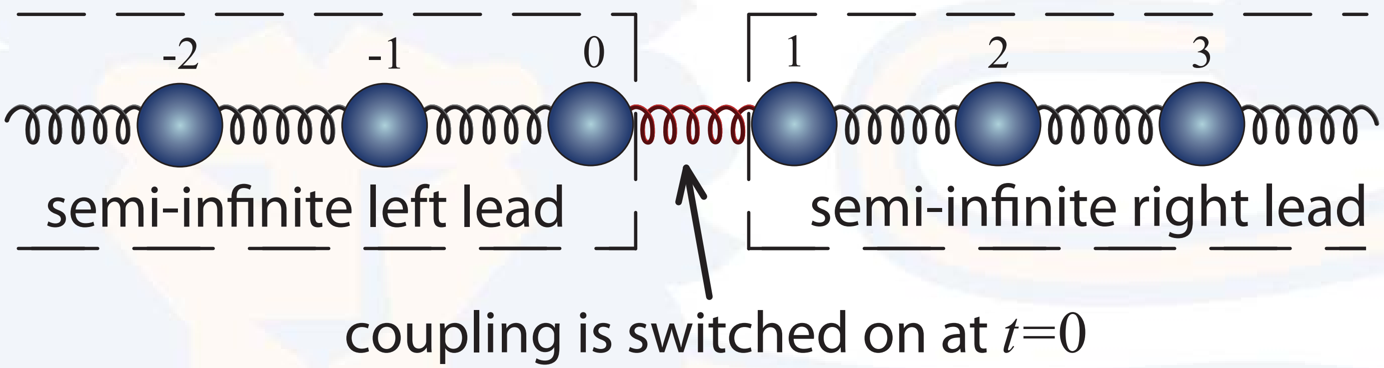
$$\sigma \approx \frac{\pi^2 k_B^2 T}{3h}, \quad T \to 0, k_0 = 0$$

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

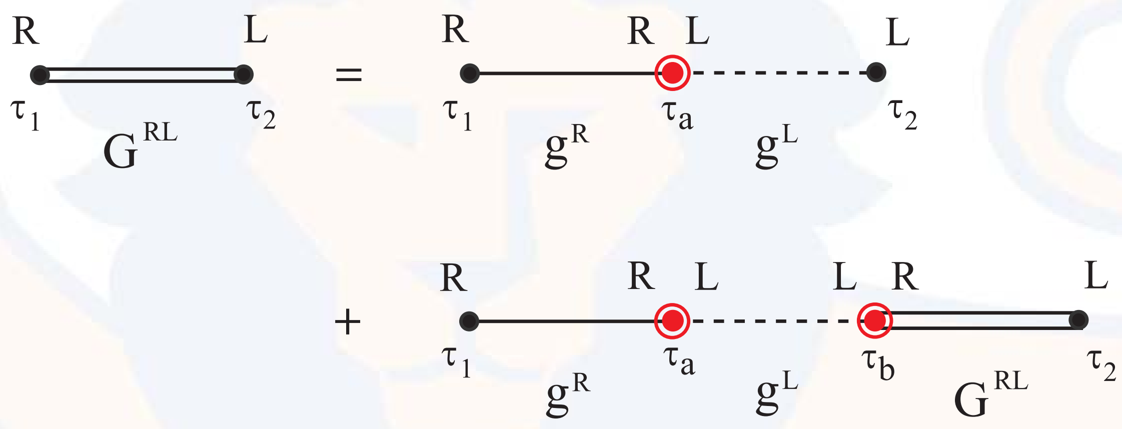


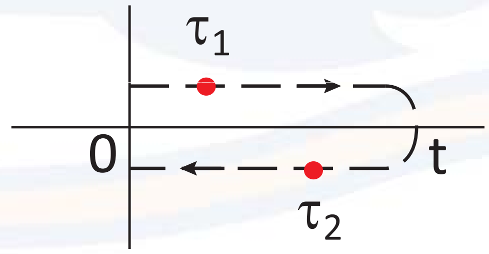
$$H_0 = H_L + H_R$$

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

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

Dyson equation on contour from 0 to *t*



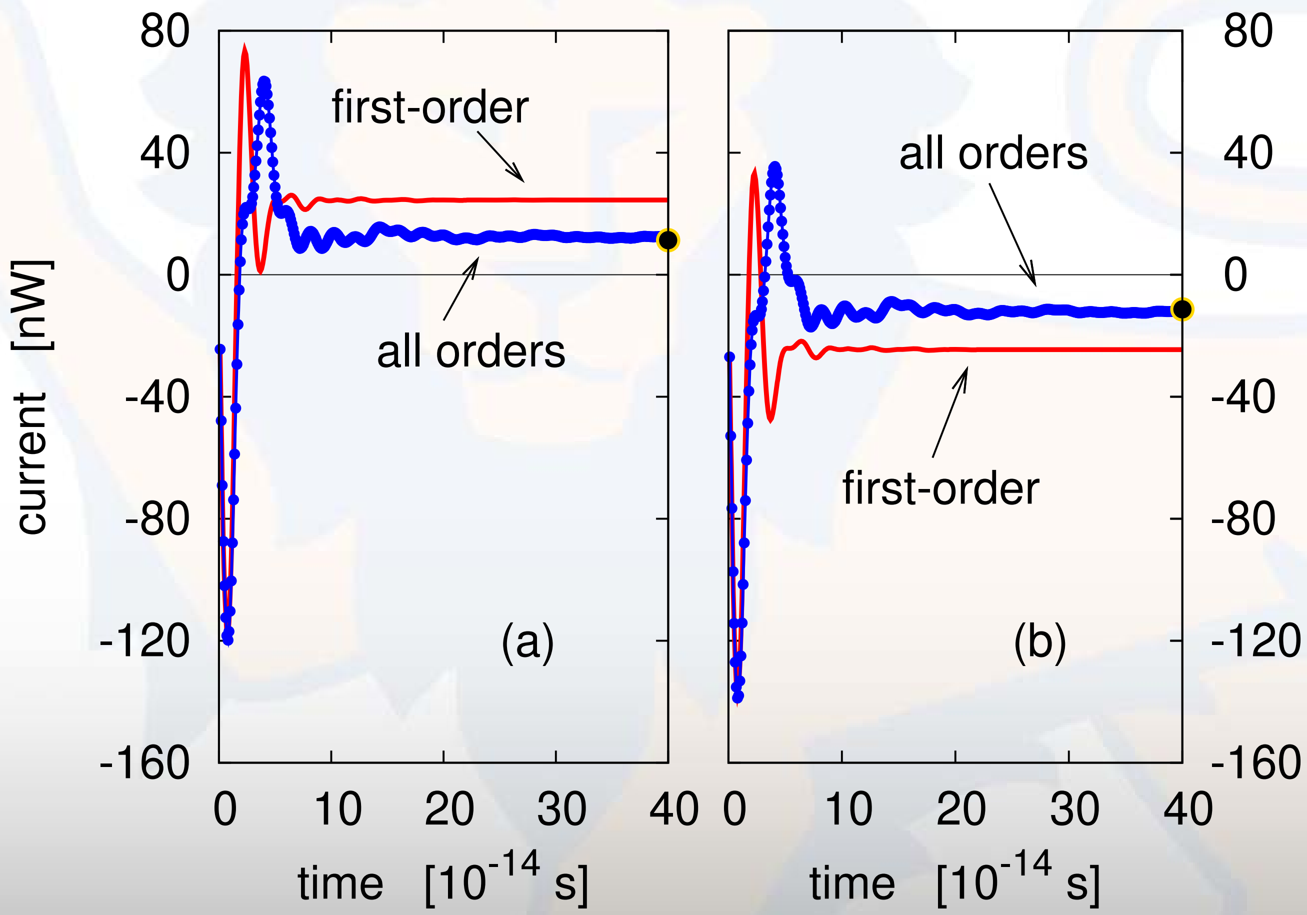


Contour C

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

$$+ \int_C d\tau_1 \int_C d\tau_2 g^R(\tau-\tau_1) V^{RL} g^L(\tau_1-\tau_2) V^{LR} G^{RL}(\tau_{2,}\tau')$$

Transient thermal current



The time-dependent current when the missing spring is suddenly connected. (a) Current flow out of left lead, (b) out of right lead. Dots are what predicted from Landauer formula. T=300K, k =0.625 eV/(Å^{2}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).

Full counting statistics

- 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, arXiv:1111.6182

Definition of generating function based on two-time measurement

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

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

$$P_a^{\,2} = P_a = |a><a|$$

$$H_L |a> = a|a>$$

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

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

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

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

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

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

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

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

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

U_x

$$U_x(t,t') = e^{ixH_L} T e^{-\frac{i}{\hbar}\int_{t'}^{t} H(t)dt} e^{-ixH_L}$$

$$= T e^{-\frac{i}{\hbar}\int_{t'}^{t} H_x(t)dt}, \qquad t \ge t'$$

$$H_x(t) = e^{ixH_L} H(t) e^{-ixH_L}$$

$$= e^{ixH_L}(H_L + H_C + H_R + H^{LC} + H^{RC})e^{-ixH_L}$$

$$= H_L + H_C + H_R + H^{RC} + e^{ixH_L} H^{LC} e^{-ixH_L}$$

$$= H_0 + H^{RC} + (u_x^L)^T V^{LC} u^C = H_0 + H_I^x$$

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

Schrödinger, Heisenberg, and interaction pictures

Schrödinger picture

$$|\Psi(t)>=U(t,t')|\Psi(t')> \qquad \rho=\sum w_i |i><i|$$

$$i\hbar\frac{\partial U(t,t')}{\partial t}=H(t)U(t,t')$$

Heisenberg picture

$$A_H(t)=U(0,t)AU(t,0), \quad |\Psi_H>=|\Psi(0)>$$

$$i\hbar\frac{\partial A_H(t)}{\partial t}=[A_H(t),H_H(t)]$$

Interaction picture

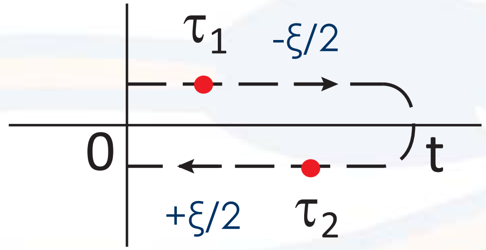
$$H=H_0+H_I$$

$$|\Psi_I(t)>=e^{\frac{i}{\hbar}H_0 t}|\Psi(t)>=S(t,t')|\Psi_I(t')>$$

$$i\hbar\frac{\partial S(t,t')}{\partial t}=H_I(t)S(t,t'), \quad S(t,t')=Te^{-\frac{i}{\hbar}\int_{t'}^{t}H_I(t'')dt''}, t>t'$$

$$A_I(t)=e^{\frac{i}{\hbar}H_0 t}Ae^{-\frac{i}{\hbar}H_0 t}$$

Compute Z in interaction picture



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

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

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

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

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

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

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

Important result

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

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

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

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

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

$$0 \text{ otherwise}$$

Long-time result, Levitov-Lesovik formula

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

$$= -\frac{1}{2}\mathrm{Tr}\left[\ln\left\{1 - \begin{pmatrix} G_0^r & G^K \\ 0 & G_0^a \end{pmatrix}\begin{pmatrix} \frac{a-b}{2} & \frac{a+b}{2} \\ -\frac{a+b}{2} & -\frac{a-b}{2} \end{pmatrix}\right\}\right]$$

$$\approx -t_M \int_{-\infty}^{+\infty} \frac{d\omega}{4\pi} \ln\det\left\{I - G_0^r\Gamma_L G_0^a\Gamma_R\left[(e^{i\xi\hbar\omega}-1)f_L + (e^{-i\xi\hbar\omega}-1)f_R + (e^{i\xi\hbar\omega}+e^{-i\xi\hbar\omega}-2)f_L f_R\right]\right\}$$

where

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

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

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

Arbitray time, transient result

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

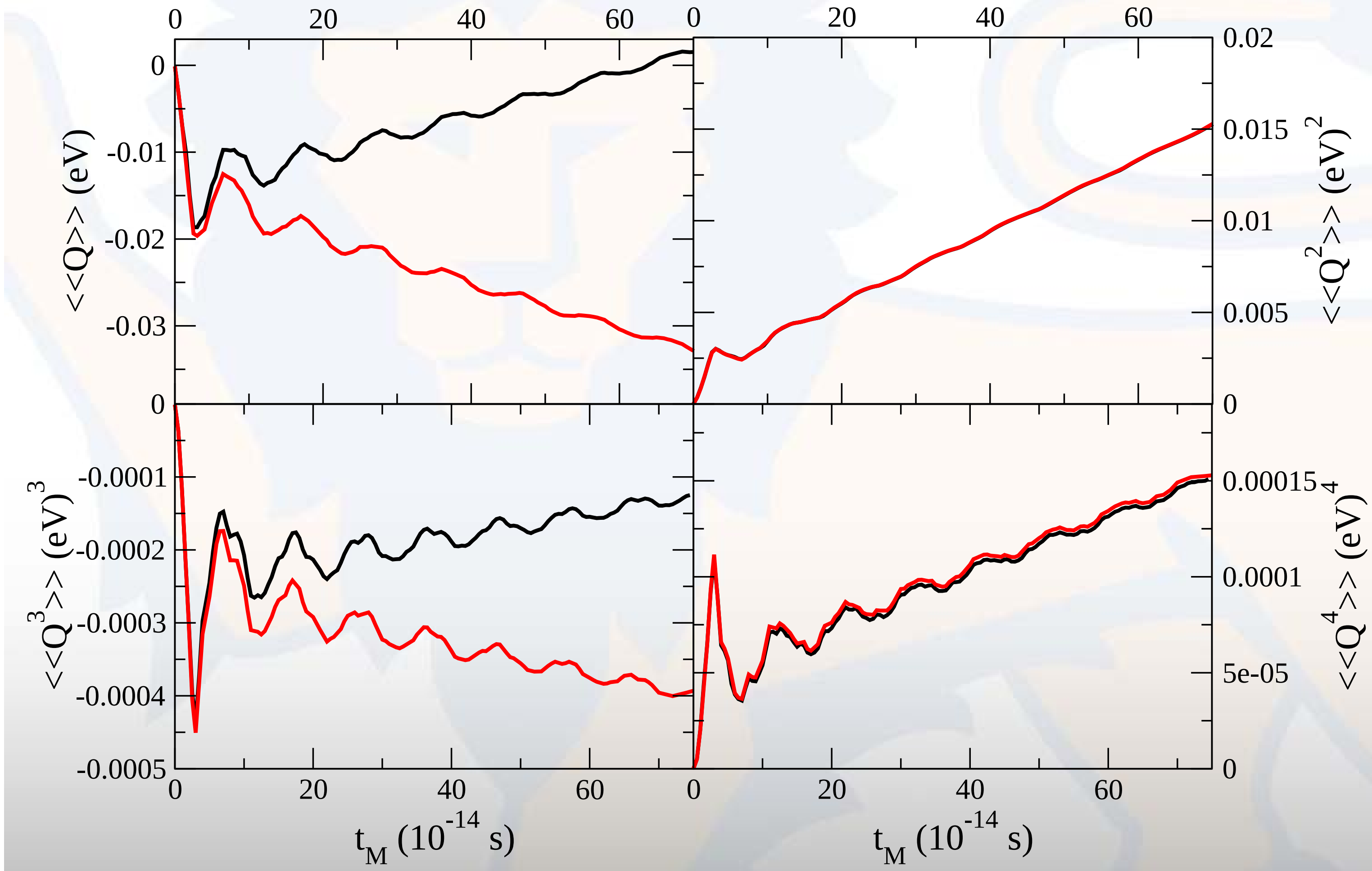
$$\langle\langle Q^n \rangle\rangle = \left.\frac{\partial^n \ln Z}{\partial(i\xi)^n}\right|_{\xi=0}$$

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

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

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

Numerical results, 1D chain



1D chain with a single site as the center. k= 1eV/(uÅ^2), k_0=0.1k, T_L=310K, T_C=300K, T_R=290K. Red line right lead; black, left lead. B. K. Agarwalla, B. Li, and J.-S. Wang, arXiv:1111.6182 .

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

Thank you