CSRC Summer School on Quantum Non-equilibrium Phenomena: Methods and Applications

Nonequilibrium Green's Function Method in Quantum Transport – Electrons, phonons, photons

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Outline

- Lecture 0: Electron Green's functions √
- ~~Lecture 1: Basics of transport theories~~
- Lecture 2: NEGF – brief history, phonon/harmonic oscillator example √
- Lecture 3: NEGF "technologies" – rules of calculus, equation of motion method, current formula √
- ~~Lecture 4: Feynman diagrammatics~~
- Lecture 5: Photons √

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).
- See also textbooks by Haug & Jauho, Rammer, Datta, Stefanucci & van Leeuwen, etc.

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.

Annihilation/creation operators

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

$$c_j c_k^\dagger + c_k^\dagger c_j = \delta_{jk}$$

$$c_j c_k + c_k c_j = 0$$

$$c_j^\dagger c_k^\dagger + c_k^\dagger c_j^\dagger = 0$$

defining property of fermion

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

Many-electron Hamiltonian and Green's functions

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

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

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

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

Perturbation theory, single electron

$H = h + V$

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

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

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

The last equation is known as Dyson or Lippmann-Schwinger equation

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

Problem for lecture zero

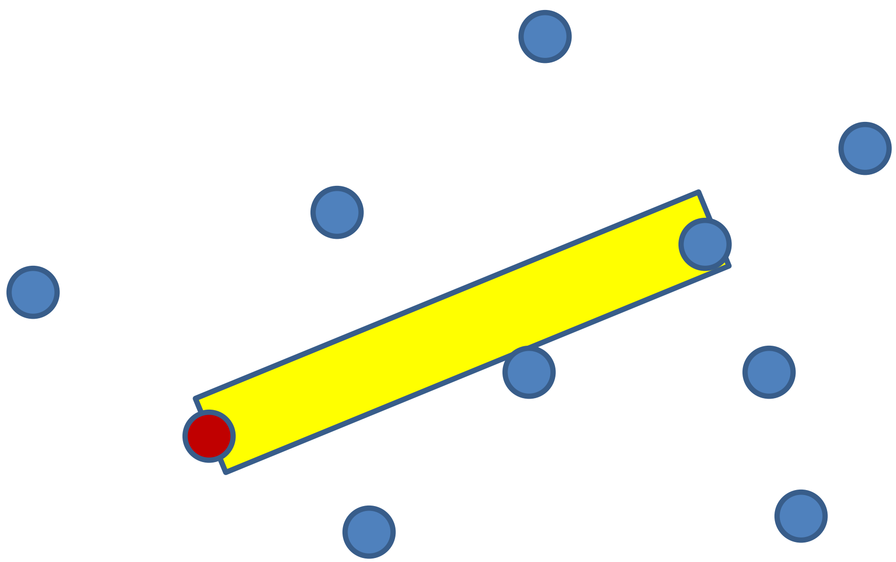
1. Assuming the many-body Hamiltonian is of the form $c^{+}Hc$, show the equivalence of two definitions of retarded Green's functions, one base on evolution operator $e^{-iHt/\hbar}$(slide 5), and one base on the anti-commutator $\{c, c^{+}\}$ for the fermion operators (slide 8).

end of lecture zero

Lecture One

Basics of thermal transport or transport in general

Mean free path (MFP)



diffusive vs ballistic regime

Clausius's problem:

How far an atom in a gas can move before colliding with another atom?

Answer:

$$l\pi d^2 n \approx 1$$

where l: MFP, d diameter of atom, n gas particle density.

Relaxation time (electrons)

- Electron makes a straight line motion, but only for a duration of τ.
- Ohm's law $\boldsymbol{j} = \sigma \boldsymbol{E}$
- and electric current $\boldsymbol{j} = -en\boldsymbol{v}$

- Kinetic theory of transport $\sigma = \frac{ne^2\tau}{m}$

See: Ashcroft/Mermin, *Solid State Physics*.

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)

Kinetic theory formula for thermal conductivity

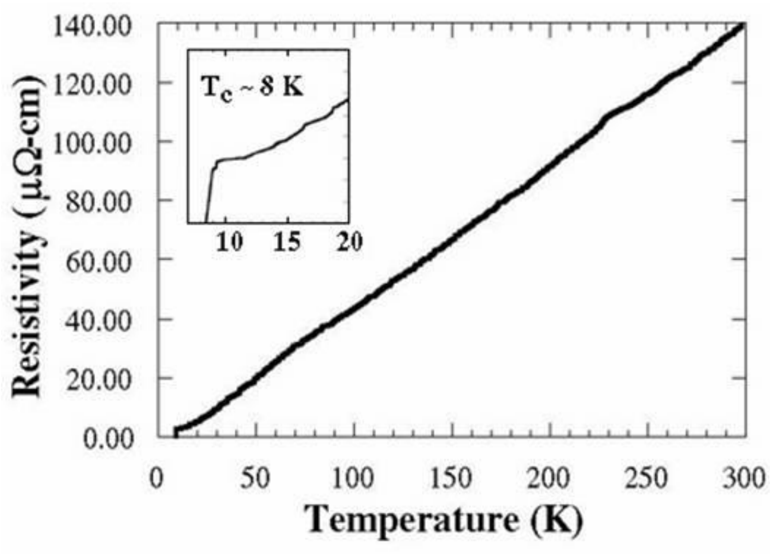
$$\kappa = \frac{1}{3} C_v v l = \frac{1}{3} C_v v^2 \tau$$

C_v: heat capacity per unit volume
v: velocity of phonon (i.e. sound velocity)

Wiedemann-Franz law (for electrons)

$$\frac{\kappa}{\sigma T} = \text{const}$$

Some features of electron transport in metal



ρ vs T for lead (Pb), $\rho \propto T$ almost in the entire temperature range and becomes superconducting at $T_c = 7.2$ K.

Simple kinetic theory gives $\rho = 1/\sigma = m/(ne^2\tau)$. Electron-phonon scattering can explain this linear dependence as self-energy ($-\mathrm{Im}\, \Sigma^r \propto 1/\tau$) due to phonon is proportional to $\langle uu \rangle \propto T$ in the classical limit. The best conductor near room temperature is Cu with resistivity around 1.6 μΩ·cm.

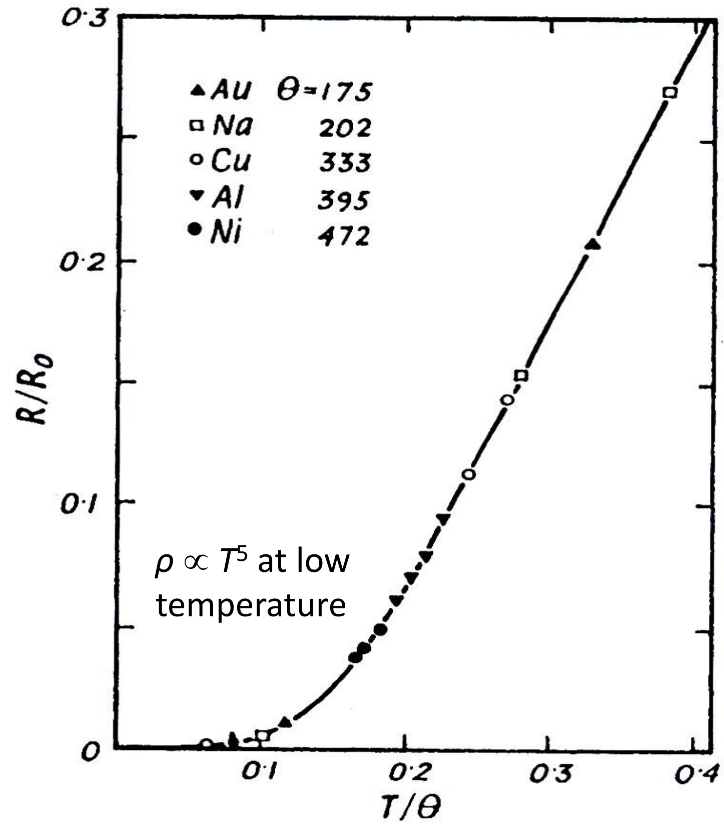
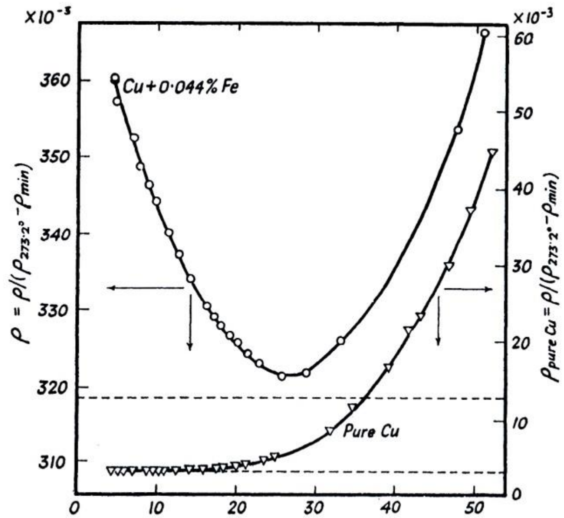
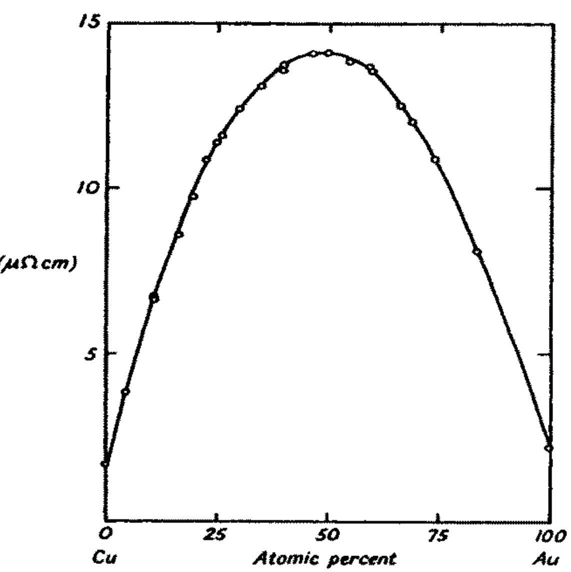


Fig. 115 of Ziman. Two-parameter fit to Grüneisen-Bloch theory to experimental data. The theory is based on Boltzmann transport equation and Debye model for phonons. The typical value of good metal resistivity is of the order of μΩ·cm (or 10 nΩ·m).

J. M. Ziman, “Electrons and Phonons,” Oxford Univ Press, 1960



Left top: Fig. 107. Due to impurity scattering, the resistance saturates to a constant. But with small amount of magnetic atoms, the resistance can go up, now known as Kondo effect.



Left bottom: Fig. 103. The disordered alloy follows $\Delta\rho \propto (1-x)x$. This is known as Nordheim’s rule (1931).

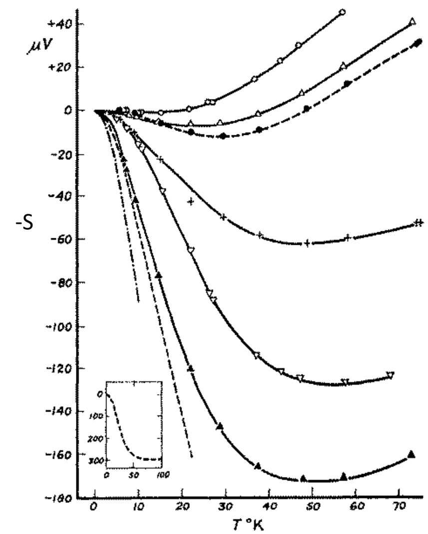
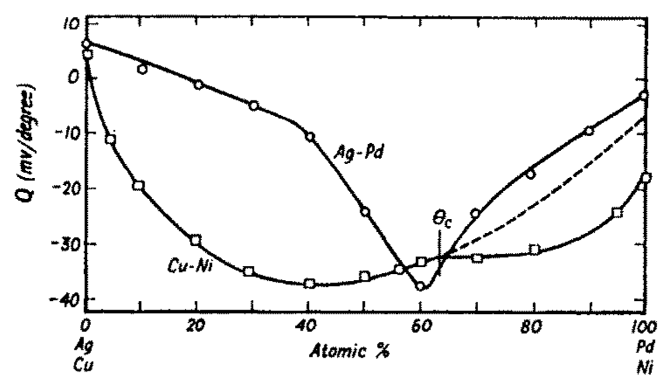
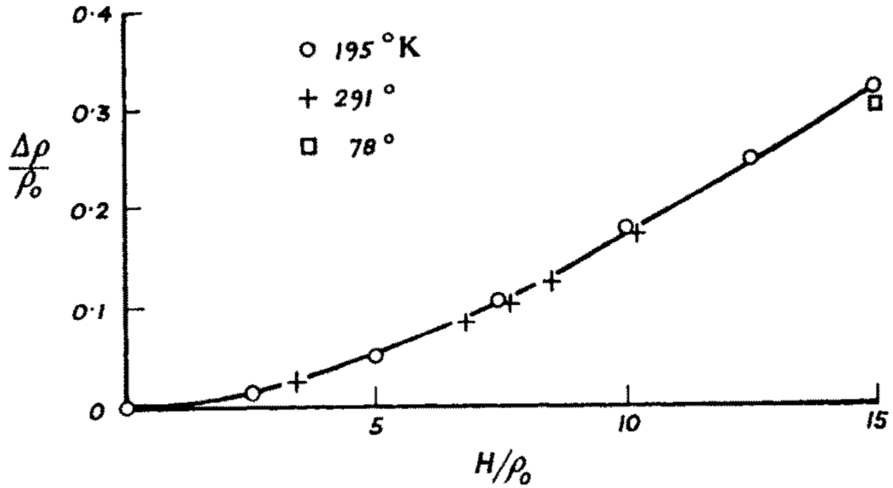


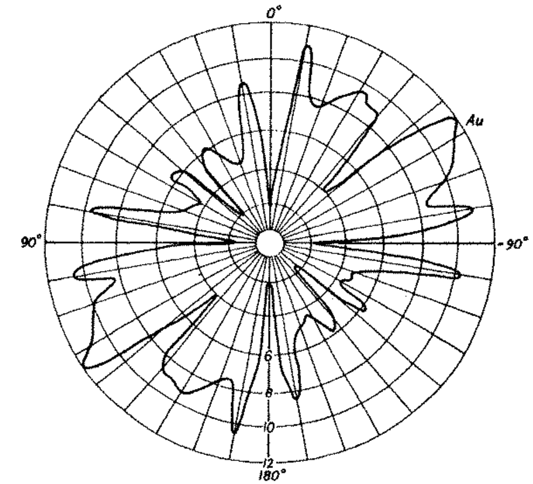
Fig. 109. Absolute thermopower of Cu and alloys at low temperatures (MacDonald & Pearson, 1953).

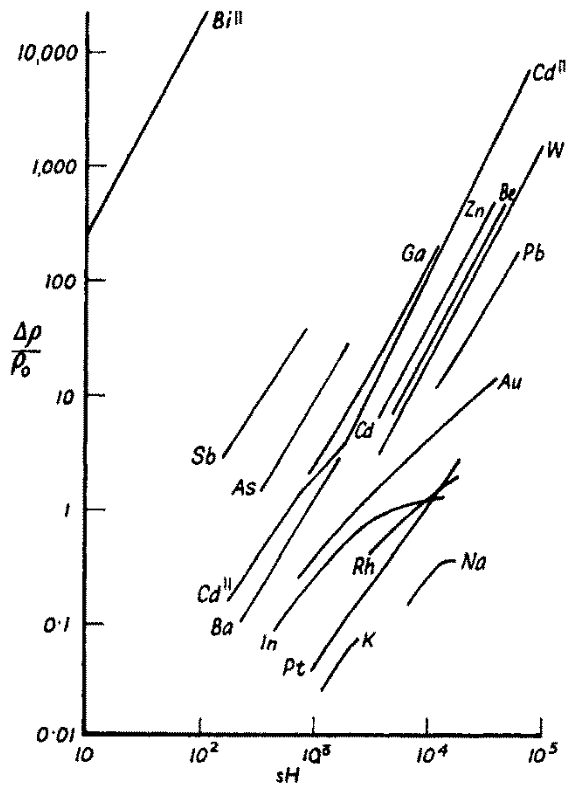
○ pure Cu, △, Cu+0·0000 at. per cent Sn; ▽, Cu+0·0026 at. per cent Sn; ▲, Cu+0·0054 at. per cent Sn; +, Cu+0·026 at. per cent Sn; ●, Cu+0·01 at. per cent Ni; – – –, 0·004 at. per cent Fe—see also inset; — · — · —, 0·03 at. per cent Fe (after Borelius, *et al.*).



Top right, Fig. 109. bottom right, Fig. 129. Thermal power S (also known as Seebeck coefficient). The Boltzmann approach gives $S = -\pi^2 k_B^2 T/(3e) \cdot \partial \ln \sigma(\varepsilon)/\partial\varepsilon|_{\varepsilon=\varepsilon_F}$.







Top left: Fig. 157. magneto-resistance of Mg. Bottom: Fig. 158. $\Delta\rho = \rho(H)-\rho(0)$, $\rho_0 = \rho(0)$. The magneto-effect can be surprisingly large, e.g. Bi. The scale seems wrong, can the magneto-effect so large? Note they are all positive (i.e. magnetic field increases resistance). Top right: Fig. 159. Anisotropic effect with respect to crystalline direction.

Kohler's rule (1938): $\Delta\rho/\rho_0=F(H/\rho_0)$. The data fall on the same curve independent of T (top left). This can be explained by Boltzmann equation under Lorentz force. $\Delta\rho \propto H^2$ is typical.

Boltzmann approach to transport

Tight-binding model

$$\hat{H} = c^{+}Hc + \frac{p^T p}{2m} + \frac{1}{2}u^T K u + \frac{1}{3}\sum T_{ijk}u_i u_j u_k + \sum c^{+}Mc \cdot u$$

Transport coefficients defined by electric and heat currents

$$j = e^2 L_0\ E + e\ L_1\ \nabla T/T,$$
$$q = -eL_1\ E - L_2\ \nabla T/T,$$

where

$$L_n = -\frac{1}{3}\int (\epsilon - \mu)^n v^2 \tau \frac{\partial f}{\partial \epsilon}\,\frac{d^3\mathbf{k}}{(2\pi)^3}, \qquad n = 0,1,2$$

Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{F}\cdot\frac{\partial f}{\partial \hbar\mathbf{k}} = \left(\frac{\partial f}{\partial t}\right)_{\mathrm{colli}} \approx -\frac{f - f_0}{\tau}$$

Green-Kubo & Kubo-Greenwood formulas

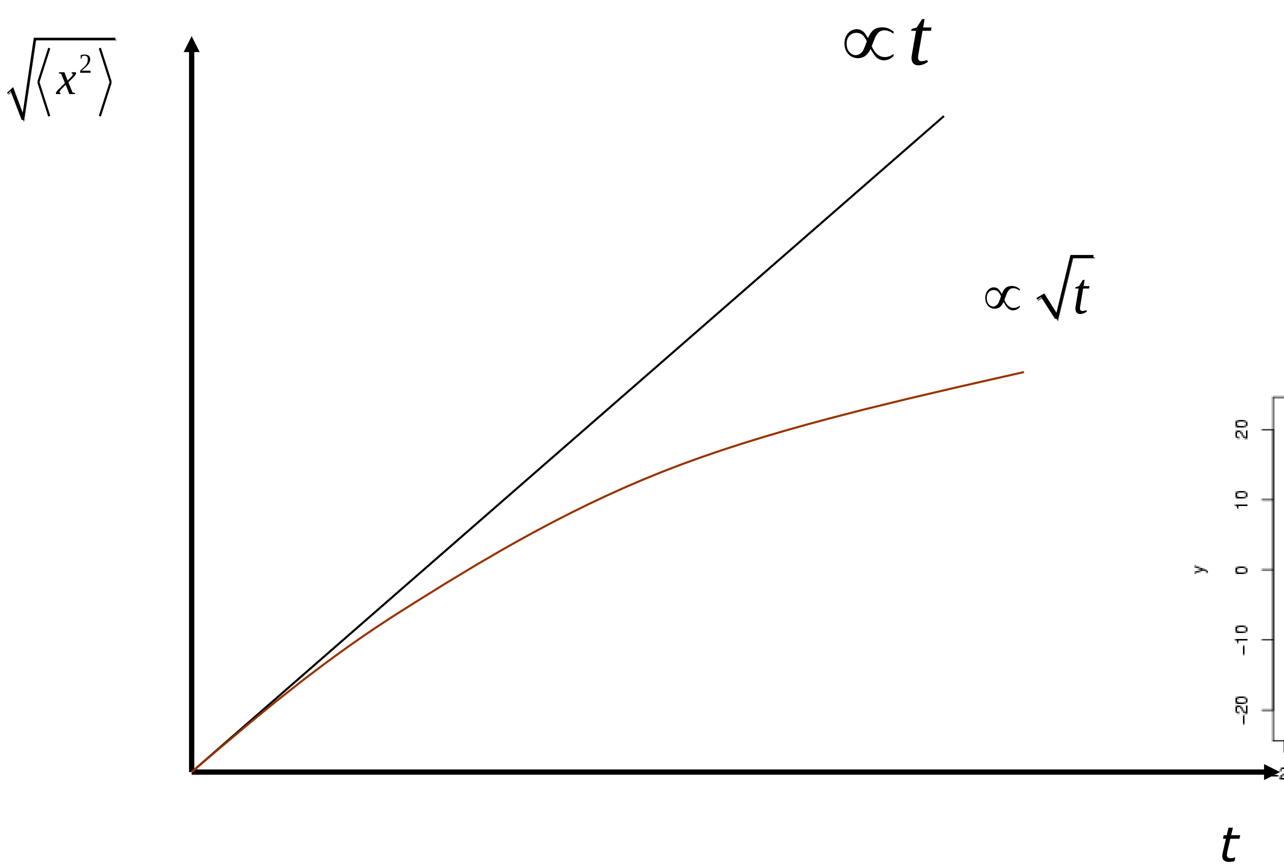
$$H_I = -b(t)\hat{B},$$

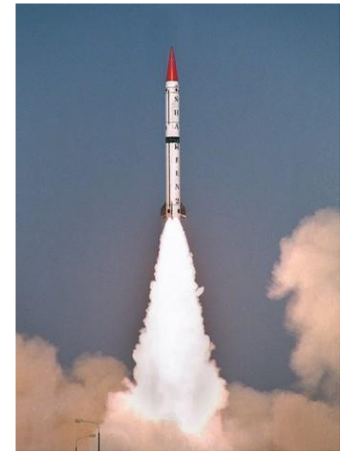
$$\langle A(t) \rangle = -\int_{t_0}^{t} G^r_{AB}(t-t')b(t')dt'$$

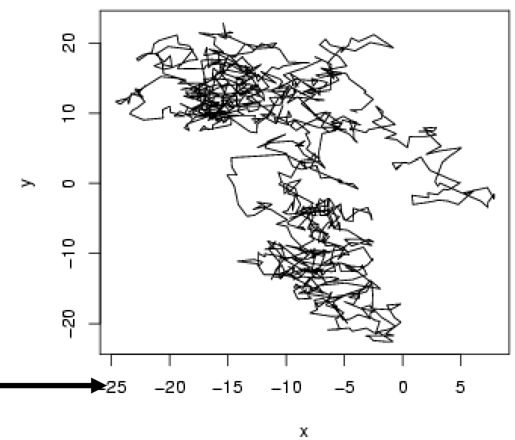
$$G^r_{AB}(t) = -\frac{i}{\hbar}\theta(t)\left\langle [\hat{A}(t), \hat{B}(0)] \right\rangle_{eq}$$

$$\sigma_{\alpha\beta} = \frac{\hbar^2 e^2}{V}\int_{-\infty}^{+\infty}\frac{dE}{\pi\hbar}\left(-\frac{\partial f}{\partial E}\right)\mathrm{Tr}\left(\mathrm{Im}\, G^r(E)V_\alpha\, \mathrm{Im}\, G^r(E)V_\beta\right)$$

Diffusive transport vs ballistic transport



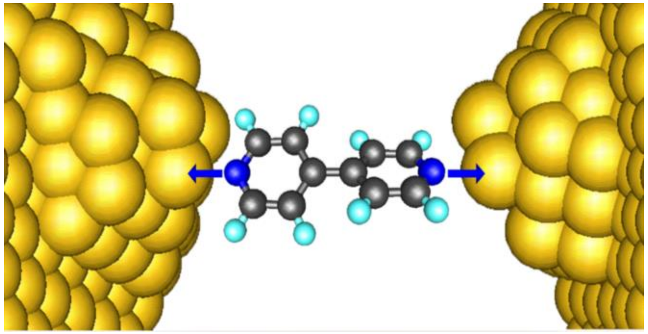




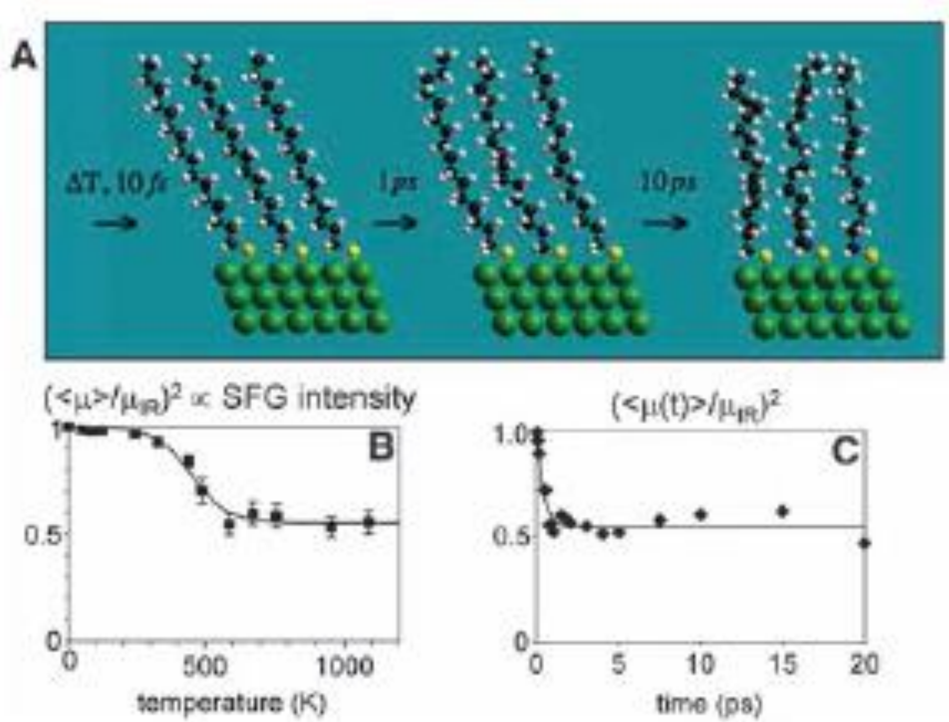
Thermal conductance

$$I = \left(T_L - T_R\right) G$$

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



Experimental report of Z Wang et al (2007)

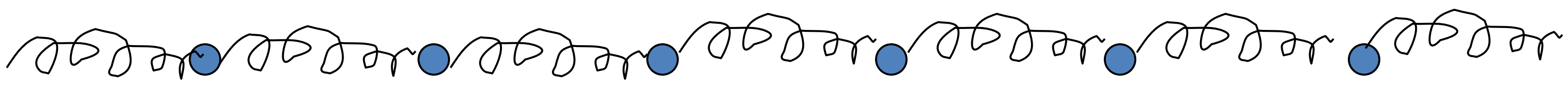


The experimentally measured thermal conductance is 50pW/K for alkane chains at 1000K, From Z Wang et al, Science 317, 787 (2007).

“Universal” thermal conductance

$$G = M\,\frac{\pi^2 k_B^2 T}{3h}$$

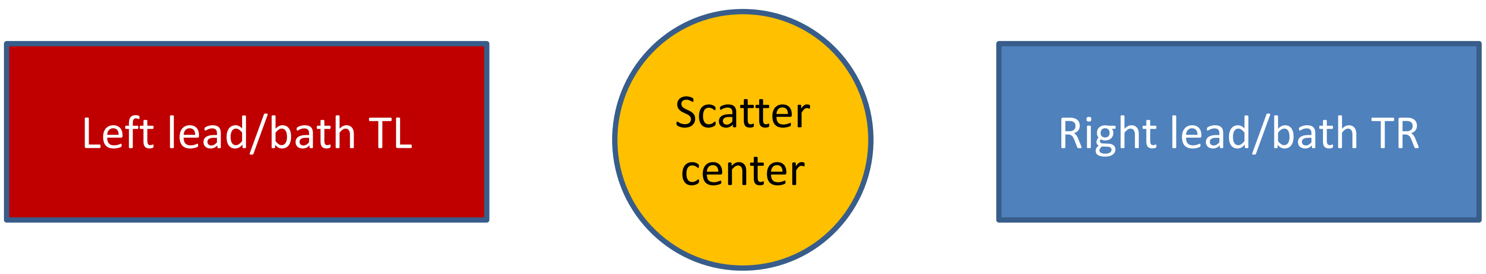
Rego & Kirczenow, PRL 81, 232 (1998).



$M = 1$

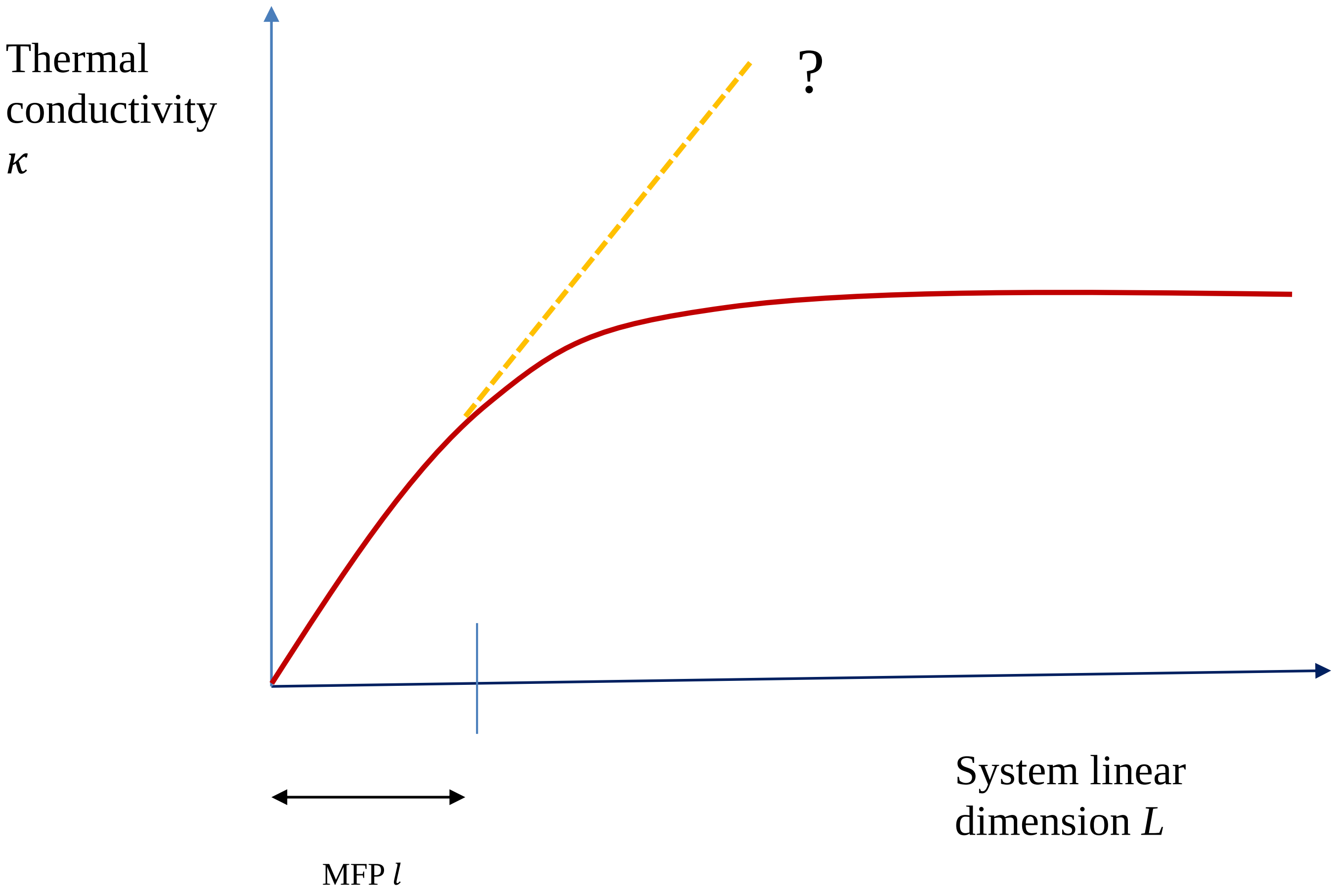
Landauer formula

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

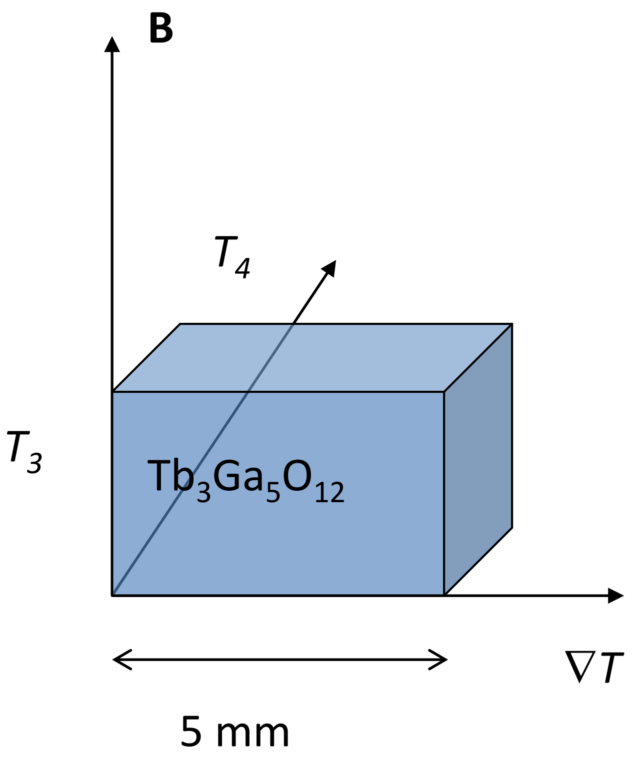


See: S Datta, "*Electronic transport in mesoscopic systems*"

From ballistic to diffusive



Phonon Hall effect



Experiments by C Strohm et al, PRL (2005), also confirmed by AV Inyushkin et al, JETP Lett (2007). Effect is small $|T_4 - T_3| \sim 10^{-4}$ kelvin in a strong magnetic field of few tesla, performed at low temperature of 5.45 K.

Ballistic model of phonon Hall effect

$$H = \frac{1}{2} p^T p + \frac{1}{2} u^T K u + u^T A p$$

where $A^T = -A$, e.g.,

$$V = \sum_n \mathbf{\Lambda} \cdot (\mathbf{U}_n \times \mathbf{P}_n)$$

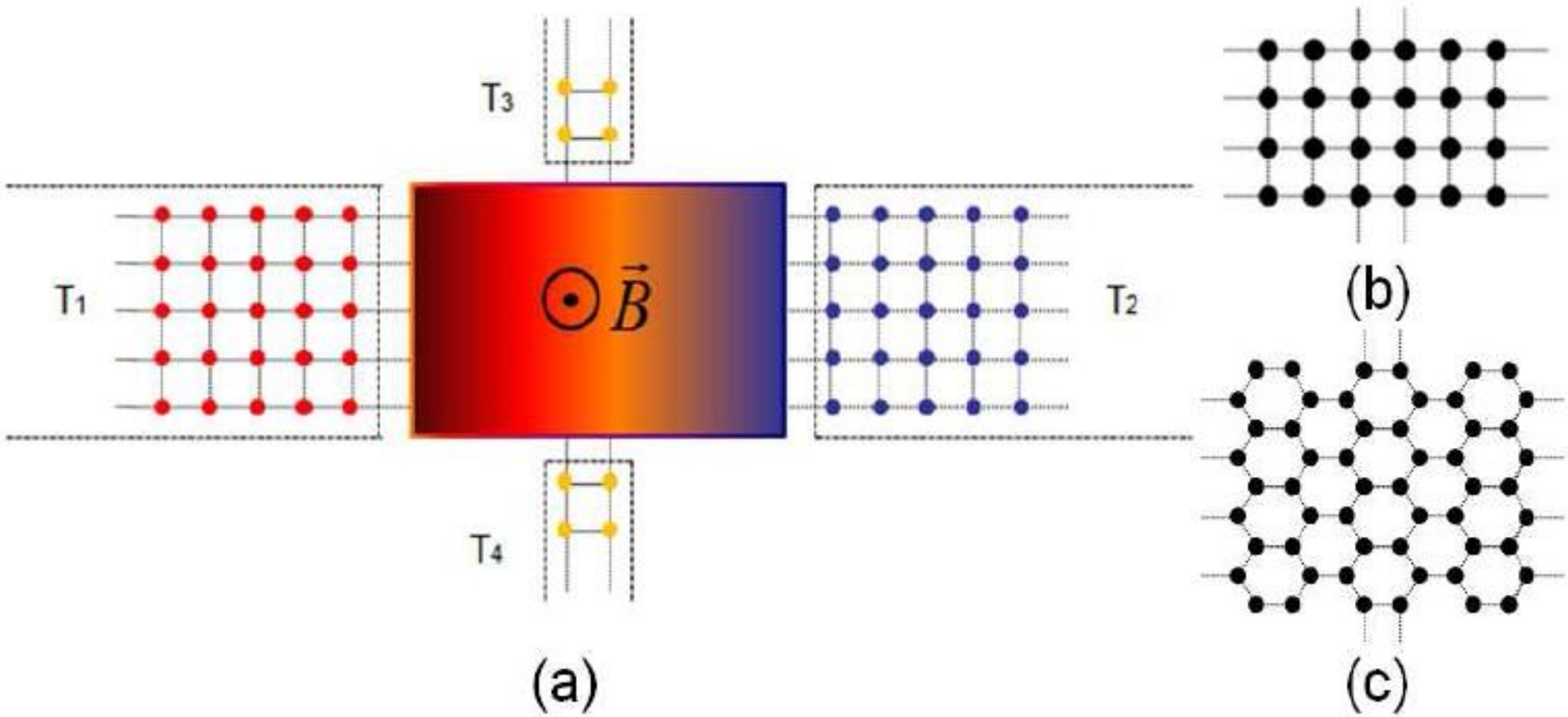
H is not positive-definite

Revised positive-definite Hamiltonian

$$H = \frac{1}{2}(p - Au)^T (p - Au) + \frac{1}{2} u^T K u$$

H is formally the same as ionic crystal in a magnetic field

Four-terminal junction structure, NEGF



$R=(T_3 - T_4)/(T_1 - T_2)$.

Hamiltonian for the four-terminal junction

$$H = \sum_{\alpha=0}^{4} H_\alpha + \sum_{\beta=1}^{4} u_\beta^T V_{\beta 0} u_0 + u_0^T A p_0,$$

$$H_\alpha = \frac{1}{2} p_\alpha^T p_\alpha + \frac{1}{2} u_\alpha^T K_\alpha u_\alpha,$$

$$A = \begin{pmatrix} 0 & +h & 0 & 0 \\ -h & 0 & 0 & 0 \\ 0 & 0 & 0 & +h \\ 0 & 0 & -h & 0 \end{pmatrix}$$

The energy current

Meir-Wingreen:

$$I_\alpha = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \hbar\omega \,\mathrm{Re}\left[\mathrm{Tr}(G^r\Sigma_\alpha^< + G^<\Sigma_\alpha^a)\right],$$

$$G^r[\omega] = \frac{1}{(\omega + i\eta)^2 I - K_0 - \Sigma^r[\omega] - A^2 + 2i\omega A},$$

Keldysh:

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

Linear response regime

$$T_\alpha = T + \Delta_\alpha, \quad \Delta_\alpha \text{ small}$$

$$I_\alpha = \sum_{\beta=1}^{4} \sigma_{\beta\alpha} (\Delta_\alpha - \Delta_\beta),$$

$$\sigma_{\beta\alpha} = \int_0^\infty \frac{d\omega}{2\pi} \hbar\omega \mathrm{Tr}(G^r \Gamma_\beta G^a \Gamma_\alpha) \frac{\partial f}{\partial T},$$

$$f = \frac{1}{\exp[\hbar\omega / (k_B T)] - 1}$$

Problems for lecture one

1. Derive the electron conductivity σ Drude formula (slide 15) following Ashcroft/Mermin.
2. Give a hand-waving derivation of the kinetic theory formula for the thermal conductivity κ (slide 17).
3. Give a derivation of the thermal conductivity (generalized to sum over the phonon modes) based on Boltzmann equation (slides 23) with a single mode relaxation approximation.

4. Derive the “universal” conductance formula (slide 28) from the Landauer formula, assuming a unit transmission $T[\omega]=1$.
5. Generalize Landauer formula so that it smoothly interpolates between ballistic regime and diffusive regime [hint: J Wang, J-S Wang APL (2006)].
6. Derive the Kubo-Greenwood formula (slide 24) .

end of lecture one

Lecture Two

History, definitions, properties of NEGF

A Brief History of NEGF

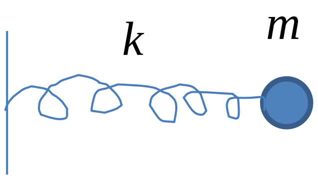
- Schwinger 1961
- Kadanoff and Baym 1962
- Keldysh 1965
- Caroli, Combescot, Nozieres, and Saint-James 1971
- Meir and Wingreen 1992

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

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

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

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

$$\left\langle aa\right\rangle = \left\langle a^\dagger a^\dagger\right\rangle = 0, \quad \left\langle a^\dagger a\right\rangle = \left\langle aa^\dagger\right\rangle - 1 = f$$

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

Heisenberg Operator/Equation

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\tilde{g}^r[\omega] = \int_{-\infty}^{+\infty} g^r(t) e^{i\omega t} dt, \qquad g^r(t) = \int_{-\infty}^{+\infty} \tilde{g}^r[\omega] e^{-i\omega t} \frac{d\omega}{2\pi}$$

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

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

$$g^a[\omega] = g^r[\omega]^*,$$

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

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

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

P for Cauchy principle value

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

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

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

Valid only in thermal equilibrium

Matsubara Green's Function

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Kramers-Kronig Relation

$$\hat{G}[z] = \int_0^{\infty} e^{izt} G^r(t) dt$$ is analytic on the upper half plane of z

$$G^r[\omega] = \hat{G}[z \to \omega + i\eta], \quad \eta \to 0^+$$

$$G_R^r[\omega] = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \mathrm{P} \frac{G_I^r[\omega']}{\omega' - \omega},$$

$$\int \mathrm{P} \frac{f(x)}{x - x_0} dx = \lim_{\varepsilon \to 0^+} \left[\int^{x_0 - \varepsilon} + \int_{x_0 + \varepsilon} \cdots \right]$$

$$G_I^r[\omega] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \mathrm{P} \frac{G_R^r[\omega']}{\omega' - \omega}$$

Eigen-mode Decomposition

$$Ku^{(j)} = \Omega_j^2 u^{(j)}, \quad S = (u^{(1)}, u^{(2)}, \cdots, u^{(N)})$$

$$u = SQ, \qquad S^T S = I$$

$$S^T K S = \begin{pmatrix} \Omega_1^2 & 0 & \cdots & 0 \\ 0 & \Omega_2^2 & 0 & \cdots \\ 0 & 0 & \cdots & \\ & \cdots & 0 & \Omega_N^2 \end{pmatrix} = \mathrm{diag}\left\{\Omega_j^2\right\}$$

$$G^{>,<,t,\bar{t},r,a}(t) = S \ \mathrm{diag}\left\{ g^{>,<,t,\bar{t},r,a}(t) \right\} S^T$$

$$G^r[\omega] = S \,\mathrm{diag}\left\{ \frac{1}{(\omega + i\eta)^2 - \Omega_j^2} \right\} S^T = \left[(\omega + i\eta)^2 - K \right]^{-1}$$

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

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

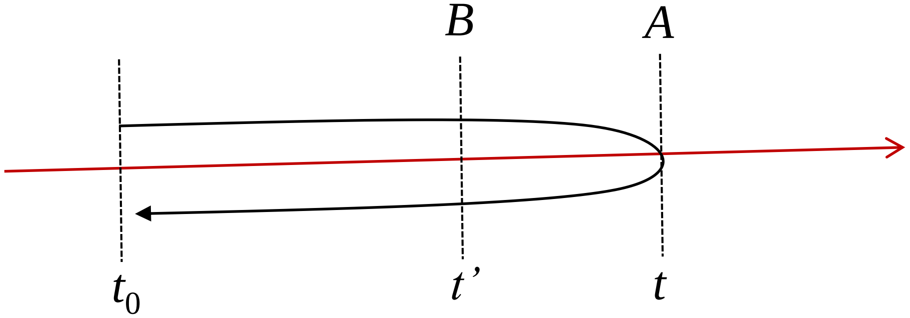
$$= \mathrm{Tr}\left[\rho(t_0)U(t_0,t)AU(t,t_0)U(t_0,t')BU(t',t_0)\right]$$

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

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

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

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



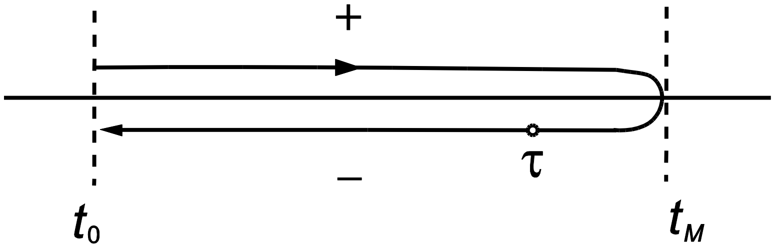
Evolution Operator on Contour

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

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

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

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

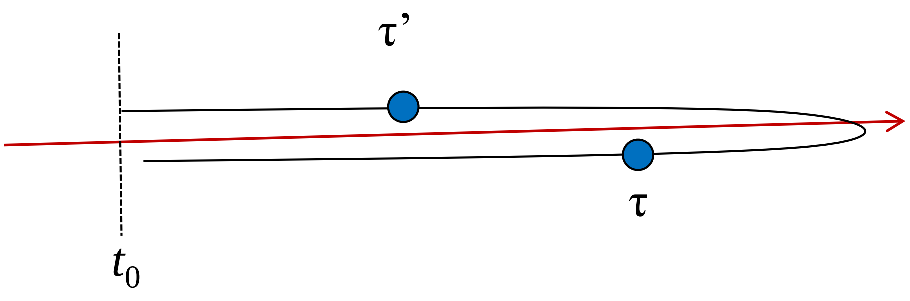


Contour-ordered Green's function

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

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

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



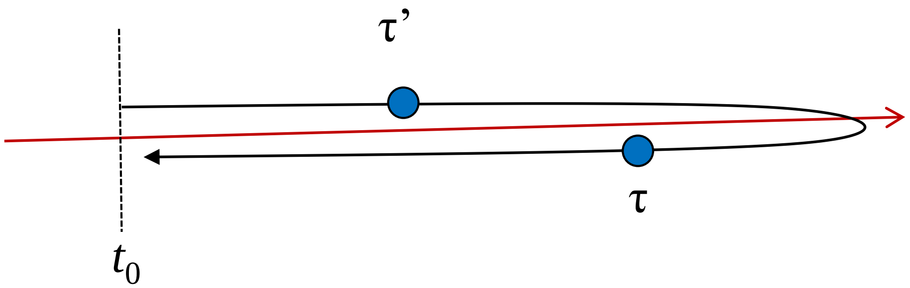
Relation to other Green's function

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

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

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

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



An Interpretation

$$H = \frac{1}{2} p^T p + \frac{1}{2} u^T K u, \quad K^T = K$$

$$V(\tau) = -F(\tau)^T u$$

$$\mathrm{Tr}\Big(U(t_M, t_0) \rho(t_0) U(t_0, t_M) \Big) =$$

$$\exp\left(-\frac{i}{2\hbar} \int_C \int_C F(\tau)^T G(\tau, \tau') F(\tau') d\tau d\tau' \right)$$

G is defined with respect to Hamiltonian *H* and density matrix ρ and assuming Wick's theorem.

Problems for lecture two

1. Express the annihilation operator a and creation operator a^+ by the position operator x and momentum operator p (slide 44). Why they have to be that form?
2. Compute the thermal average values $<aa>$, $<a^+a^+>$, $<aa^+>$, and $<a^+a>$ for the simple harmonic oscillator (slide 45).
3. For the harmonic oscillator, work out the expressions for various Green's functions defined in terms of a, a^+, instead of u (slide 47 - 50). Discuss the advantage and disadvantage of both. [Hint: Piet Brower's lecture notes, "Theory of many-particle systems".]

4. Verify the equations for g^r on slides 49 and 50.
5. For the harmonic oscillator, verify the claim that we can obtain g^r in frequency domain from the Matsubara function by the substitution $i\omega_n \rightarrow \omega + i\eta$ (bottom of slide 52).
6. Prove the "fluctuation-dissipation" theorem for equilibrium systems, $G^< = (G^r - G^a)f$, using the Lehmann representation. Here f is the Bose function $\frac{1}{e^{\beta\hbar\omega} - 1}$.

7. Prove the Kramers-Kronig relation and state the condition needed for its validity (slide 58).
8. Explain the meaning of slide 63 from first line to the second line.
9. Derive the retarded Green’s function of photon for a free field (no interaction) and discuss how it differs from the time-ordered one (at zero temperature) [Hint. Mahan, “Many-particle physics”,3rd ed, Chap.2.10]

end of lecture two

Lecture three

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

Calculus on the contour

- Integration on (Keldysh) contour

$$\int f(\tau)d\tau = \sum_{\sigma=\pm} \int_{-\infty}^{+\infty} f^{\sigma}(t)\sigma dt = \int_{-\infty}^{+\infty} f^{+}(t)dt - \int_{-\infty}^{+\infty} f^{-}(t)dt$$

- Differentiation on contour

$$\frac{df(\tau)}{d\tau} \rightarrow \frac{df^{\sigma}(t)}{dt}$$

Theta function and delta function

- Theta function $\theta(\tau,\tau') = \begin{cases} 1 & \text{if } \tau \text{ is later than } \tau' \text{ along the contour} \\ 0 & \text{otherwise} \end{cases}$

$$\theta(\tau,\tau') \quad \to \quad \theta^{\sigma\sigma'}(t,t') = \begin{cases} \theta^{++}(t,t') = \theta(t-t') \\ \theta^{--}(t,t') = \theta(t'-t) \\ \theta^{+-}(t,t') = 0 \\ \theta^{-+}(t,t') = 1 \end{cases}$$

- Delta function on contour

$$\delta(\tau,\tau') = \frac{d\theta(\tau,\tau')}{d\tau} \quad \to \quad \delta^{\sigma\sigma'}(t,t') = \sigma\delta_{\sigma\sigma'}\delta(t-t')$$

where $\theta(t)$ and $\delta(t)$ are the ordinary Heaviside theta and Dirac delta functions

Transformation/Keldysh Rotation

$$A \to A_{jj'}(\tau,\tau') \to A_{jj'}^{\sigma\sigma'}(t,t')$$

$$\bar{A}^{\sigma\sigma'} \equiv \sigma A^{\sigma\sigma'} \quad \text{or} \quad \bar{A} = \begin{pmatrix} A^{t} & A^{<} \\ -A^{>} & -A^{\bar{t}} \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad R = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad RR^T = I$$

$$\breve{A} = R^T \sigma_z A R = R^T \bar{A} R = \begin{pmatrix} A^{r} & A^{K} \\ A^{\bar{K}} & A^{a} \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} A^{t} - A^{<} + A^{>} - A^{\bar{t}} & A^{t} + A^{\bar{t}} + A^{<} + A^{>} \\ A^{t} + A^{\bar{t}} - A^{<} - A^{>} & A^{<} - A^{\bar{t}} + A^{t} - A^{>} \end{pmatrix},$$

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

Convolution, Langreth Rule

$$AB\cdots D \equiv \int d\tau_2 d\tau_3 \cdots d\tau_n A(\tau_1,\tau_2)B(\tau_2,\tau_3)\cdots D(\tau_n,\tau_{n+1})$$

$$C = AB \quad \rightarrow \quad \bar{C} = \bar{A}\bar{B} \quad \rightarrow \quad \breve{C} = \breve{A}\breve{B}$$

$$\begin{pmatrix} C^r & C^K \\ 0 & C^a \end{pmatrix} = \begin{pmatrix} A^r & A^K \\ 0 & A^a \end{pmatrix}\begin{pmatrix} B^r & B^K \\ 0 & B^a \end{pmatrix}$$

or $\quad C^r = A^r B^r, \;\; C^a = A^a B^a, \; C^K = A^r B^K + A^K B^a$

$$\breve{G} = \breve{g} + \breve{g}\breve{\Sigma}\breve{G} \quad \rightarrow \quad G^r = g^r + g^r \Sigma^r G^r \quad \rightarrow \quad G^r = \left((g^r)^{-1} - \Sigma^r\right)^{-1}$$

$$G^K = g^K + g^r \Sigma^r G^K + g^r \Sigma^K G^a + g^K \Sigma^a G^a,$$

$$G^< = (1 + G^r \Sigma^r) g^< (1 + \Sigma^a G^a) + G^r \Sigma^< G^a$$

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.

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

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

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

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

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

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

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

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

$$= -K G(\tau,\tau') - \delta(\tau,\tau') I$$

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:

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

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

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

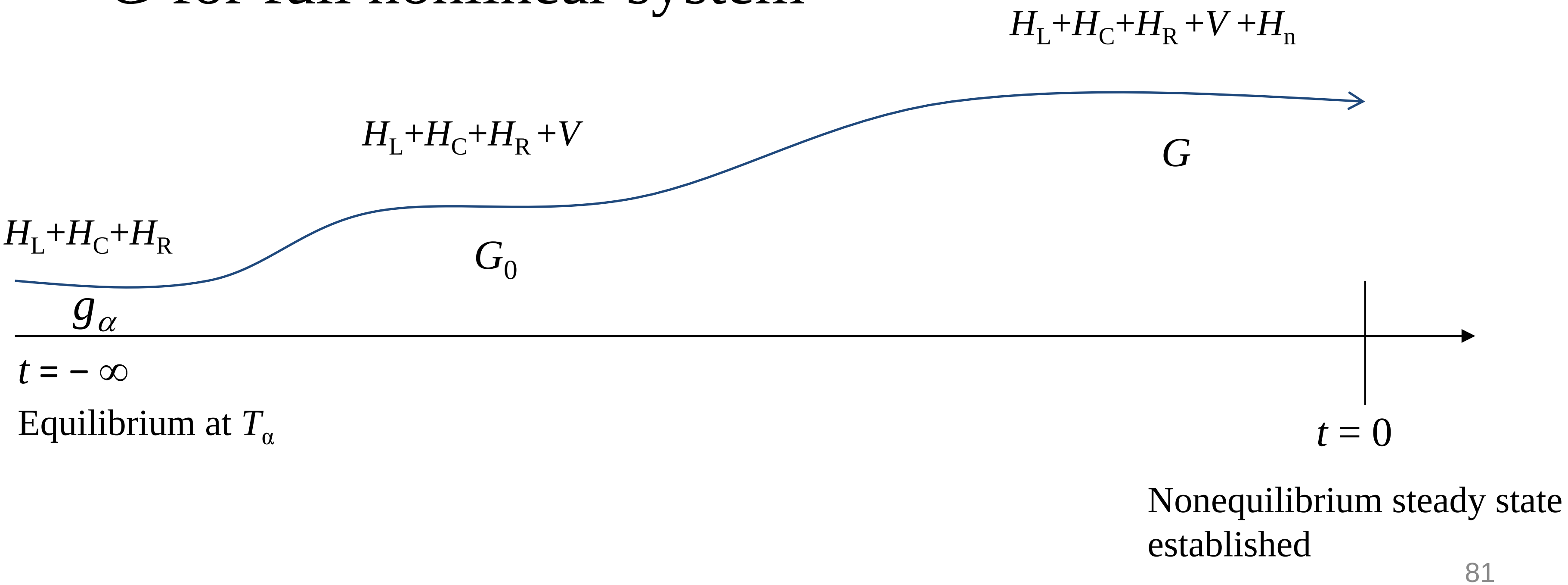
$$G^< = f(G^r - G^a), \quad G^> = e^{\beta\hbar\omega} G^<$$

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

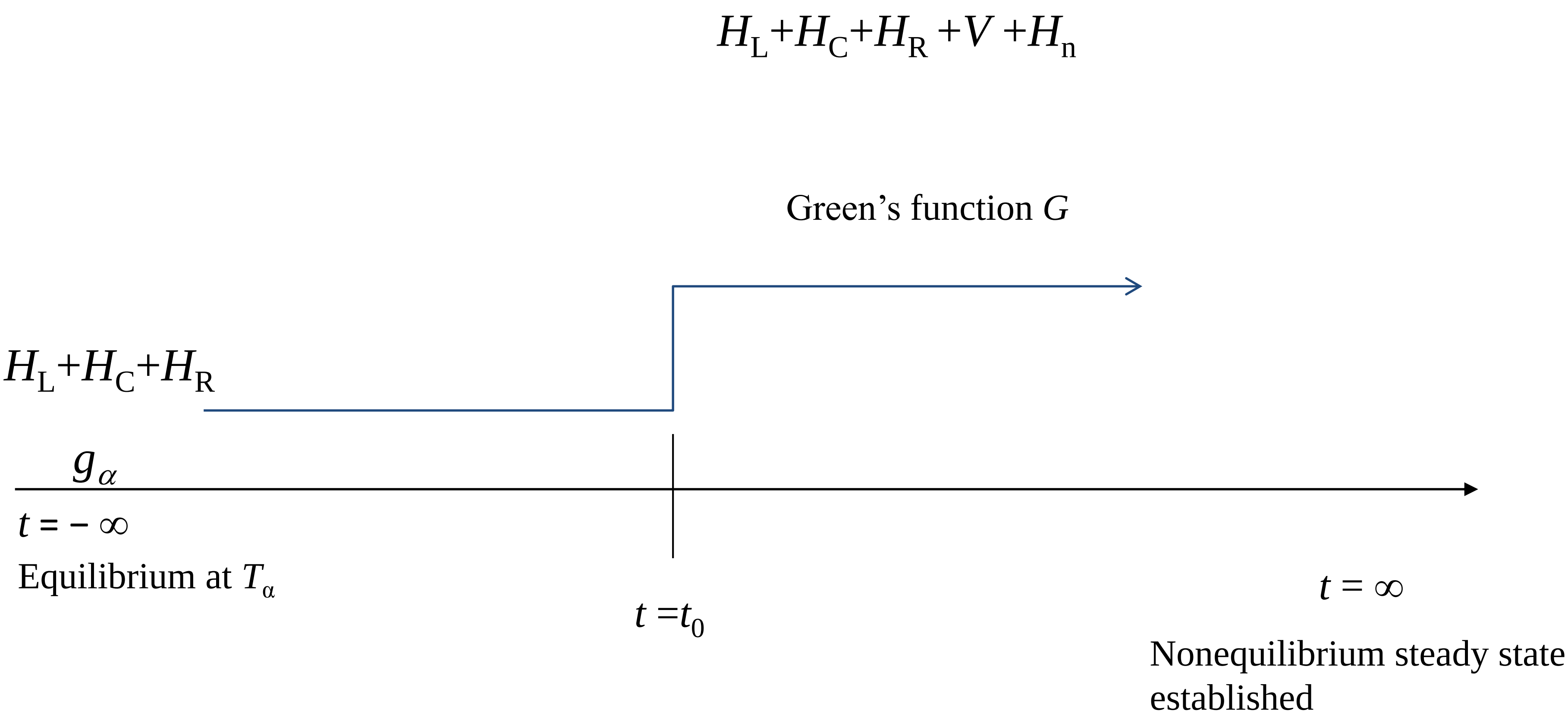
c and *d* can be fixed by initial/boundary condition.

Junction system, adiabatic switch-on

- g_α for isolated systems when leads and centre are decoupled
- G_0 for ballistic system
- G for full nonlinear 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

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

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

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

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

Force Constant Matrix

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

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

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

Relation between g and G_0

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}

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

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

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

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

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

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

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

Equation of Motion Way (ballistic system)

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

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

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

$$G(\tau,\tau') = g(\tau,\tau') + \int_C d\tau'' g(\tau,\tau'') V G(\tau'',\tau')$$

The Langreth theorem

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

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

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

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

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

$$D^r=A^rB^rC^r,$$

$$D^<=A^rB^rC^<+A^rB^<C^a+A^<B^aC^a$$

Dyson equations and solution

$$G_0 = g_C + g_C \Sigma G_0,$$
$$G = G_0 + G_0 \Sigma_n G$$

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

$$G^r = \left((G_0^r)^{-1} - \Sigma_n^r\right)^{-1},$$
$$G^< = G^r \Sigma_n^< G^a + (I + G^r \Sigma_n^r) G_0^< (I + \Sigma_n^a G^a)$$
$$= G^r (\Sigma^< + \Sigma_n^<) G^a$$

Energy current

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

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

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

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

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

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

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

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

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

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

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

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

- 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

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

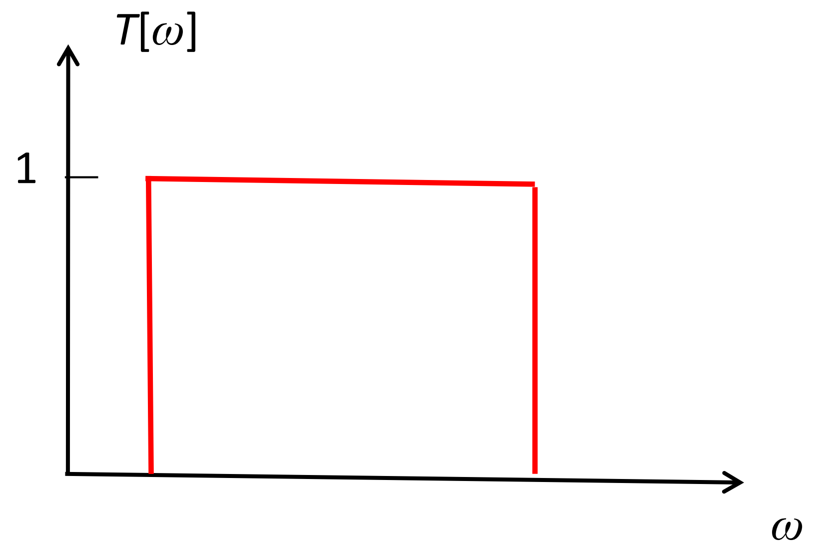
$$K^R = \begin{bmatrix} 2k+k_0 & -k & 0 & \cdots \\ -k & 2k+k_0 & -k & 0 \\ 0 & -k & 2k+k_0 & -k \\ 0 & 0 & -k & \cdots \end{bmatrix}$$

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

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

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

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

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

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

General recursive algorithm for g

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

$$\begin{aligned}
& s \leftarrow k_{00} \\
& e \leftarrow k_{11} \\
& \alpha \leftarrow k_{01} \\
& \mathrm{do}\,\{ \\
& \qquad g \leftarrow \left((\omega + i\eta)^2 I - e\right)^{-1} \\
& \qquad \beta \leftarrow \alpha^T \\
& \qquad s \leftarrow s + \alpha g \beta \\
& \qquad e \leftarrow e + \alpha g \beta + \beta g \alpha \\
& \qquad \alpha \leftarrow \alpha g \alpha \\
& \}\ \mathrm{while}\,(|\alpha| > \varepsilon) \\
& g_{00} \leftarrow \left((\omega + i\eta)^2 I - s\right)^{-1}
\end{aligned}$$

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

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

Problems for lecture three

1. Work out the detail of Keldysh rotation and Langreth rules (slide 73,74).
2. On slide 76, what is the meaning of t_0^+? And why we need to define Heisenberg operator starting at the same point?
3. Derive the integral form of equation from the differential form for G_{LC} (slide 86) and state clearly the implicit assumption made for the validity of the integral form.

4. On slide 80, how to fix the constants *c* and *d* for the retarded, advanced, and time-ordered Green's functions?
5. Derive the contour ordered Dyson equation, slides 86-88.
6. Derive the two different forms of Keldysh equations on bottom of slide 90.
7. Derive the Meir-Wingreen formula and the Caroli formula (slide 91 - 93).
8. Verify the results on slide 95-98 for 1D chain. In particular, show that the transmission function $T[\omega]=1$.

end of lecture three

Lecture four

Feynman diagrammatic expansion, Hedin equations

Diagrammatic representation of expansion results, e.g., Meyer expansion for equation of states

Grand potential:

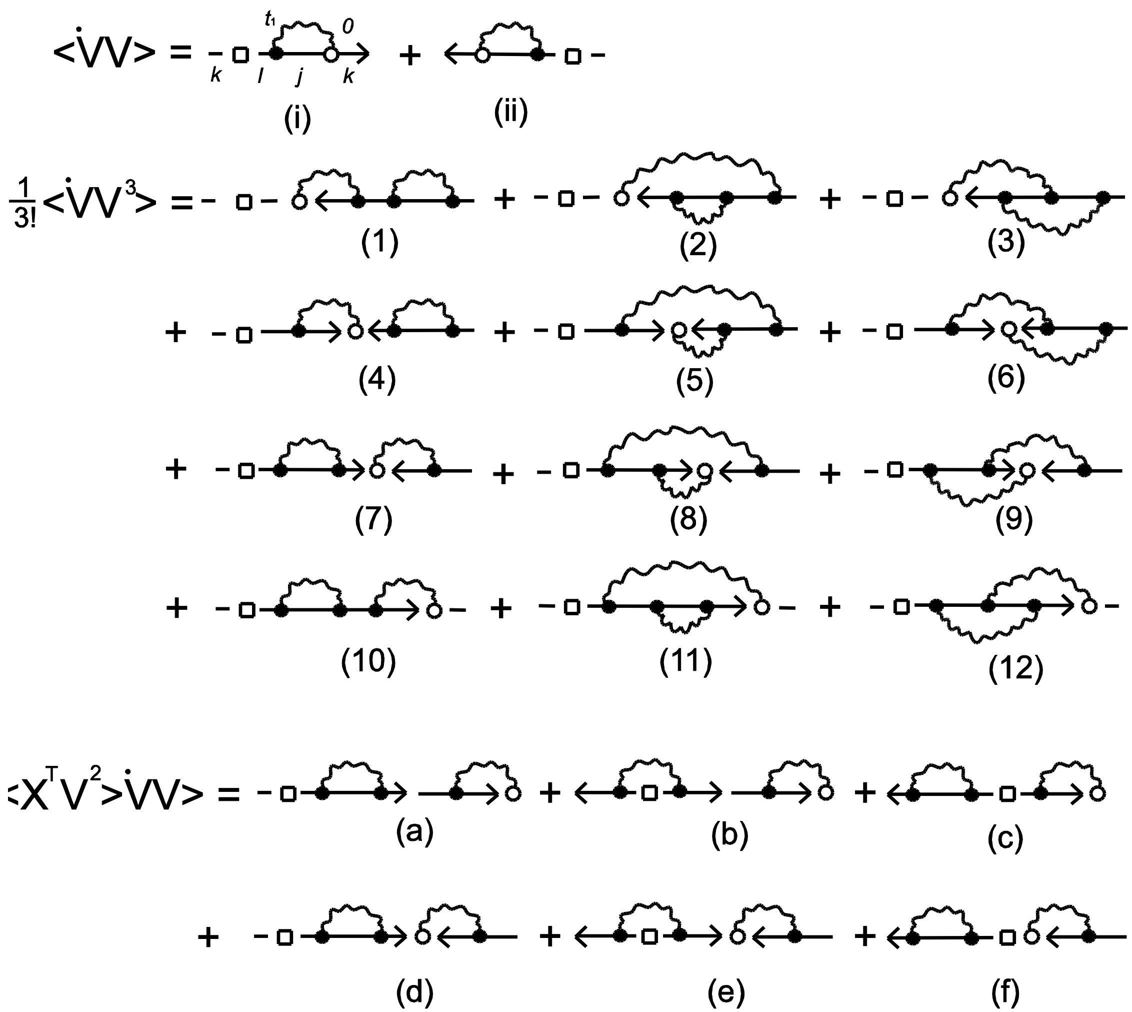
Ξ = 1 + x [o] + ½! x^2 [o   o + o---o] + 1/3! x^3 [….]

ln Ξ = x [o] + ½! x^2 [o---o] + 1/3! x^3 [….]

Equation of state

$pV/(k_B T) = N$ – 1/2 [o---o] – 1/3 [o---o with third vertex o above, joined to both (triangle)] – 1/8 [3 o---o with o---o above, joined vertically (square) + …]

Diagrammatics in higher order quantum master equations



Diagrams representing the terms for current $\dot{V}$ or $[X^T, V]$. Open circle has time t=0, solid dots have dummy times. Arrows indicate ordering and pointing from time -∞ to 0. Note that (4) is cancelled by (c); (7) by (d).

From Wang, Agarwalla, Li, and Thingna, Front. Phys. (2013), DOI: 10.1007/s11467-013-0340-x.

Feynman diagrammatic method

- The Wick theorem
- Cluster decomposition theorem, factor theorem
- Dyson equation
- Vertex function
- Vacuum diagrams and Green’s function

Handling interaction

Transform to interaction picture, $H = H_0 + H_n$

$$\Psi_I(t) = e^{i\frac{H_0}{\hbar}(t-t_0)}\Psi_S(t) = e^{i\frac{H_0}{\hbar}(t-t_0)}U(t,t_0)\Psi_H = S(t,t_0)\Psi_I(t_0)$$

$$S(t,t') = e^{i\frac{H_0}{\hbar}(t-t_0)}U(t,t')e^{-i\frac{H_0}{\hbar}(t'-t_0)}$$

$$\rho_I(t) = e^{i\frac{H_0}{\hbar}(t-t_0)}U(t,t_0)\rho_H U(t_0,t)e^{-i\frac{H_0}{\hbar}(t-t_0)}$$

$$A_I(t) = e^{i\frac{H_0}{\hbar}(t-t_0)}A_s e^{-i\frac{H_0}{\hbar}(t-t_0)} = e^{i\frac{H_0}{\hbar}(t-t_0)}U(t,t_0)A_H(t)U(t_0,t)e^{-i\frac{H_0}{\hbar}(t-t_0)}$$

Scattering operator S

$$\langle A(t)B(t')\rangle = \mathrm{Tr}\left[\rho_H A_H(t) B_H(t')\right] \qquad t < t'$$

$$= \mathrm{Tr}[\rho_I U(t_0,t) e^{-i\frac{H_0}{\hbar}(t-t_0)} A(t) e^{i\frac{H_0}{\hbar}(t-t_0)} U(t,t_0) U(t_0,t') e^{-i\frac{H_0}{\hbar}(t'-t_0)} B(t') e^{i\frac{H_0}{\hbar}(t'-t_0)} U(t',t_0)]$$

$$= \mathrm{Tr}[\rho_I S(t_0,t) A(t) S(t,t') B(t') S(t',t_0)]$$

$$i\hbar\frac{\partial}{\partial t} S(t,t') = H_n^I(t) S(t,t'), \qquad H_n^I(t) = e^{i\frac{H_0}{\hbar}(t-t_0)} H_n^S e^{-i\frac{H_0}{\hbar}(t-t_0)}$$

$$S(t,t') = T e^{-\frac{i}{\hbar}\int_{t'}^{t} H_n^I(t'')dt''}, \qquad t > t'$$

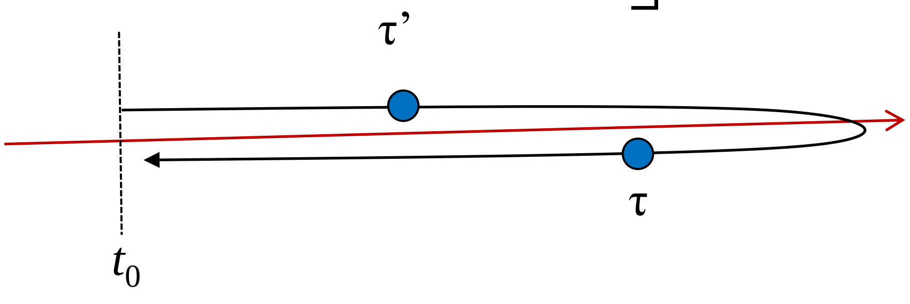
Contour-ordered Green's function

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

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

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

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



Perturbative expansion of contour ordered Green's function

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

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

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

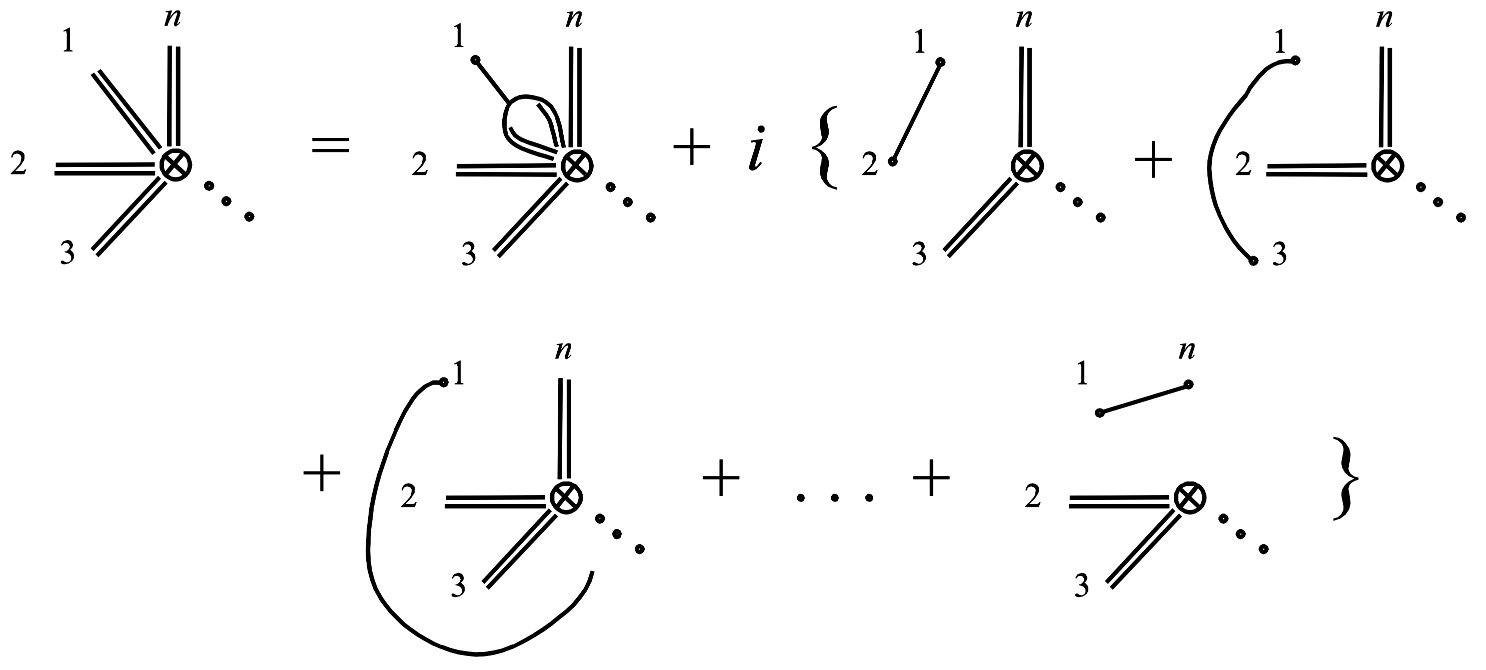
$$\left.\times \iiint \frac{1}{3}\sum_{opq} T_{opq}(\tau_4,\tau_5,\tau_6) u_o(\tau_4) u_p(\tau_5) u_q(\tau_6) d\tau_4 d\tau_5 d\tau_6\right\rangle$$

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

$\downarrow$ (Wick's 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



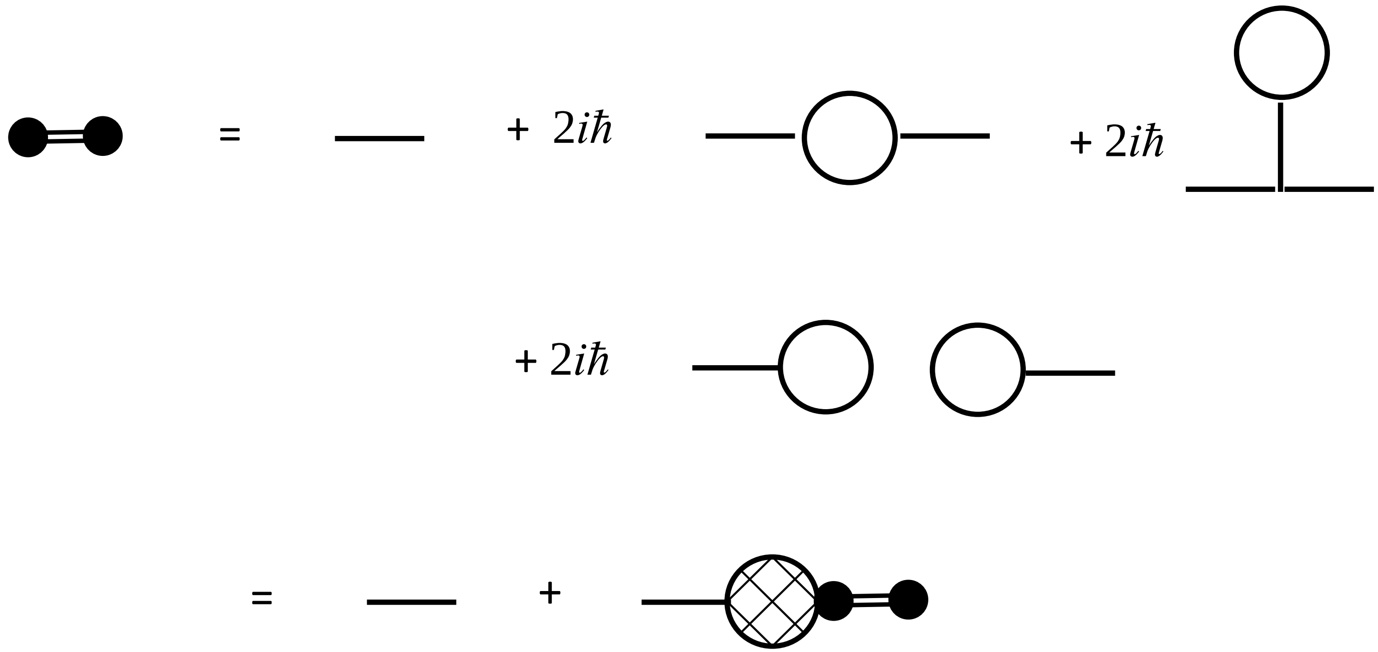
Single line $G_0(\tau, \tau')$

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

n-double line vertex

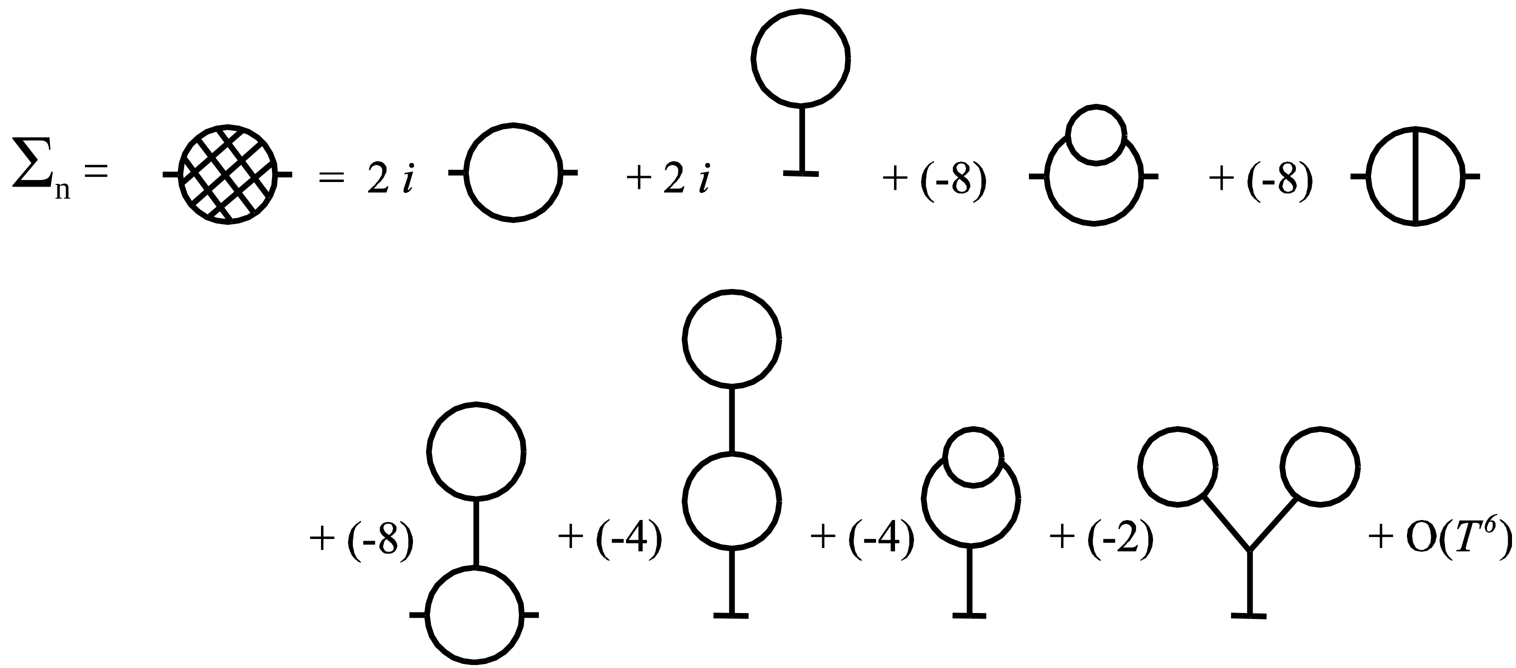
$$G_{j_1 j_2 \cdots j_n}(\tau_1, \tau_2, \cdots, \tau_n) = -\frac{i}{\hbar}\left\langle T_C u_{j_1}(\tau_1) u_{j_2}(\tau_2) \cdots u_{j_n}(\tau_n) \right\rangle$$

Diagrammatic representation of the expansion



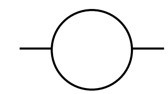
$$G(\tau,\tau') = G_0(\tau,\tau') + \int\int G_0(\tau,\tau_1)\Sigma_n(\tau_1,\tau_2)G(\tau_2,\tau')\,d\tau_1 d\tau_2$$

Self -energy expansion

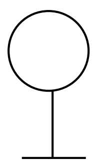


Explicit expression for self-energy

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

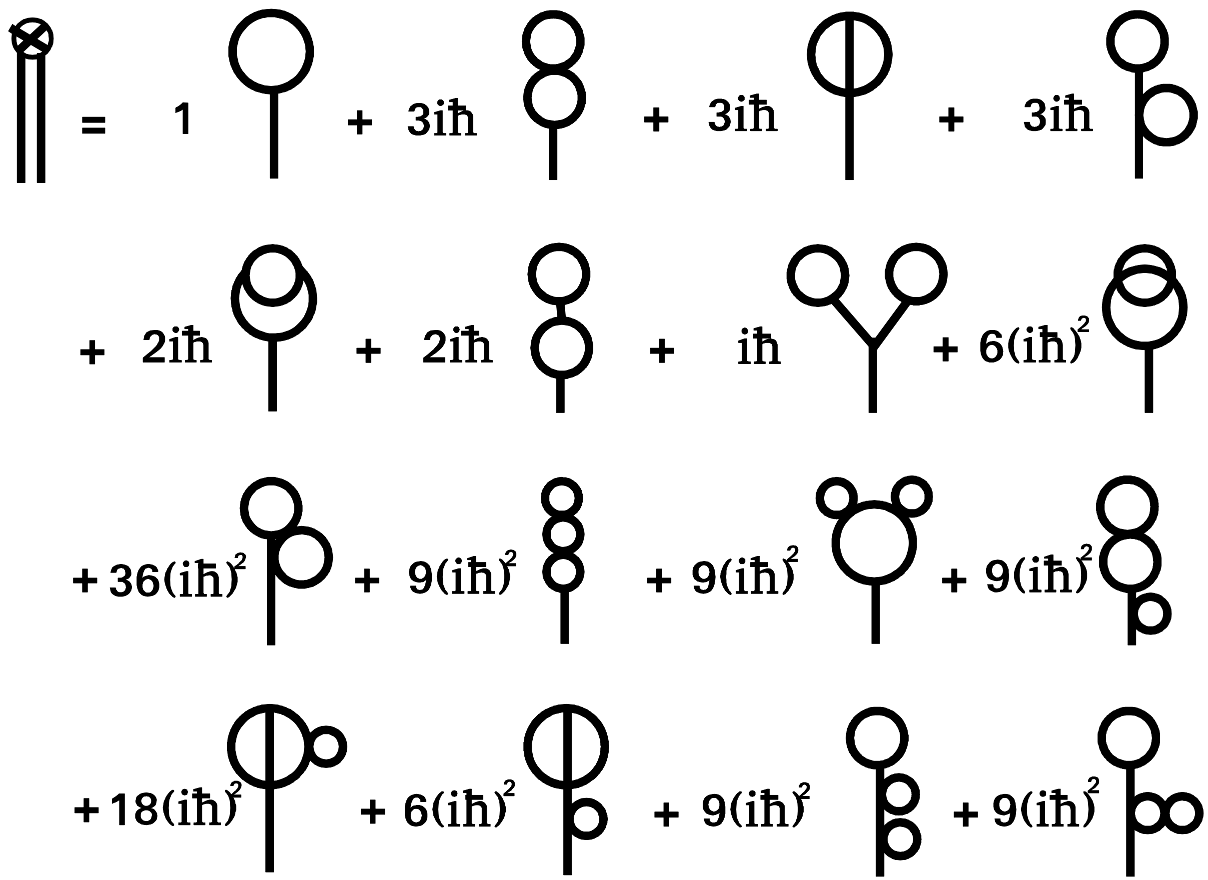


$$+2i\sigma\delta_{\sigma,\sigma'}\sum_{lmrs,\sigma''}\sigma'' T_{jkl}T_{mrs}\int_{-\infty}^{+\infty} G_{0,lm}^{\sigma\sigma''}[0]G_{0,rs}^{\sigma''\sigma''}[\omega']\frac{d\omega'}{2\pi}$$



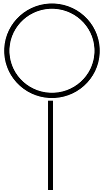
$$+O(T_{ijk}^{4})$$

One-Point Green's Function



Average displacement, thermal expansion

One-point Green's function



$$G_j(\tau) = -\frac{i}{\hbar}\left\langle T_C u_j(\tau)\right\rangle$$

$$= \sum_{lmn}\int d\tau' d\tau'' d\tau''' T_{lmn}(\tau',\tau'',\tau''')G^0_{lm}(\tau',\tau'')G^0_{nj}(\tau''',\tau)$$

$$G_j = \sum_{lmn} T_{lmn} G^>_{lm}(t=0) G^r_{nj}[\omega = 0]$$

$$\alpha_j = \frac{i\hbar}{M}\times\frac{1}{x_j}\times\frac{dG_j}{dT}$$

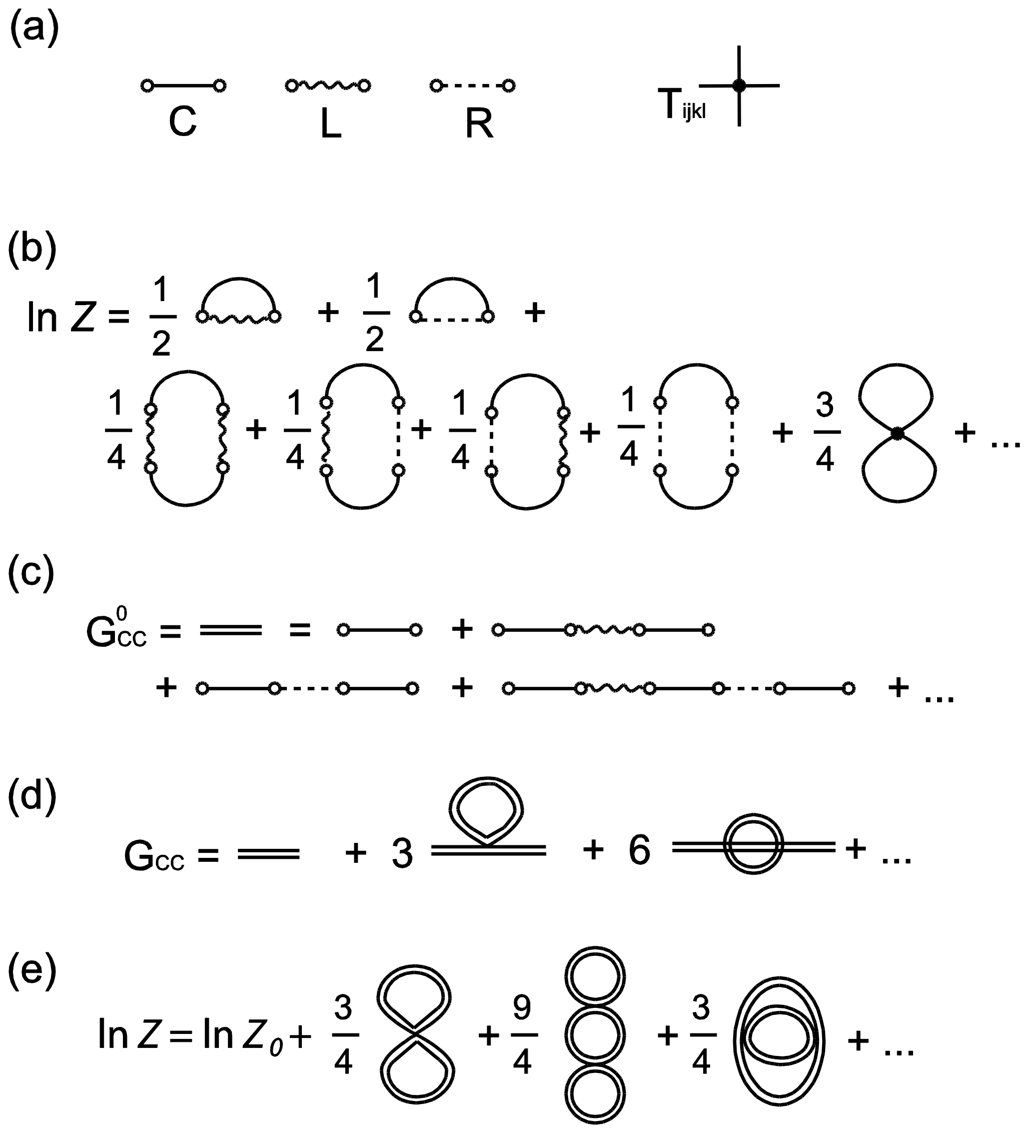
“Partition Function”

$$Z = \mathrm{Tr}\left[\rho(t_0)U(t_0,t)U(t,t_0)\right]$$

$$= \mathrm{Tr}\left[\rho(t_0)T_c e^{-\frac{i}{\hbar}\int_C \left(V_I(\tau)+H_I^n(\tau)\right)d\tau}\right]$$

$$\equiv 1$$

Diagrammatic Way



Feynman diagrams for the nonequilibrium transport problem with quartic nonlinearity. (a) Building blocks of the diagrams. The solid line is for g_C, wavy line for g_L, and dash line for g_R; (b) first few diagrams for ln Z; (c) Green's function $G^0{}_{CC}$; (d) Full Green's function G_{CC}; and (e) re-sumed ln Z where the ballistic result is ln Z_0 = (1/2) Tr ln (1 –$g_C\Sigma$). The number in front of the diagrams represents extra combinatorial factor.

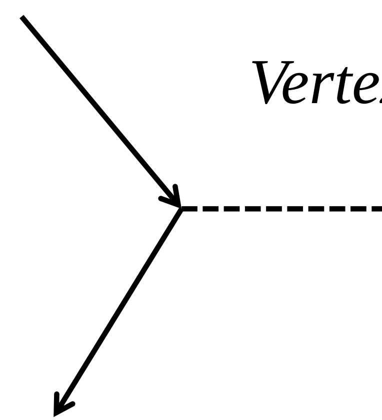
Electron phonon interaction

- Free electrons + free phonons + ep interactions

$$H_{ep} = \sum_{jkl} M_{jk}^{l} c_j^{+} c_k u_l = c^{+} \mathbf{M} c \cdot \mathbf{u}$$

G_0

D_0



Vertex M

Hedin equations (electron-phonon system)

$$\Sigma(1,2) = i\hbar \int d(3456) M(14;5) G(4,6) \Gamma(62;3) D(5,3)$$

$$\Pi(1,2) = -i\hbar \int d(3467) M(34;1) G(4,6) \Gamma(67;5) G(7,3^{+})$$

$$\Gamma(12;3) = M(12;3) + \int d(4567) \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6) \Gamma(67;3) G(7,5)$$

Functional Derivative

$$I[G] = \int dx F(G(x))$$

$$\delta I = I[G+\delta G] - I[G] = \int dx \frac{\delta I}{\delta G} \delta G(x)$$

Problems for lecture four

1. Give a proof of the expansion rule on slide 111, using the equation of motion method.
2. Work out the first few terms of Feynman-Dyson expansion for the (contour ordered) electron Green's function G and phonon Green's function D and identify the lowest order self-energies (the Hartree, Fock, and polarization diagrams). Give the explicit expressions in energy/frequency space.

3. Verify the “one-point” Green’s function result for the T_{ijk} interaction for phonons on slide 116.
4. Derive the Hedin equations for the electron-phonon system.

end of lecture four

Lecture Five

Green’s function for scalar and vector photons

Scalar photon

Hamiltonian: $H = H_e + H_\phi + H_{\text{int}}$

electron: $H_e = c^\dagger H c$

scalar photon: $H_\phi = -\frac{\varepsilon_0}{2}\int d^3\mathbf{r}\left[\left(\frac{\dot\phi}{\tilde c}\right)^2 + \left(\nabla\phi\right)^2\right], \qquad \tilde c \to \infty$

Interaction: $H_{\text{int}} = -e\sum_{j\in\text{system}} c_j^\dagger c_j \phi(\mathbf{r}_j)$

Green's functions: $D(\mathbf{r},t;\mathbf{r}',t') = -\frac{i}{\hbar}\left\langle T_c \phi(\mathbf{r},t)\phi(\mathbf{r}',t')\right\rangle$

$$G_{jk}(t;t') = -\frac{i}{\hbar}\left\langle T_c c(j,t) c^\dagger(k,t')\right\rangle$$

Meir-Wingreen/Caroli formulas

$$J = -\int_{-\infty}^{+\infty} \frac{d\omega}{4\pi} \hbar\omega \mathrm{Tr}\left(D^{>}\Pi_\alpha^{<} - D^{<}\Pi_\alpha^{>} \right)$$

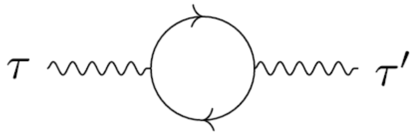
Random phase approximation (RPA)

$$D^{>,<} = D^r \Pi^{>,<} D^a$$

$$D^r = v + v\Pi^r D^r, \qquad D^a = \left(D^r \right)^\dagger$$

$$\Pi_{jk}(\tau,\tau') = -i\hbar e^2 G_{jk}(\tau,\tau') G_{kj}(\tau',\tau)$$

Assuming local equilibrium

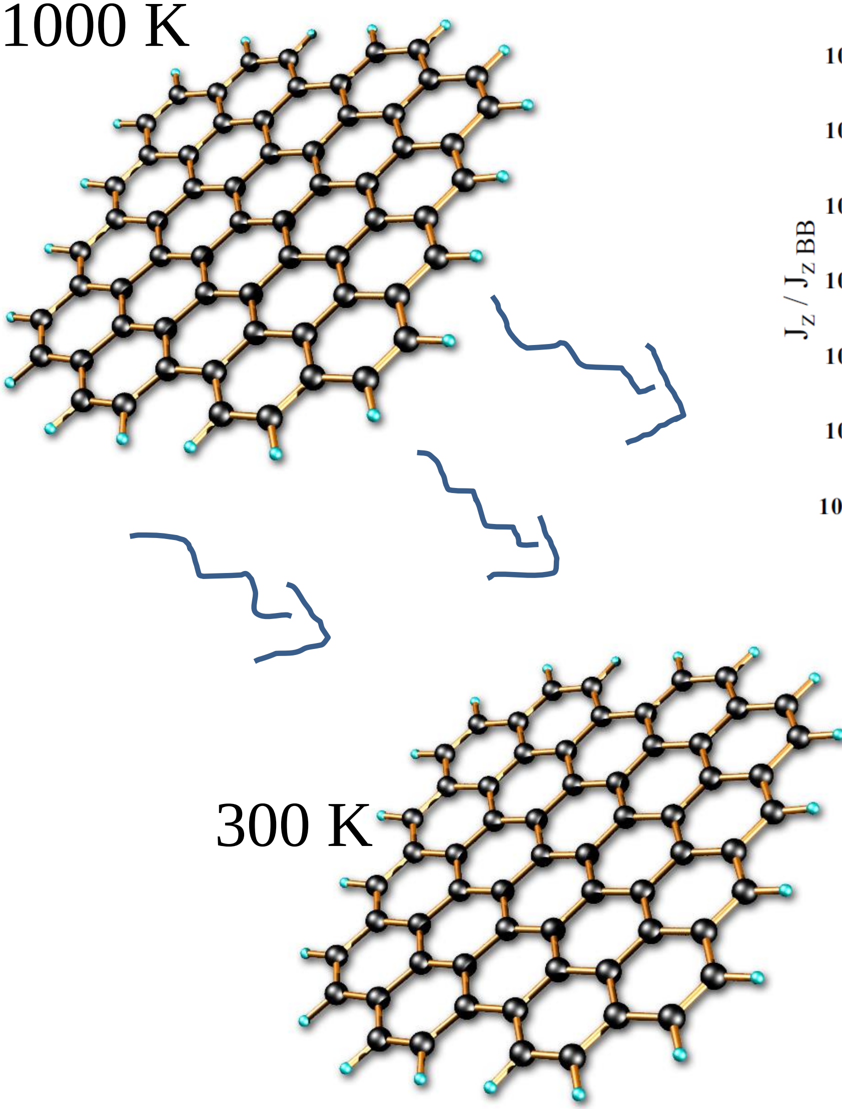


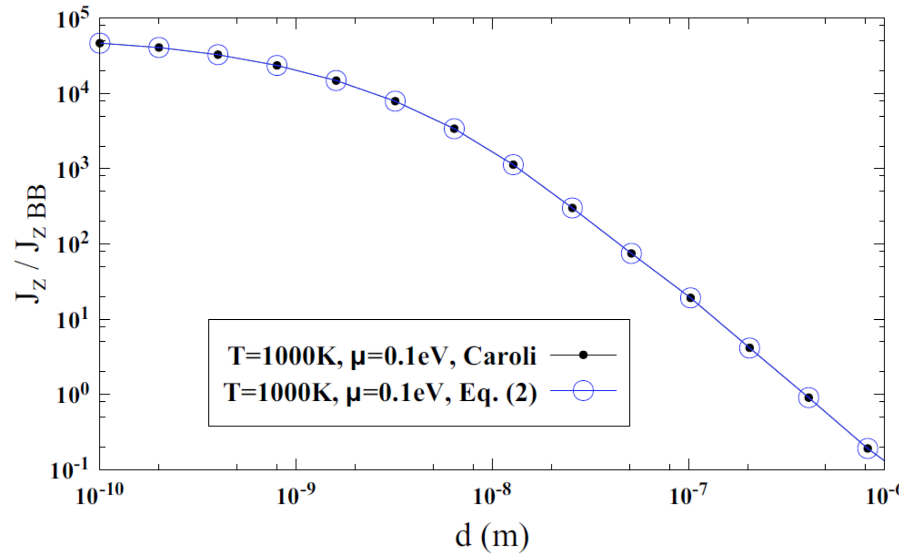
$$\Pi_\alpha^{<} = N_\alpha \left(\Pi_\alpha^r - \Pi_\alpha^a \right), \quad \Pi_\alpha^{>} = (N_\alpha + 1)\left(\Pi_\alpha^r - \Pi_\alpha^a \right)$$

$$J_1 = \int_0^\infty \frac{d\omega}{2\pi} \hbar\omega T(\omega)\left(N_1 - N_2 \right), \quad T(\omega) = \mathrm{Tr}\left(D^r \Gamma_1 D^a \Gamma_2 \right)$$

$$\Gamma_\alpha = i\left(\Pi_\alpha^r - \Pi_\alpha^a \right), \qquad \alpha = 1, 2$$

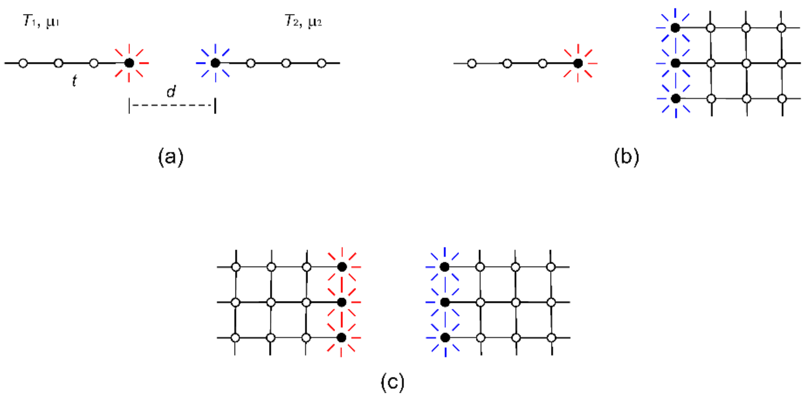
Two graphene sheets



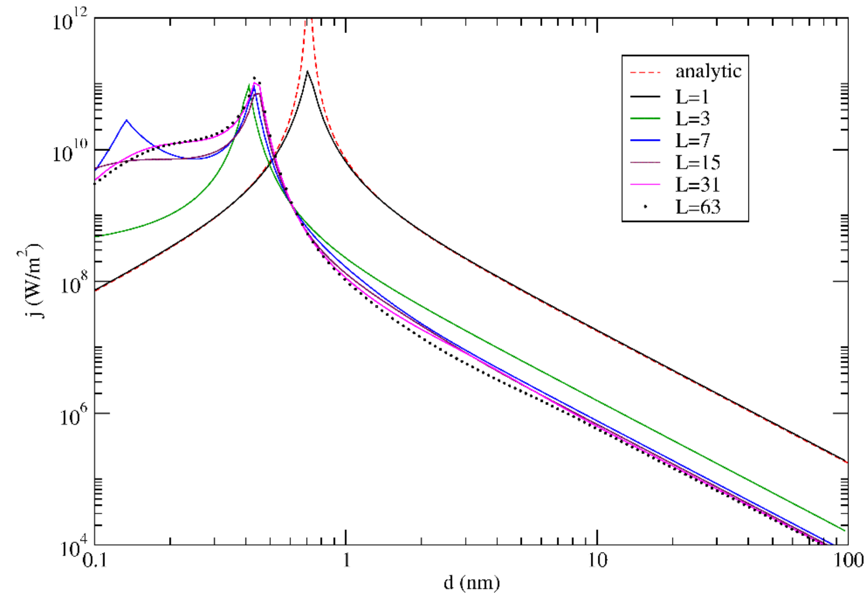


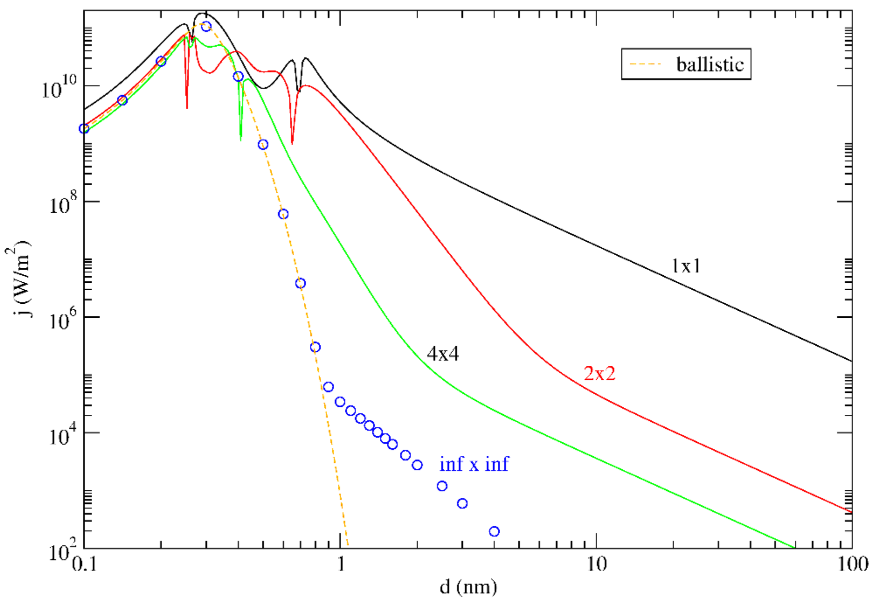
Ratio of heat flux to blackbody value for graphene as a function of distance *d*, J_{zBB} = 56244 W/m^2. From PRB 96, 155437 (2017), J.-H. Jiang and J.-S. Wang.

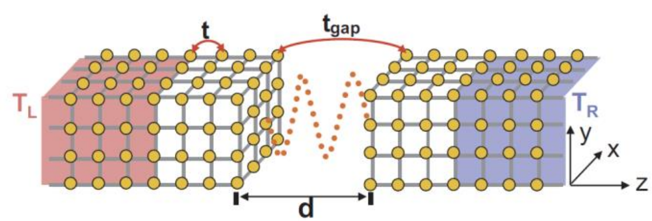
Metal surfaces and tip



: dot and surface.

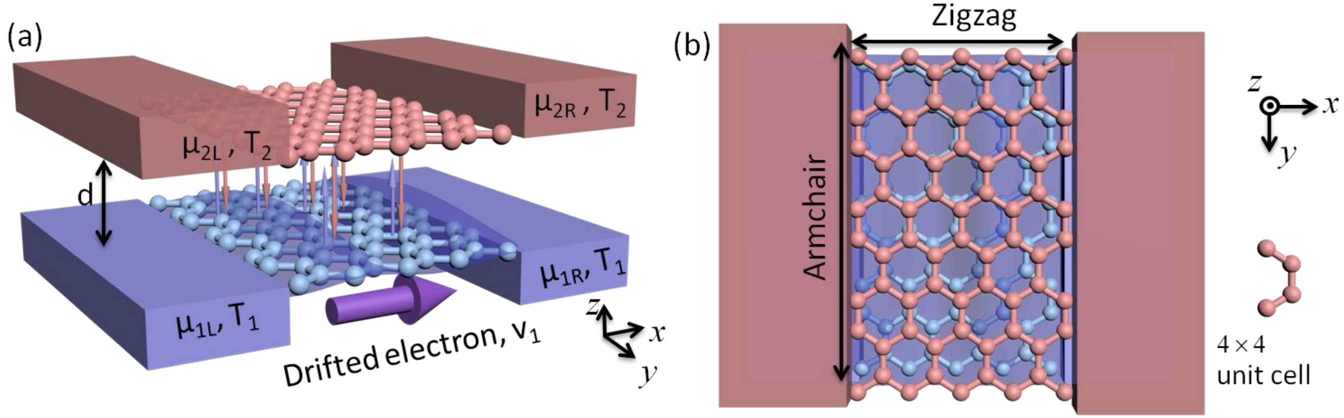




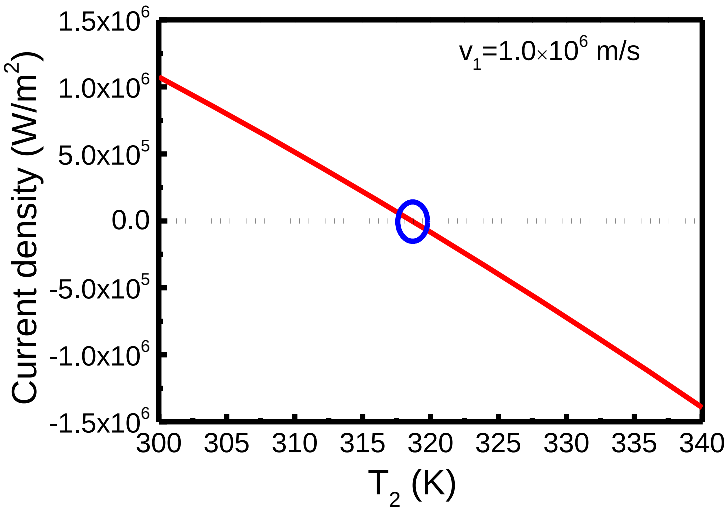


: cubic lattice parallel plate geometry. From Z.-Q. Zhang, et al. Phys. Rev. B 97, 195450 (2018); Phys. Rev. E 98, 012118 (2018).

Current-carrying graphene sheets



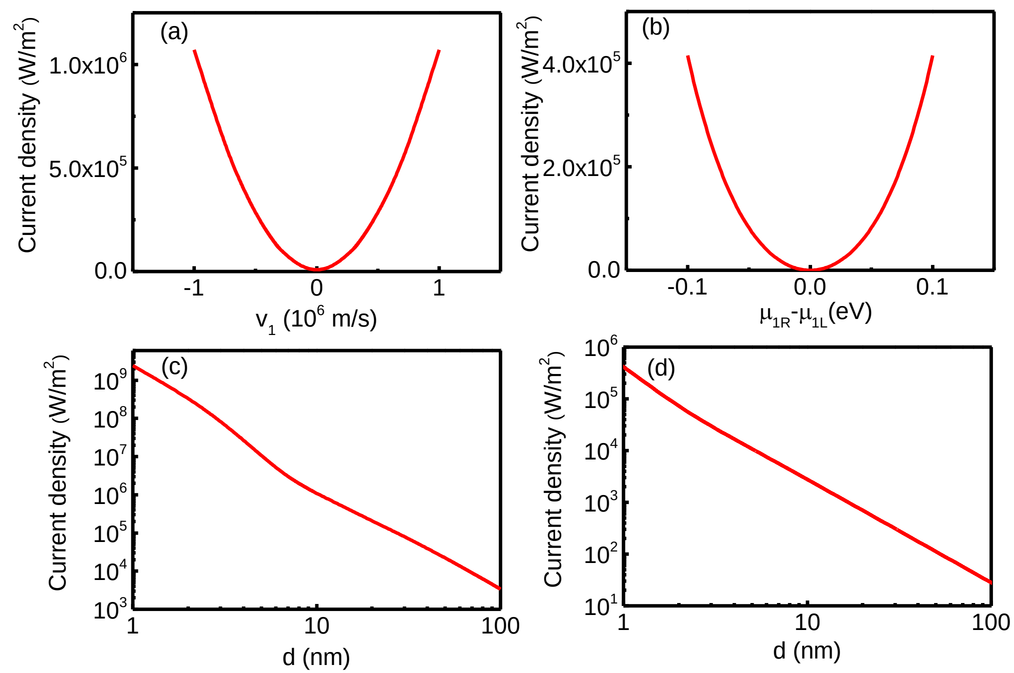
Current-induced heat transfer



↑ : Double-layer graphene. T_1=300K, varying T_2 at distance d = 10 nm, chemical potential at 0.1 eV.

From Peng & Wang, arXiv:1805.09493.

↓ : T_1=T_2=300 K. (a) and (c) infinite system (fluctuational electrodynamics), (b) and (d) 4×4 cell finite system with four leads (NEGF).



Green's function for vector photon

$$D^{\alpha\beta}(\mathbf{r},\tau;\mathbf{r}'\tau') = -\frac{i}{\hbar}\left\langle T_C A^{\alpha}(\mathbf{r},\tau)A^{\beta}(\mathbf{r}',\tau')\right\rangle$$

$$A^{\alpha}(\mathbf{r},t) = \sum_{\mathbf{q},\sigma=1,2}\sqrt{\frac{\hbar}{2\varepsilon_0\omega_{\mathbf{q}}V}}\,e^{\alpha}(\mathbf{q},\sigma)\left(a_{\mathbf{q},\sigma}e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_{\mathbf{q}}t)} + \text{h.c.}\right)$$

A: vector potential (component A^{α}),
V: volume,
e: polarization vector.

Electrons & electrodynamics

$$\hat{H} = \sum_{l,l'} c_l^\dagger H_{ll'} c_{l'} \exp\left[-\frac{i}{\hbar} e \int_{l'}^{l} \mathbf{A}\cdot d\mathbf{l} \right] + \sum_l q_l \varphi(\mathbf{r}_l)$$

$$+\frac{1}{2}\int dV \left[-\varepsilon_0 \left(\nabla\varphi\right)^2 + \varepsilon_0 \left(\frac{\partial \mathbf{A}}{\partial t}\right)^2 + \frac{1}{\mu_0}\left(\nabla\times\mathbf{A}\right)^2 \right]$$

$$\approx H_e + H_\gamma + H_{\text{int}}$$

$$H_{\text{int}} = \sum_{\alpha=(l,\mu)} I_\alpha A^\alpha, \quad \mu = 0, x, y, z$$

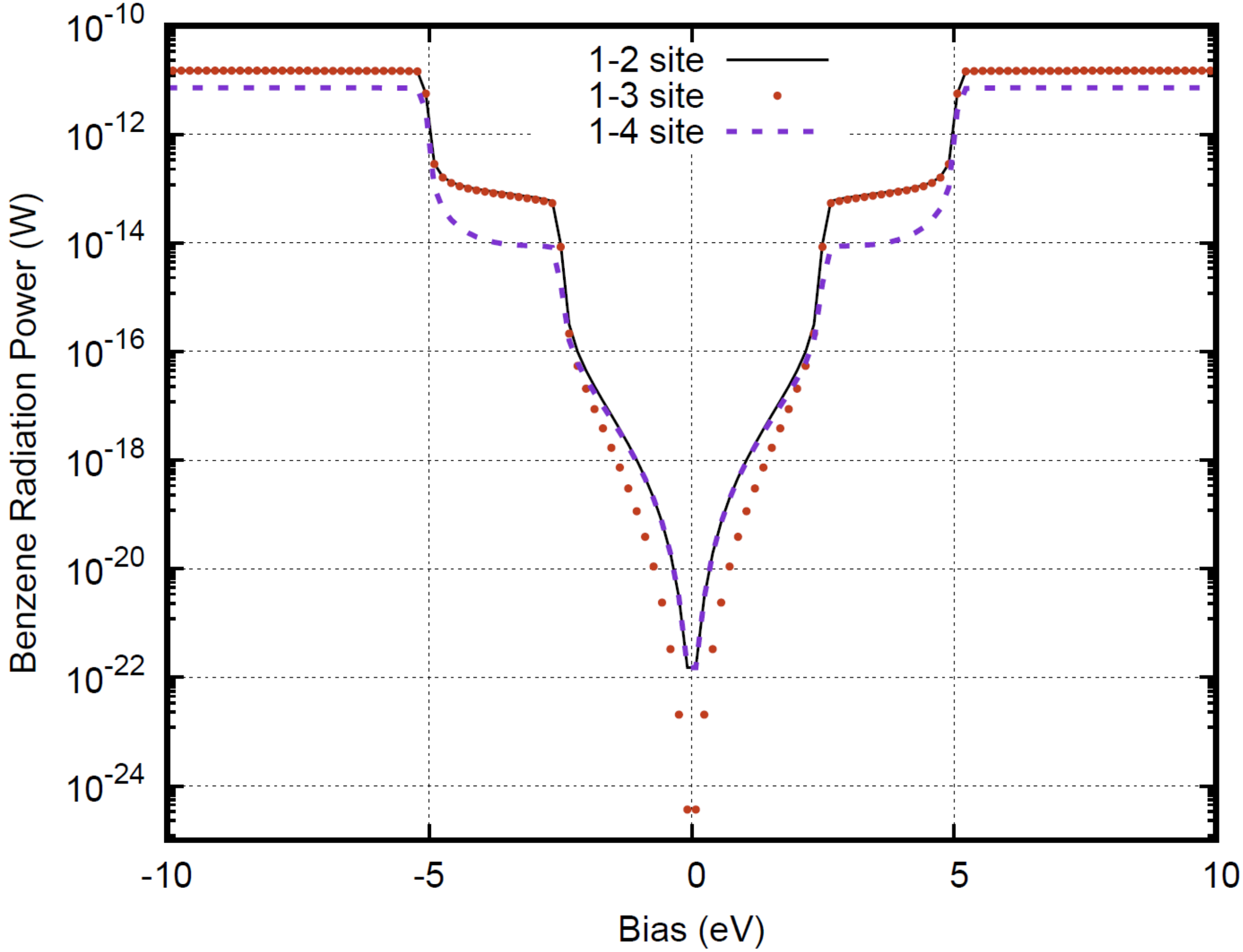
$$A^\mu \to \begin{pmatrix} \varphi \\ A_x \\ A_y \\ A_z \end{pmatrix}, \quad I_{l\mu} \to \left(q_l, -\mathbf{I}_l\right)$$

$$\Pi_{\alpha\beta}(\tau,\tau') = \frac{1}{i\hbar}\left\langle T_c I_\alpha(\tau) I_\beta(\tau') \right\rangle_0 \quad \leftarrow \text{RPA}$$

$$\mathbf{I}_l = \frac{1}{2}\sum_{l'} \frac{ie}{\hbar} c_l^\dagger H_{ll'} c_{l'} \left(\mathbf{R}_l - \mathbf{R}_{l'}\right) + \text{h.c.}$$

$$D = D_0 + D_0 \Pi D$$

Radiative energy current of a benzene molecule under voltage bias



Benzene molecule modeled as a 6-carbon ring with hopping parameter t = 2.54 eV, lead coupling Γ = 0.05 eV. Unpublished work by Zuquan Zhang.

end of lecture five

The end of lectures

These powerpoint slides can be found at
https://www.physics.nus.edu.sg/~phywjs
Under the heading of talks (CSRC-lectures-2019.pptx)