KITP, UC Santa Barbara - Emerging regimes and implications of quantum and thermal fluctuational electrodynamics

Nonequilibrium Green's Functions – definition, fluctuation-dissipation theorem, Meir-Wingreen formula, etc

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Outline

- Lecture 0: Electron Green's functions
- Lecture 1: NEGF – brief history, phonons/harmonic oscillator example
- Lecture 2: NEGF "technologies" – equation of motion method, Langreth rules, heat current formula (Meir-Wingreen, Landauer).

References

- J.-S. Wang, J. Wang, and J. T. Lü, "Quantum thermal transport in nanostructures," Eur. Phys. J. B **62**, 381 (2008).

- J.-S. Wang, B. K. Agarwalla, H. Li, and J. Thingna, "Nonequilibrium Green's function method for quantum thermal transport," Front. Phys. **9**, 673 (2014).

- J.-S. Wang, J. Peng, Z.-Q. Zhang, Y.-M. Zhang, and T. Zhu, "Transport in electron-photon systems", manuscript in preparation.

Lecture Zero

Green's function for free electrons

Single electron quantum mechanics

$$i\hbar \frac{d\Psi}{dt} = H\Psi, \quad \Psi(t) = e^{-i\frac{Ht}{\hbar}}\Psi(0)$$

We define the (retarded) Green's function by

$$G^r(t) = -\frac{i}{\hbar}\theta(t)e^{-iHt/\hbar}, \quad \theta(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases}$$

then

$$\Psi(t) = i\hbar G^r(t)\Psi(0), \qquad t > 0$$

Green's function in energy space

Fourier transform to E space

$$\tilde{G}(E) = \int_{-\infty}^{+\infty} G(t) e^{iEt/\hbar - \eta t/\hbar} dt = -\frac{i}{\hbar} \int_{0}^{+\infty} e^{i\frac{E+i\eta-H}{\hbar}} dt$$

$$= \left(E + i\eta - H\right)^{-1}, \quad \eta \to 0^{+}$$

$(z - H)^{-1}$ is called resolvent of the operator H.

Perturbation theory, single electron

$$H = h + V$$

use $A^{-1} = B^{-1} + B^{-1}(B - A)A^{-1}$

Let $\left(G^r\right)^{-1} = A = z - H, \quad \left(g^r\right)^{-1} = B = z - h, \quad z = E + i\eta$

then $G^r = g^r + g^r V G^r$

The last equation is known as the Dyson equation,
equivalent to the Lippmann-Schwinger equation

Annihilation/creation operators

$$\left(c_j\right)^2 = 0, \quad \left(c_j^\dagger\right)^2 = 0, \qquad \leftarrow \text{Pauli exclusion principle}$$

$$\left.\begin{aligned} c_j c_k^\dagger + c_k^\dagger c_j &= \delta_{jk} \\ c_j c_k + c_k c_j &= 0 \\ c_j^\dagger c_k^\dagger + c_k^\dagger c_j^\dagger &= 0 \end{aligned}\right\} \text{defining property of fermion}$$

$$c_j^\dagger \,|\, 0 > = |\, 1_j >$$

Many-electron Hamiltonian and Green's functions

$$\hat{H} = c^{\dagger} H c, \qquad c = \begin{pmatrix} c_1 \\ c_2 \\ \dots \\ \\ c_N \end{pmatrix}$$

Annihilation operator c is a column vector, H is N by N matrix.
$\{A, B\} = AB + BA$

$$G^{r}_{jk}(t,t') = -\frac{i}{\hbar}\theta(t-t')\left\langle \{c_j(t), c_k^{\dagger}(t')\} \right\rangle$$

$$G^{>}_{jk}(t,t') = -\frac{i}{\hbar}\left\langle c_j(t) c_k^{\dagger}(t') \right\rangle$$

Why Green's functions?

- Solutions to differential equations
- Retarded Green's function is related to the linear response theory
- Im G^r gives electron density of states
- Related to (non-equilibrium) physical observables such as the electron or energy current

end of lecture zero

Lecture Two

History, definitions, properties of NEGF

A Brief History of NEGF

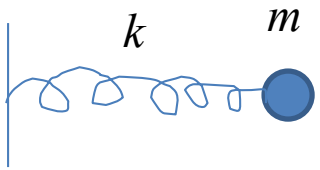
- Schwinger 1961
- Kadanoff and Baym 1962
- Keldysh 1965
- Caroli, Combescot, Nozieres, and Saint-James 1971
- Meir and Wingreen 1992

Equilibrium Green's functions using a harmonic oscillator as an example

- Single mode harmonic oscillator is a very important example to illustrate the concept of Green's functions as any phononic system (vibrational degrees of freedom in a collection of atoms) and photonic system at ballistic (linear) level can be thought of as a collection of independent oscillators in eigenmodes. Equilibrium means that system is distributed according to the Gibbs canonical distribution.

Harmonic Oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2, \quad u = x\sqrt{m}$$



$$H = \frac{1}{2}\dot{u}^2 + \frac{1}{2}\Omega^2 u^2 = \hbar\Omega\left(a^\dagger a + \frac{1}{2}\right), \qquad \Omega = \sqrt{\frac{k}{m}}$$

$$u = \sqrt{\frac{\hbar}{2\Omega}}\left(a + a^\dagger\right), \qquad [x, p] = i\hbar, \quad [a, a^\dagger] = 1$$

Eigenstates, Quantum Mech/Stat Mech

$$H|n\rangle = E_n|n\rangle, \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\Omega, \quad n = 0,1,2,\cdots$$

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$\rho = \frac{e^{-\beta H}}{\mathrm{Tr}\left(e^{-\beta H}\right)}, \qquad \beta = \frac{1}{k_B T}$$

$$\langle aa\rangle = \langle a^\dagger a^\dagger\rangle = 0, \quad \langle a^\dagger a\rangle = \langle aa^\dagger\rangle - 1 = N$$

$$\langle\cdots\rangle = \mathrm{Tr}(\rho\cdots), \qquad N = \frac{1}{e^{\beta\hbar\Omega} - 1}$$

Heisenberg Operator/Equation

$$O(t) = e^{i\frac{Ht}{\hbar}} O e^{-i\frac{Ht}{\hbar}}$$

$$\frac{dO(t)}{dt} = \frac{1}{i\hbar}[O(t), H]$$

O: Schrödinger operator
$O(t)$: Heisenberg operator

$$\frac{da(t)}{dt} = \frac{1}{i\hbar}[a(t), H] = \frac{1}{i\hbar}[a(t), \hbar\Omega(a^\dagger(t)a(t) + \frac{1}{2})]$$

$$= -i\Omega\, a(t)$$

$$a(t) = ae^{-i\Omega t}, \quad a^\dagger(t) = a^\dagger e^{+i\Omega t}$$

Defining >, <, t, $\bar{t}$ Green's Functions

$$g^{>}(t,t') = -\frac{i}{\hbar}\langle u(t)u(t')\rangle, \qquad i = \sqrt{-1}$$

$$u(t) = \sqrt{\frac{\hbar}{2\Omega}}\left(a(t) + a^{\dagger}(t)\right), \qquad a(t) = a\,e^{-i\Omega t}$$

$$g^{>}(t,t') = -\frac{i}{2\Omega}\left[Ne^{i\Omega(t-t')} + (1+N)e^{-i\Omega(t-t')}\right]$$

$$g^{<}(t,t') = -\frac{i}{\hbar}\langle u(t')u(t)\rangle = g^{>}(t',t)$$

$$g^{t}(t,t') = -\frac{i}{\hbar}\langle Tu(t)u(t')\rangle = \theta(t-t')g^{>}(t,t') + \theta(t'-t)g^{<}(t,t')$$

$$g^{\bar{t}}(t,t') = -\frac{i}{\hbar}\langle \bar{T}u(t)u(t')\rangle = \theta(t'-t)g^{>}(t,t') + \theta(t-t')g^{<}(t,t')$$

$$\theta(t) = \begin{cases} 1, & \text{if } t > 0 \\ \frac{1}{2}, & \text{if } t = 0 \\ 0, & \text{if } t < 0 \end{cases}$$

T: time order

$\bar{T}$: anti-time order

Retarded and Advanced Green's functions

$$g^r(t,t') = -\frac{i}{\hbar}\theta(t-t')\langle[u(t),u(t')]\rangle$$

$$= -\theta(t-t')\frac{\sin\Omega(t-t')}{\Omega},$$

$$g^a(t,t') = \frac{i}{\hbar}\theta(t'-t)\langle[u(t),u(t')]\rangle = g^r(t',t)$$

$$\ddot{g}^r(t) + \Omega^2 g^r(t) = -\delta(t), \qquad \text{with } g^r(t) = 0 \text{ for } t < 0$$

Fourier Transform

$$\int_{-\infty}^{+\infty} \qquad \int_{-\infty}^{+\infty} \qquad \frac{d\omega}{2\pi}$$

$$g^r[\omega] = -\int_{-\infty}^{+\infty} \theta(t) \frac{\sin(\Omega t)}{\Omega} e^{i\omega t - \eta t} dt$$

$$= \frac{1}{(\omega + i\eta)^2 - \Omega^2}, \quad \eta \to 0^+$$

$$g^a[\omega] = g^r[\omega]^*, \qquad N = \frac{1}{e^{\beta\hbar\Omega} - 1}$$

$$g^<[\omega] = -\frac{i\pi}{\Omega}\left[N\delta(\omega - \Omega) + (1 + N)\delta(\omega + \Omega)\right]$$

Plemelj formula, fluctuation-dissipation, Kubo-Martin-Schwinger condition

P for Cauchy principle value

$$\frac{1}{x+i\eta} = P\frac{1}{x} - i\pi\delta(x)$$

$$g^{<}[\omega] = \left(g^{r}[\omega] - g^{a}[\omega]\right)N(\omega)$$

$$g^{>}[\omega] = e^{\beta\hbar\omega} g^{<}[\omega],$$

$$g^{<}(t) = g^{<}(-t + i\beta\hbar)$$

Valid only in thermal equilibrium

Matsubara Green's Function

$$g^M(\tau,\tau') = -\frac{1}{\hbar}\left\langle T_\tau \tilde{u}(\tau)\tilde{u}(\tau')\right\rangle$$

$$= -\frac{1}{2\Omega}\left[Ne^{\Omega(\tau-\tau')} + (1+N)e^{-\Omega(\tau-\tau')}\right]$$

where $0 \le \tau,\tau' \le \beta\hbar,\ \tilde{u}(\tau) = u(-i\tau) = e^{\frac{H\tau}{\hbar}} u e^{-\frac{H\tau}{\hbar}}$

$$g^M(\tau) = g^M(\tau+\beta\hbar)$$

$$\breve{g}^M[i\omega_n] = \int_0^{\beta\hbar} g^M(\tau)e^{i\omega_n\tau}d\tau, \quad \omega_n = \frac{2\pi n}{\beta\hbar}, \quad n = \cdots,-1,0,1,2,\cdots$$

$$g^r[\omega] = \breve{g}^M[i\omega_n \to \omega + i\eta]$$

Nonequilibrium Green's Functions

- By "nonequilibrium", we mean, either the Hamiltonian is explicitly time-dependent after t_0, or the initial density matrix ρ is not a canonical distribution.

- We'll show how to build nonequilibrium Green's function from the equilibrium ones through product initial state or through the Dyson equation.

Definitions of General Green's functions (phonon/displacement)

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

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

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

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

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

Relations among Green's functions

$$G^r - G^a = G^> - G^< = -iA$$

$$G^t + G^{\bar{t}} = G^> + G^< = G^K, \qquad G^r = G^t - G^<$$

$$G^t - G^{\bar{t}} = G^r + G^a, \qquad G^a = G^< - G^{\bar{t}}$$

$$G^>_{jk}(t,t') = G^<_{kj}(t',t)$$

$$G^r_{jk}(t,t') = G^a_{kj}(t',t)$$

Steady state, Fourier transform

$$G(t,t') = G(t-t'),$$

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

$$G^r[\omega]^\dagger = G^a[\omega]$$

Equilibrium Green's Function, Lehmann Representation

$$H\,|\,n> = E_n\,|\,n>, \qquad \rho = \frac{e^{-\beta H}}{Z}, \quad Z = \sum_n e^{-\beta E_n}$$

$$u_j(t) = e^{i\frac{Ht}{\hbar}} u_j e^{-i\frac{Ht}{\hbar}}, \qquad \sum_m |\,m><m\,| = 1$$

$$G^{>}_{jk}(t) = -\frac{i}{\hbar}\mathrm{Tr}\left[\rho u_j(t) u_k(0)\right]$$

$$= -\frac{i}{\hbar}\sum_n e^{-\beta E_n} <n\,|\,u_j(t) u_k(0)\,|\,n> \frac{1}{Z}$$

$$= -\frac{i}{\hbar}\sum_{n,m} e^{-\beta E_n + i\frac{(E_n - E_m)t}{\hbar}} <n\,|\,u_j\,|\,m><m\,|\,u_k\,|\,n> \frac{1}{Z}$$

Fluctuation-Dissipation Theorem (Callen-Welton 1951)

$$G^{<}(\omega) = N(\omega)\big(G^{r}(\omega) - G^{a}(\omega)\big)$$

$$G^{>}(\omega) = (1 + N(\omega))\big(G^{r}(\omega) - G^{a}(\omega)\big)$$

Fluctuations: $< uu >$
Linear response: $u = -G^{r} f$, f is force
Dissipation: $-\omega$ Im $G^{r}\, f^{2}$

Pictures in Quantum Mechanics

- Schrödinger picture: O, $\Psi(t) = U(t,t_0)\Psi(t_0)$

- Heisenberg picture: $O(t) = U(t_0,t)OU(t,t_0)$, ρ_0, where the evolution operator U satisfies

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

$$U(t,t') = Te^{-\frac{i}{\hbar}\int_{t'}^{t} H_{t''}dt''}, \qquad t > t'$$

See, e.g., Fetter & Walecka, "Quantum Theory of Many-Particle Systems."

Calculating correlation

$$\langle A(t)B(t')\rangle = \mathrm{Tr}\left[\rho A(t)B(t')\right] \qquad t > t'$$

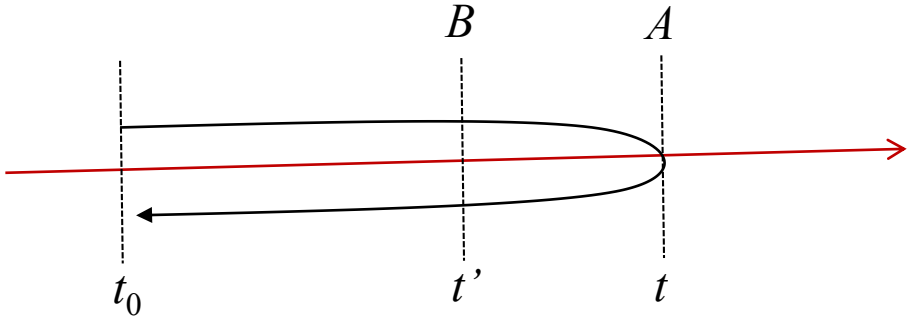
$$= \mathrm{Tr}\left[\rho(t_0)U(t_0,t)AU(t,t_0)U(t_0,t')BU(t',t_0)\right]$$

$$= \mathrm{Tr}\left[\rho(t_0)U(t_0,t)AU(t,t')BU(t',t_0)\right]$$

$$= \mathrm{Tr}\left[\rho(t_0)T_C e^{-\frac{i}{\hbar}\int_C H_\tau d\tau} A_t B_{t'}\right],$$

$$U(t,t') = Te^{-\frac{i}{\hbar}\int_{t'}^{t} H_{t''}dt''},$$

$$U(t,t')U(t',t'') = U(t,t'')$$



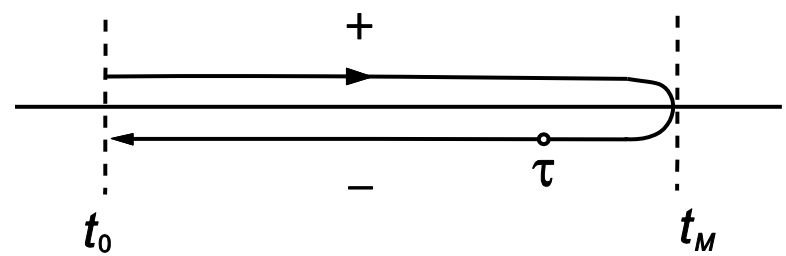
Evolution Operator on Contour

$$U(\tau_2,\tau_1) = T_c \exp\left(-\frac{i}{\hbar}\int_{\tau_1}^{\tau_2} H_\tau d\tau\right), \qquad \tau_2 \succ \tau_1$$

$$U(\tau_3,\tau_2)U(\tau_2,\tau_1) = U(\tau_3,\tau_1), \qquad \tau_3 \succ \tau_2 \succ \tau_1$$

$$U(\tau_1,\tau_2) = U(\tau_2,\tau_1)^{-1}, \qquad \tau_1 \prec \tau_2$$

$$O(\tau) = U(t_0^+,\tau)OU(\tau,t_0^+)$$



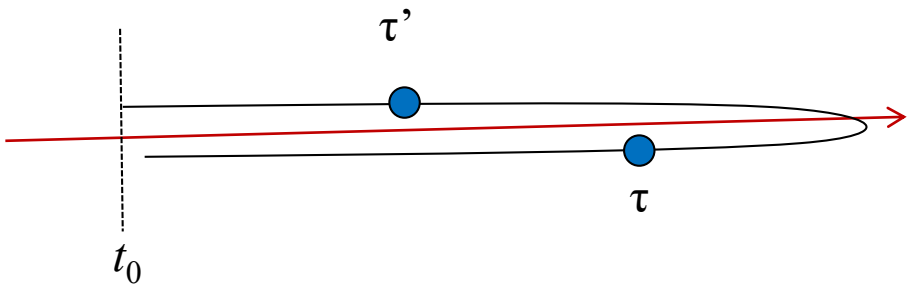
Keldysh contour

Contour-ordered Green's function

$$G(\tau,\tau') = -\frac{i}{\hbar}\left\langle T_C u(\tau) u(\tau')^T \right\rangle$$

$$= \mathrm{Tr}\left[\rho(t_0) T_C u_\tau u_{\tau'}{}^T e^{-\frac{i}{\hbar}\int_C H_\tau d\tau} \right]$$

Contour order: the operators earlier on the contour are to the right. See, e.g., H. Haug & A.-P. Jauho.



Relation to real-time Green's functions

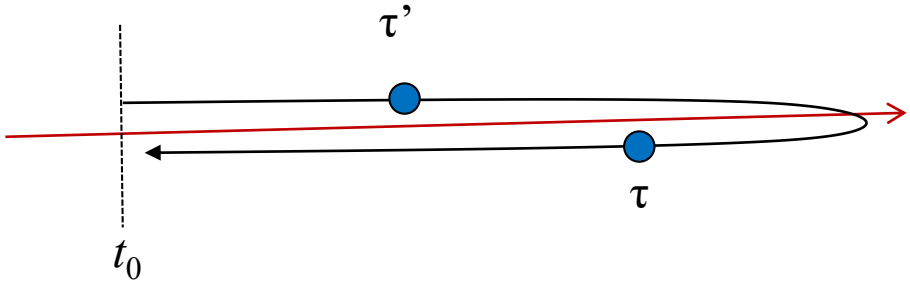
$$\tau \to (t,\sigma), \quad \text{or} \quad \tau = t^{\sigma}, \quad \sigma = \pm$$

$$G(\tau,\tau') \to G^{\sigma\sigma'}(t,t') \quad \text{or} \quad G = \begin{bmatrix} G^{t} & G^{<} \\ G^{>} & G^{\bar{t}} \end{bmatrix}$$

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

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

$$G^{r} = G^{t} - G^{<}$$



end of lecture two

Lecture three

Calculus on contour, equation of motion method, current, etc

Equation of Motion Method

- The advantage of equation of motion method is that we don't need to know or pay attention to the distribution (density operator) ρ. The equations can be derived quickly.
- The disadvantage is that we have a hard time justified the initial/boundary condition in solving the equations.

- *Diagrammatic expansion (initial product states satisfy Wick's theorem)*

Heisenberg Equation on Contour

$$U(\tau_2,\tau_1) = T_c \exp\left(-\frac{i}{\hbar}\int_{\tau_1}^{\tau_2} H_\tau d\tau\right), \qquad \tau_2 \succ \tau_1$$

$$O(\tau) = U(t_0^+,\tau) O U(\tau, t_0^+)$$

$$i\hbar \frac{dO(\tau)}{d\tau} = [O(\tau), H]$$

Express contour order using theta function

$$G(\tau,\tau') = -\frac{i}{\hbar}\left\langle T_C u(\tau) u(\tau')^T \right\rangle$$

$$= \left(-\frac{i}{\hbar}\right)\left\langle u(\tau) u(\tau')^T \right\rangle \theta(\tau,\tau') + \left(-\frac{i}{\hbar}\right)\left\langle u(\tau') u(\tau)^T \right\rangle^T \theta(\tau',\tau)$$

Operator $A(\tau)$ is the same as $A(t)$ as far as commutation relation or effect on wavefunction is concerned

$$[u(\tau), \dot{u}(\tau)^T] = i\hbar I$$

Equation of motion for contour ordered Green's function

$$\frac{\partial}{\partial\tau}G(\tau,\tau') = \left(-\frac{i}{\hbar}\right)\left\langle \dot{u}(\tau)u(\tau')^T\right\rangle\theta(\tau,\tau') + \left(-\frac{i}{\hbar}\right)\left\langle u(\tau')\dot{u}(\tau)^T\right\rangle^T\theta(\tau',\tau)$$

$$+\left(-\frac{i}{\hbar}\right)\left\langle u(\tau)u(\tau')^T\right\rangle\delta(\tau,\tau') + \left(-\frac{i}{\hbar}\right)\left\langle u(\tau')u(\tau)^T\right\rangle^T\left(-\delta(\tau',\tau)\right)$$

$$=\left(-\frac{i}{\hbar}\right)\left\langle T_C\dot{u}(\tau)u(\tau')^T\right\rangle$$

$$\frac{\partial^2}{\partial\tau^2}G(\tau,\tau') = \left(-\frac{i}{\hbar}\right)\left\langle \ddot{u}(\tau)u(\tau')^T\right\rangle\theta(\tau,\tau')$$

$$+\left(-\frac{i}{\hbar}\right)\left\langle \dot{u}(\tau)u(\tau')^T\right\rangle\delta(\tau,\tau') + \left(-\frac{i}{\hbar}\right)\left\langle u(\tau')\dot{u}(\tau)^T\right\rangle^T\left(-\delta(\tau',\tau)\right)$$

$$=\left(-\frac{i}{\hbar}\right)\left\langle T_C\ddot{u}(\tau)u(\tau')^T\right\rangle + \left(-\frac{i}{\hbar}\right)\left\langle [\dot{u}(\tau),u(\tau')^T]\right\rangle\delta(\tau,\tau')$$

$$=\left(-\frac{i}{\hbar}\right)\left\langle T_C(-Ku(\tau)u(\tau')^T)\right\rangle - \delta(\tau,\tau')I$$

$$=-KG(\tau,\tau') - \delta(\tau,\tau')I$$

Equations for Green's functions

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

$$\downarrow$$

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

$$\downarrow$$

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

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

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

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:

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

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

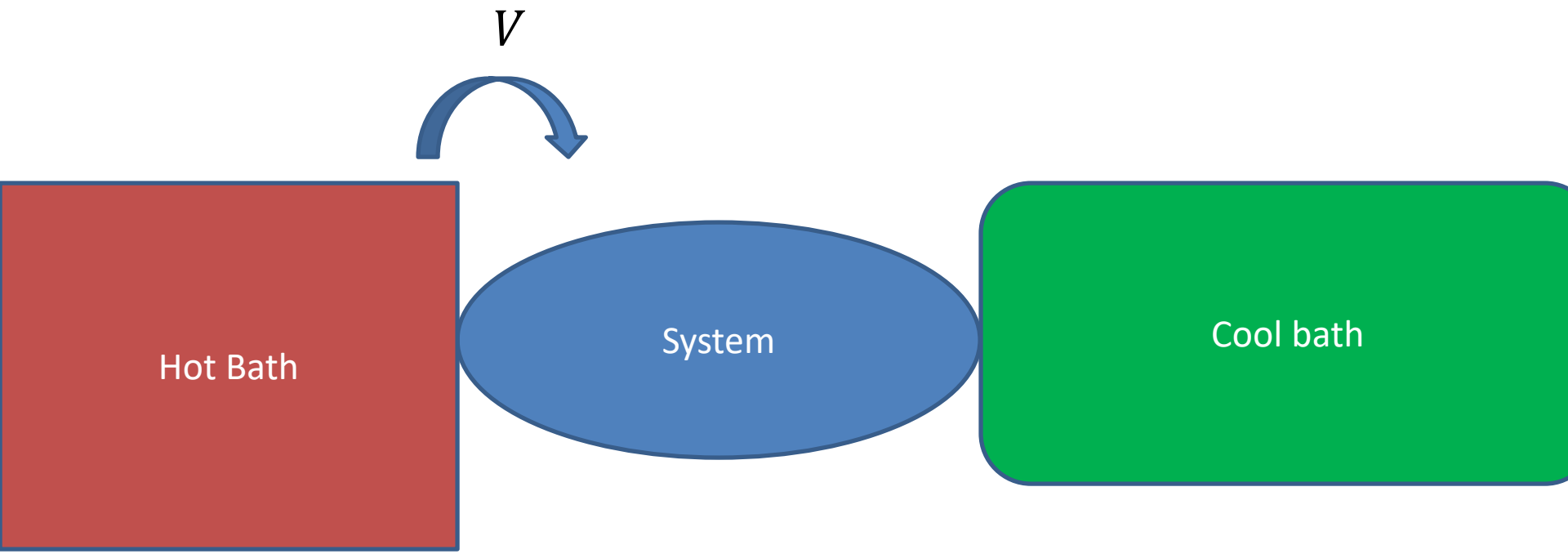
$$G^r[\omega] = G^a[\omega]^+ = \left((\omega + i\eta)^2 I - K\right)^{-1}, \quad \eta \to 0^+$$

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

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

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

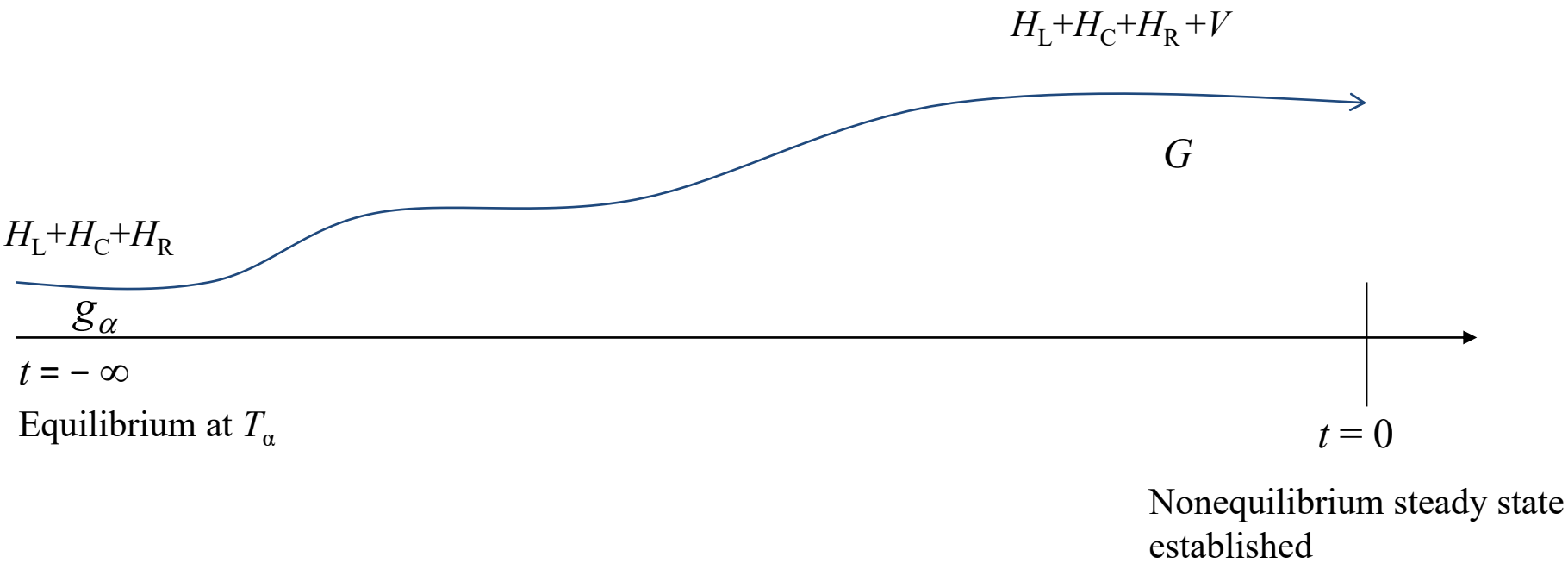
Junction system



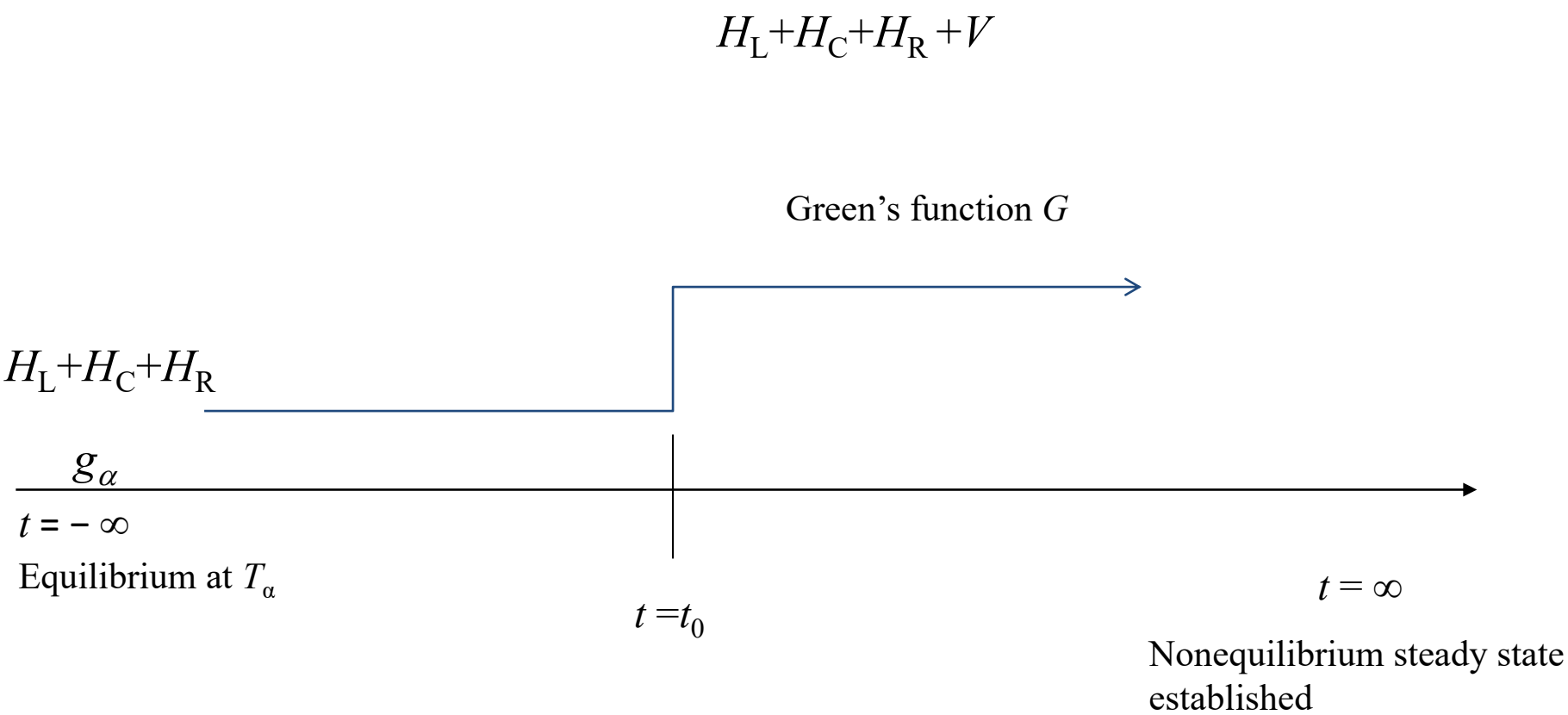
Key point: reducing from an infinite size problem to finite degrees of the center through self-energy.

Junction system, adiabatic switch-on

- g_α for isolated systems where leads and centre are decoupled
- G for coupled ballistic nonequilibrium system



Sudden Switch-on



Three regions

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

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

Heisenberg equations of motion in three regions

$$H = H_L + H_C + H_R + u_L^T V^{LC} u_C + u_R^T V^{RC} u_C + H_n,$$

$$H_\alpha = \frac{1}{2}\dot{u}_\alpha^T \dot{u}_\alpha + \frac{1}{2} u_\alpha^T K^\alpha u_\alpha,$$

$$\ddot{u}_C = \frac{1}{i\hbar}\left[\frac{1}{i\hbar}[u_C, H], H\right] = -K^C u_C - V^{CL} u_L - V^{CR} u_R + \cancel{\frac{1}{i\hbar}[\dot{u}_C, H_n]},$$

$$\ddot{u}_\alpha = -K^\alpha u_\alpha - V^{\alpha C} u_C, \qquad \alpha = L, R$$

Force Constant Matrix

$$K = \begin{pmatrix} K^L & V^{LC} & 0 \\ V^{CL} & K^C & V^{CR} \\ 0 & V^{RC} & K^R \end{pmatrix},$$

$$H = \frac{1}{2} p^T p + \frac{1}{2} \begin{pmatrix} u_L^T & u_C^T & u_R^T \end{pmatrix} K \begin{pmatrix} u_L \\ u_C \\ u_R \end{pmatrix}$$

$$p = \dot{u} = \begin{pmatrix} \dot{u}_L \\ \dot{u}_C \\ \dot{u}_R \end{pmatrix}$$

Relation between g and G

Equation of motion for G_{LC}

$$G_{LC}(\tau,\tau') = -\frac{i}{\hbar}\left\langle T_C u_L(\tau) u_C(\tau')^T \right\rangle,$$

$$\frac{\partial^2}{\partial\tau^2} G_{LC}(\tau,\tau') = -\frac{i}{\hbar}\left\langle T_C \ddot{u}_L(\tau) u_C(\tau')^T \right\rangle$$

$$= -K^L G_{LC}(\tau,\tau') - V^{LC} G_{CC}(\tau,\tau'),$$

$$G_{LC}(\tau,\tau') = \int g_L(\tau,\tau'') V^{LC} G_{CC}(\tau'',\tau')\, d\tau'',$$

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

Dyson equation for G_{CC}

$$G_{CC}(\tau,\tau') = -\frac{i}{\hbar}\left\langle T_C u_C(\tau) u_C(\tau')^T \right\rangle,$$

$$\frac{\partial^2}{\partial\tau^2} G_{CC}(\tau,\tau') = -\frac{i}{\hbar}\left\langle T_C \ddot{u}_C(\tau) u_C(\tau')^T \right\rangle - I\delta(\tau,\tau')$$

$$= -K^C G_{CC}(\tau,\tau') - V^{CL} G_{LC}(\tau,\tau') - V^{CR} G_{RC}(\tau,\tau') - I\delta(\tau,\tau')$$

$$= -K^C G_{CC}(\tau,\tau') - \int V^{CL} g_L(\tau,\tau'') V^{LC} G_{CC}(\tau'',\tau')\, d\tau''$$

$$- \int V^{CR} g_R(\tau,\tau'') V^{RC} G_{CC}(\tau'',\tau')\, d\tau'' - I\delta(\tau,\tau'),$$

$$G_{CC}(\tau,\tau') = g_C(\tau,\tau') + \iint g_C(\tau,\tau_1)\Sigma(\tau_1,\tau_2) G_{CC}(\tau_2,\tau') d\tau_1 d\tau_2,$$

$$\Sigma(\tau,\tau') = V^{CL} g_L(\tau,\tau') V^{LC} + V^{CR} g_R(\tau,\tau') V^{RC}$$

The Langreth theorem

$$C(\tau,\tau') = \int A(\tau,\tau'')B(\tau'',\tau')\,d\tau'' \rightarrow \sum_{\sigma''=\pm}\int_{-\infty}^{+\infty} A^{\sigma\sigma''}(t,t'')B^{\sigma''\sigma'}(t'',t')\sigma''\,dt''$$

$$C^r(t,t') = C^t - C^< = \int A^r(t,t'')B^r(t'',t')\,dt'' \quad \rightarrow \quad C^r[\omega] = A^r[\omega]B^r[\omega]$$

$$C^<(t,t') = \int A^r(t,t'')B^<(t'',t')\,dt'' + \int A^<(t,t'')B^a(t'',t')\,dt''$$

$$\rightarrow \quad C^<[\omega] = A^r[\omega]B^<[\omega] + A^<[\omega]B^a[\omega]$$

$$D(\tau,\tau') = \iint A(\tau,\tau_1)B(\tau_1,\tau_2)C(\tau_2,\tau')\,d\tau_1 d\tau_2 \quad \rightarrow$$

$$D^r = A^r B^r C^r,$$

$$D^< = A^r B^r C^< + A^r B^< C^a + A^< B^a C^a$$

Dyson equations and solution

g : isolated center
G : center coupled to baths
$\Sigma_\alpha = V^{C\alpha} g_\alpha V^{\alpha C}$, $\Sigma = \Sigma_L + \Sigma_R$

$$G = g + g\Sigma G,$$

$$\Downarrow$$

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

$$G^< = G^r \Sigma^< G^a$$ (Keldysh equation)

Energy current

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

$$= i\hbar \int_{t_0}^{t} \left[G_{CC}^r(t,t') \frac{\partial \Sigma_L^<(t',t)}{\partial t} + G_{CC}^<(t,t') \frac{\partial \Sigma_L^a(t',t)}{\partial t} \right] dt'$$

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

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

Meir-Wingreen formula, symmetric form

$$J_\alpha = -\int_{-\infty}^{+\infty} \frac{d\omega}{4\pi} \hbar\omega \,\mathrm{Tr}\left(G^{>}\Sigma_\alpha^{<} - G^{<}\Sigma_\alpha^{>} \right), \quad \alpha = L, R$$

Landauer/Caroli formula

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

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

FDT for baths: $i\Sigma^<_\alpha = N_\alpha \Gamma_\alpha$

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

$$G^< = G^r \Sigma^< G^a, \qquad i\Sigma^< = N_L \Gamma_L + N_R \Gamma_R$$

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

1D calculation

- In the following we give a complete calculation for a simple 1D chain (the baths and the center are identical) with on-site coupling and nearest neighbor couplings. This example shows the steps needed for more general junction systems, such as the need to calculate the “surface” Green’s functions.

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

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

Solution of g

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

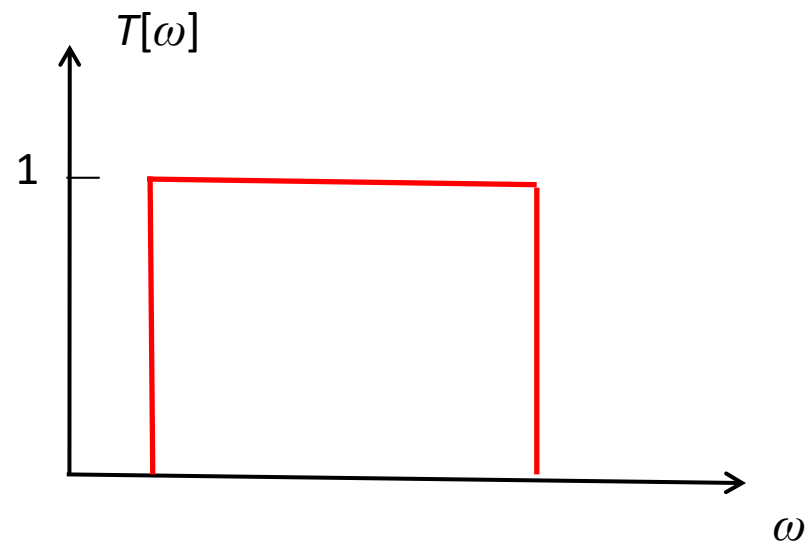
$$K^R=\begin{bmatrix} 2k+k_0 & -k & 0 & \cdots \\ -k & 2k+k_0 & -k & 0 \\ 0 & -k & 2k+k_0 & -k \\ 0 & 0 & -k & \cdots \end{bmatrix}$$

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

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

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

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

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

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

K. Schwab, et al, Nature 404, 974 (2000)

General recursive algorithm for g

$$K^R = \begin{bmatrix} k_{00} & k_{01} & 0 & \cdots \\ k_{10} & k_{11} & k_{01} & 0 \\ 0 & k_{10} & k_{11} & \cdots \\ \vdots & 0 & k_{10} & \ddots \end{bmatrix}$$

$$\eta \approx 10^{-5}$$

$$\varepsilon \approx 10^{-14}$$

$$s \leftarrow k_{00}$$

$$e \leftarrow k_{11}$$

$$\alpha \leftarrow k_{01}$$

do {

$$g \leftarrow \left((\omega + i\eta)^2 I - e\right)^{-1}$$

$$\beta \leftarrow \alpha^T$$

$$s \leftarrow s + \alpha g \beta$$

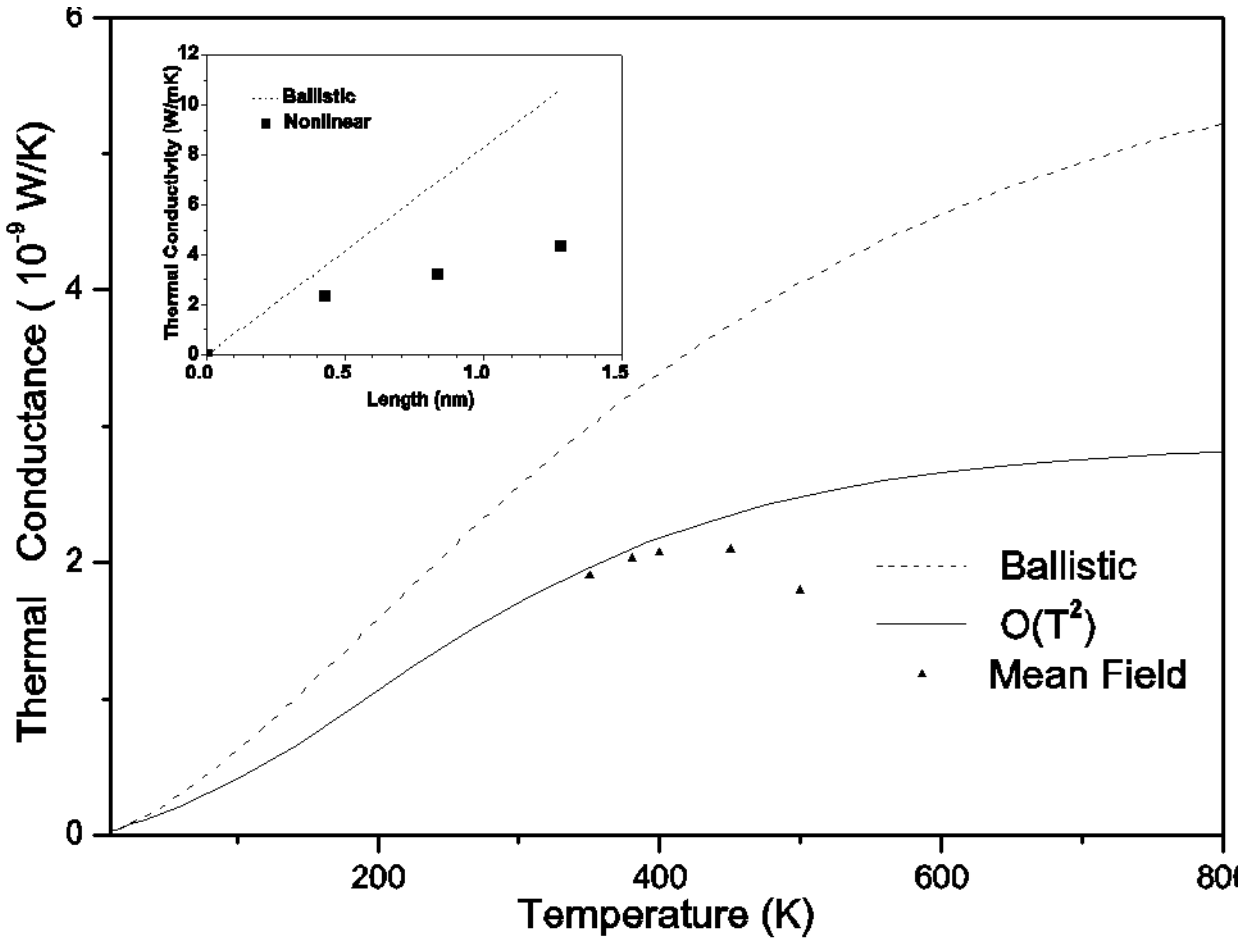
$$e \leftarrow e + \alpha g \beta + \beta g \alpha$$

$$\alpha \leftarrow \alpha g \alpha$$

} while $(|\alpha| > \varepsilon)$

$$g_{00} \leftarrow \left((\omega + i\eta)^2 I - s\right)^{-1}$$

(8,0) carbon nanotube



J.-S. Wang, J. Wang, N. Zheng, PRB 74, 033408 (2006).

Main figure: center region one unit cell (0.43 nm). Inset: length dependence of thermal conductivity at 300K.