제3회 전자구조계산 겨울학교

제1원리 양자수송 계산 – 강의 1

1st-Principles Quantum Transport Calculations

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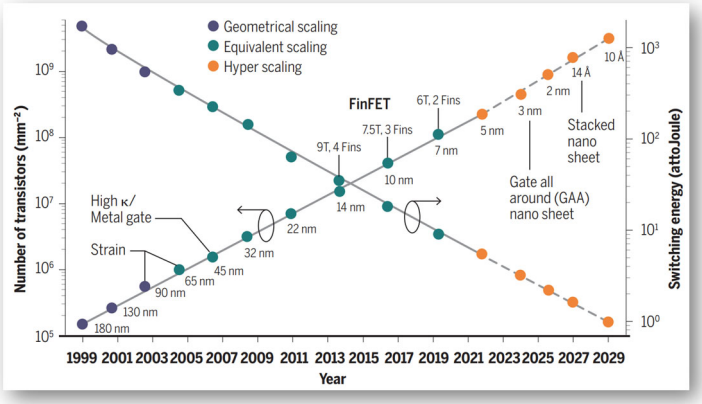
2023년 1월 20일 (금)

KAIST EE

Background: "75 Years of Transistors"







John Bardeen,
William Shockley &
Walter Brattain



Physics 1956



Robert Noyce & Gordon Moore
(Intel)



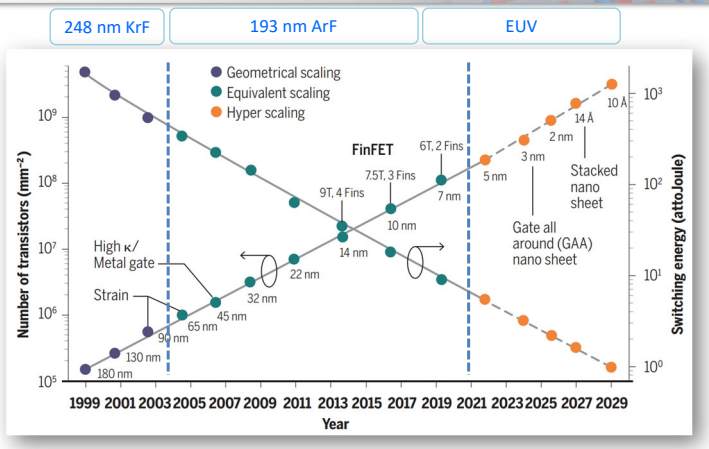
Jack Kilby
(Texas Instruments)

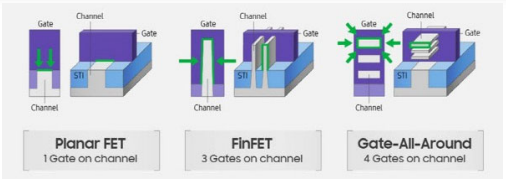


Physics 2000

Background: "75 Years of Transistors"

- Geometrical (classical) scaling
- Equivalent (effective) scaling
  - FinFET
  - Strained Si
  - High-k metal gate
- Hyper/Functional scaling
  - GAA nano sheet
  - Sub-Boltzmann FET (e.g. NCFET)
  - Embedded NVM
  - 3D stacked logic
  - …



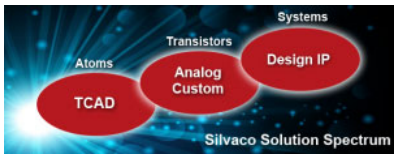


TCAD: Opportunities for 1st-principles community

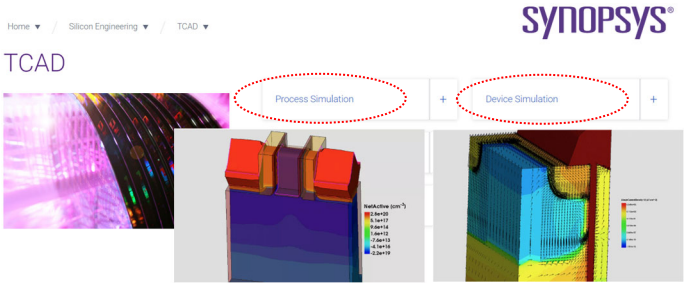
- Technology Computer Aided Design (TCAD) for semiconductor devices
- TCAD ⇔ Electronic Design Automation (EDA)
- Synopsis, Silvaco, etc.
- Types of TCAD:
  - Process TCAD
  - Device TCAD
  - *Compact models (e.g. SPICE transistor models)*



SILVACO



SYNOPSYS



Recent trends: atomistic TCAD

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TCAD



Technology Computer Aided Design (TCAD)

Simulation of semiconductor processing, device operation and interconnect characterization for technology development and manufacturing.

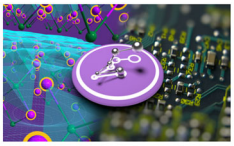
SILVACO





Home ▾ / Silicon Engineering ▾ / Atomic-Scale Modeling ▾

QuantumATK - Atomistic Simulation Software



Atomic-Scale Modeling for Semiconductor & Materials Research

The exponential growth in computer power in combination with new advancement in algorithms has in recent years enabled the practical application of atomic-scale modeling to the R&D of new materials and product design across a broad range of high tech industries.

Recent trends: atomistic TCAD

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TCAD



Process Simulation + | Device Simulation +

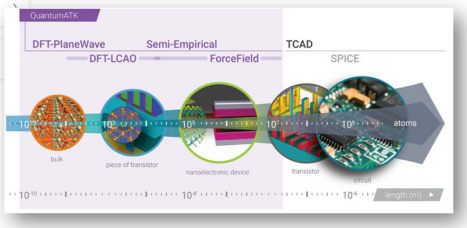
Interconnect Simulation + | Framework

Structure Editor › | Calibration & Services

Density Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)



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QuantumATK - Atomistic Simulation Software



Atomic-Scale Modeling for Semiconductor & Materials Research

The exponential growth in computer power in combination with new advancement in algorithms has in recent years enabled the practical application of atomic-scale modeling to the R&D of new materials and product design across a broad range of high tech industries.

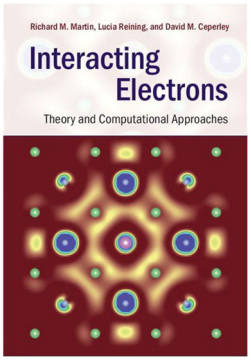
@ DTU , Copenhagen

- 2003: Atomistix
- 2008: QuantumWise
- 2017: Acquired by Synopsys

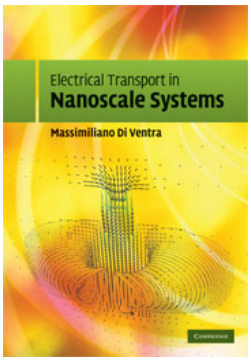


Kurt Stokbro

References

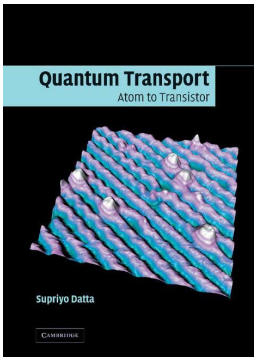


R. M. Martin, L. Reining, & D. M. Ceperley (Cambridge, 2016)



M. Di Ventra (Cambridge, 2008)

Datta



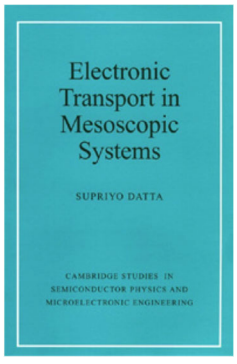
S. Datta (Cambridge, 2005)



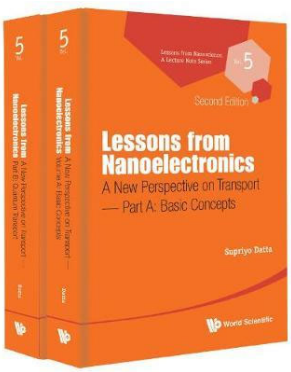




References

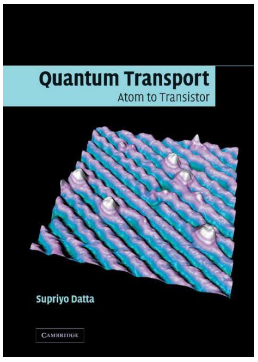


S. Datta (Cambridge, 1997)



S. Datta (World Scientific, 2017)

Datta



S. Datta (Cambridge, 2005)

온라인 강의:

- https://nanohub.org/resources/6172
- https://nanohub.org/courses/FON1
- https://nanohub.org/courses/fon2

추천 공부/숙제:

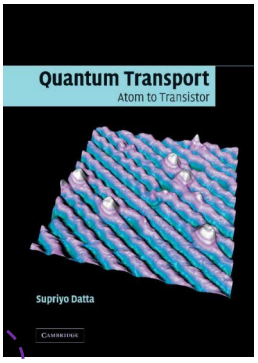
- Matlab 코드 → Python 번역



Key concepts: Quantum Mechanics/Transport

QM 101		*Advanced QM*
• 1-electron	→	many-electron
Self-consistent field (Ch. 3)		
• 1D	→	3D
Basis functions (Ch. 4)		
• Atom	→	Solid
Bandstructure (Ch. 5)		*Brillouin zone, Bloch theorem*
Subbands (Ch. 6)		*quantum confinement, DOS*
This Lecture *Capacitance (Ch. 7)*		*effective-mass Hamiltonian*
• Closed	→	Open
Level broadening (Ch. 8)		
• Equilibrium	→	Non-equilibrium
Coherent transport (Ch. 9)		
Non-coherent transport (Ch. 10)		*e-photon/phonon coupling*
Capacitance (Ch. 7), Transistor (Ch. 11)		

Datta



S. Datta (Cambridge, 2005)



S. Datta

강의 계획

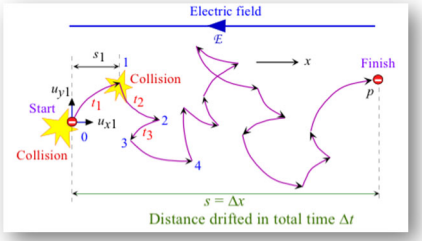
강의 1: 열린 양자계(Open quantum systems)

강의 2: 비평형 양자계(Non-equilibrium quantum systems)

강의 3: 양자수송의 새로운 관점 – 다공간 여기

Quantum transport: Why?

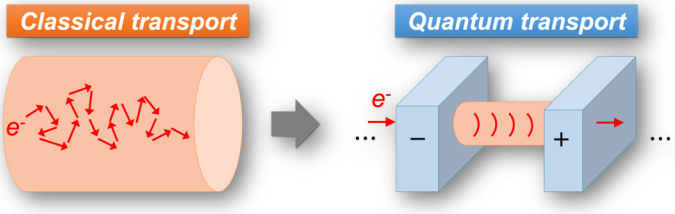
- Q: μ_d, v_d, τ, D, etc. in nanoscale?
- e.g. Relaxation time (τ) : mean time between collisions



u : Mean speed ($\neq$ drift velocity)

$\ell = u\tau$ Mean free path

- What we need:



Quantum transport: 1st-principles?

		Transport nature		Theory	
0.1 mm	*Macroscopic dimensions*				
10 μm		(3) Diffusive	$L \gg \lambda$	Drift-Diffusion eq.	
			$R_c \ll R_{ch}$		
1 μm					
0.1 μm		(2) Quasi-ballistic	$L \approx \lambda$	Boltzmann eq.	
			$R_c \approx R_{ch}$		
10 nm					
1 nm		(3) Ballistic	$L \ll \lambda$	NEGF	
			$R_c \gg R_{ch}$		
0.1 nm	*Atomistic dimensions*				

Top-down → *Conventional textbook ?*

Need to rewrite textbook! → *Bottom-up*

Quantum transport: 1st-principles?

Transport nature

"Transmission"

$$T(E) = \frac{\lambda(E)}{\lambda(E)+L}$$

0.1 mm *Macroscopic dimensions*

10 μm



(3) Diffusive $L \gg \lambda$ $T = \frac{\lambda}{L} \ll 1$

1 μm

0.1 μm



(2) Quasi-ballistic $L \approx \lambda$ $T < 1$

10 nm



1 nm

(3) Ballistic $L \ll \lambda$ $T \approx 1$

Atomistic dimensions

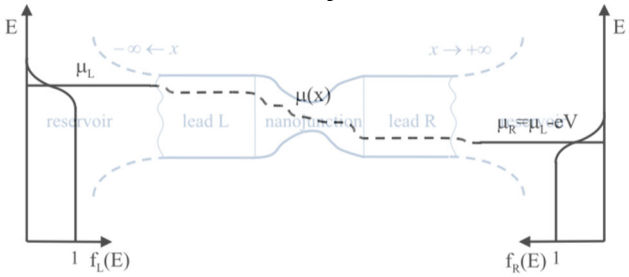
0.1 nm

Focus of this lecture "1st-principles"

Bottom-up

Landauer "picture" for quantum transport

"conductance from transmission"





Rolf William Landauer (1927~1999)

- Landauer formula:

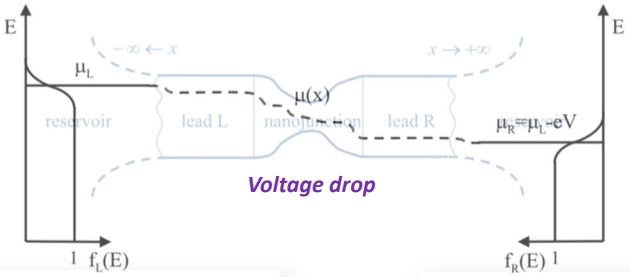
$$I = \frac{2e^2}{h} T\, V \longrightarrow G = \frac{I}{V} = \frac{2e^2}{h} T$$

where "quantum of conductance" (or "quantum of resistance"):

$$G_0 = \frac{I}{V} \equiv \frac{2e^2}{h} = 77.6\ \mu\text{S} = (12.8\ \text{kW})^{-1}$$

Landauer "picture" for quantum transport

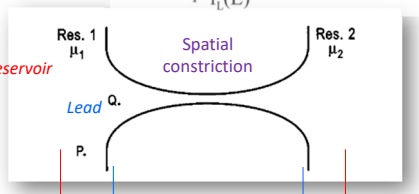
"… it is a viewpoint, not a specific equation."

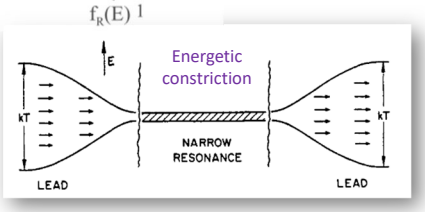




Rolf William Landauer
(1927~1999)

Contacts





$$G_B = \frac{2e^2}{h}\frac{T}{1-T}$$

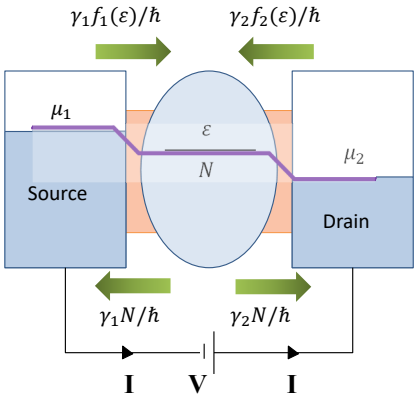
$$G_B = \frac{2e^2}{h}T$$

R. Landauer, *Z. Phys. B* **68**, 217 (1987)
R. Landauer, *J. Phys. Condens. Matter* **43**, 8099 (1989)
R. Landauer, *Phys. Scr.* **T42**, 110 (1992)
Y. Imry & R. Landauer, *Rev.Mod. Phys.* **71**, S306 (1999)

Quantum transport: Open + Non-equilibrium

"Landauer" viewpoint: Open + Non-Equilibrium Conditions

Contacts → Open



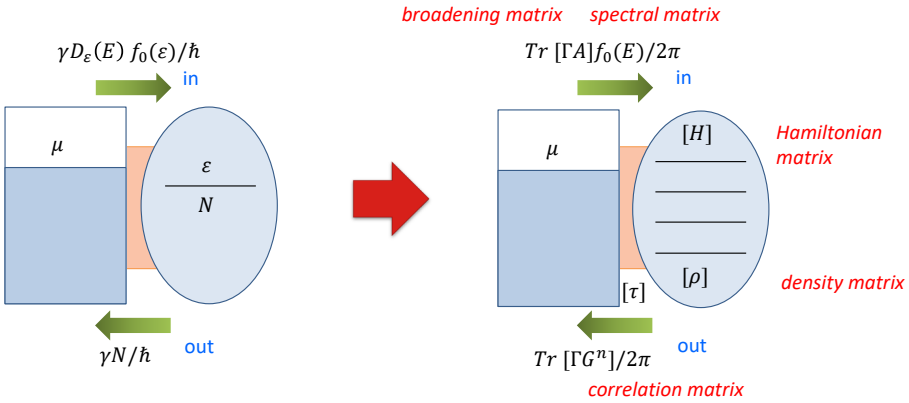
Voltage drop → Non-Equilibrium

Standard theory: Non-Equilibrium Green's Function (NEGF)

Lecture 1: Open quantum systems

cf. Datta Ch. 8

- To develop the understanding, we will use the 1-contact model (i.e. no current)
- Also keep in mind of the physical meaning of many-body quantities

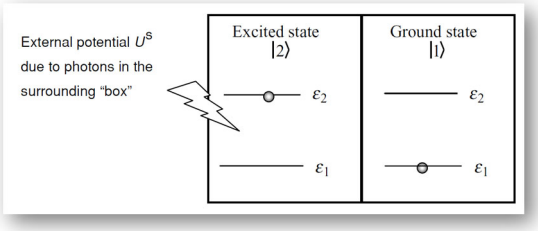


$$E\psi = H\psi + \Sigma\psi + s$$

out in

Q. Why does an atom emit light?

cf. Datta Ch. 10.1



- Using the eigenfunctions of $[H]$ as our basis:

$$i\hbar \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

→Solution:

$$\psi_1(t) = \psi_1(0) e^{-i\varepsilon_1 t/\hbar}$$
$$\psi_2(t) = \psi_2(0) e^{-i\varepsilon_2 t/\hbar}$$

→Probability:

$$P_1(t) = P_1(0)$$
$$P_2(t) = P_1(0)$$

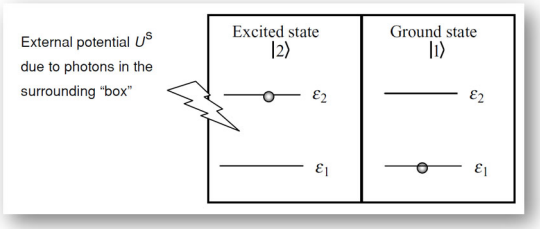
- Following the Schrodinger equation in this form, an electron should not "fall"!

→ What's missing?

Zero-point fluctuations or EM noise even @ absolute 0 K.

→ What are the solution?

Q. Why does an atom emit light?



- Solution?

$$i\hbar \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

→ NON-Hermitian Hamiltonian :

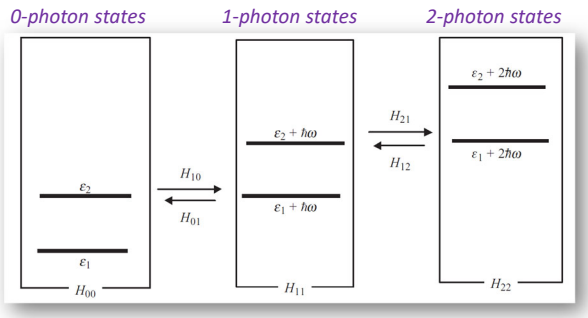
$$i\hbar \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \varepsilon_1 & [U_S]_{12} \\ [U_S]_{21} & \varepsilon_2 \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

such that

$$[U_S]_{12} \neq 0 \;\&\; [U_S]_{21} = 0 \;@\; 0\,\mathrm{K}$$

$$[U_S]_{12} > [U_S]_{21} \;@\; T > 0\,\mathrm{K}$$

Q. Why does an atom emit light?



- Better solution?

→ Electron + Photon as one big many-particle system:

$$\hat{H} = \hat{H}_e \otimes \hat{\mathbb{I}}_e + \hat{\mathbb{I}}_{ph} \otimes \hat{H}_{ph} + \hat{H}_{e-ph} \quad \& \quad |\Psi_{e,ph}\rangle = |\Psi_e\rangle\,|\Psi_{ph}\rangle$$

e.g.

$$i\hbar \begin{Bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{Bmatrix} = \begin{bmatrix} H_{00} & H_{01} & 0 \\ H_{10} & H_{11} & H_{12} \\ 0 & H_{21} & H_{22} \end{bmatrix} \begin{Bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{Bmatrix} \text{ with } \{\Psi_N\} = \begin{Bmatrix} \psi_{1,N} \\ \psi_{2,N} \end{Bmatrix}$$

Green's functions (GFs): Mathematical definition

- Generally (see e.g. wikipedia):

$$Lu(x) = f(x) \quad \rightarrow \quad LG(x,s) = \delta(x-s)$$

response impulse

- For QM (Schrödinger equation):

$$(E-H)\psi = 0 \quad \rightarrow \quad (E-H)G(E;x,y) = \delta(x-y) \quad \text{or} \quad (E\mathbf{1}-\mathbf{H})\mathbf{G}(E) = \mathbf{1}$$

with b.c. $\lim_{|x-y|\to 0} G(E;x,y) = 0$

→ retarded GF: $\mathbf{G}^R(E) = [E\mathbf{1} - \mathbf{H} + i\boldsymbol{\delta}]^{-1}$

advanced GF: $\mathbf{G}^A(E) = [E\mathbf{1} - \mathbf{H} - i\boldsymbol{\delta}]^{-1}$

where $\boldsymbol{\delta} \equiv [\delta] \equiv 0^+[\mathbb{I}]$

Preliminaries: Basis functions & Spectral funtion

cf. Datta Ch. 4.3 & 8.2

- Eigenstate basis (representation) $\phi_\alpha(\vec{r})$

→ $$[H] = \begin{bmatrix} \varepsilon_1 & 0 & 0 & \\ 0 & \varepsilon_2 & 0 & \cdots \\ 0 & 0 & \varepsilon_3 & \\ & \cdots & & \cdots \end{bmatrix}$$

- Consider: "local density of states (DOS)":

$$D(\vec{r};E) = \sum_\alpha \delta(E-\varepsilon_\alpha)\,|\phi_\alpha(\vec{r})|^2$$

- Can define "spectral function" (generalization of DOS

← diagonal elements (divided by 2π) of the "spectral function")

$$A(\vec{r},\vec{r}';E) = 2\pi \sum_\alpha \delta(E-\varepsilon_\alpha)\,\phi_\alpha(\vec{r})\phi_\alpha^*(\vec{r}')$$

$$[A](E) = \sum_\alpha \delta(E-\varepsilon_\alpha)\,\{\phi_\alpha\}\{\phi_\beta\}^+$$

real space basis

unitary transformation

eigenstate basis

Local DOS & Spectral function

cf. Datta Ch. 8.2

- @ eigenstate basis (representation) $\phi_\alpha(\vec{r})$:

$$[A(E)] = 2\pi \begin{bmatrix} \delta(E-\varepsilon_1) & 0 & 0 & \\ 0 & \delta(E-\varepsilon_2) & 0 & \cdots \\ 0 & 0 & \delta(E-\varepsilon_3) & \\ & \cdots & & \cdots \end{bmatrix}$$

- Total DOS:

$$D(E) = \frac{1}{2\pi} Trace[A(E)] = \sum_\alpha \delta(E-\varepsilon_\alpha)$$

- Sum rule: Total number of states at any point integrated over all energy → 1

$$\int d\vec{r} \int_{-\infty}^{\infty} dE \; D(\vec{r};E) = 1$$

@ eigenstate basis, since since $\int_{-\infty}^{\infty} dE\, \delta(E-\epsilon) = 1$ →

$$\int_{-\infty}^{\infty} \frac{dE}{2\pi} [A(E)] = \begin{bmatrix} 1 & 0 & 0 & \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \\ & \cdots & & \cdots \end{bmatrix}$$

GFs ↔ Spectral function

- $[A(E)]$ from $[G(E)]$: Note the mathematical identity

$$2\pi\delta(E-E_n) = i\left[\frac{2\delta}{(E-E_n)^2+\delta^2}\right]_{\delta\to 0^+} = i\left[\frac{1}{E-E_n+i\delta} - \frac{1}{E-E_n-i\delta}\right]$$

or

$$2\pi\delta([E\mathbb{I}-H]) = i\{[(E+i\delta)\mathbb{I}-H]^{-1} - [(E-i\delta)\mathbb{I}-H]^{-1}\}$$

or

$$\mathbf{A}(E) = i[\mathbf{G}(E) - \mathbf{G}^+(E)] \qquad \textit{"spectral function"}$$

where

$$\mathbf{G}^R(E) = [(E+i\delta)\mathbb{I}-\mathbf{H}]^{-1} \qquad \textit{"retarded GF"}$$
$$\mathbf{G}^A(E) = [(E-i\delta)\mathbb{I}-\mathbf{H}]^{-1} \qquad \textit{"advanced GF"}$$

Density → Density matrix @ Equilibrium

cf. Datta Ch. 4.3

- Similarly, consider equilibrium "density" for a multi-electron system:

$$n(\vec{r}) = \sum_{occ\ \alpha} \underbrace{|\phi_\alpha(\vec{r})|^2}_{\text{probability densities}} \rightarrow \sum_\alpha f_0(\varepsilon_\alpha - \mu)|\phi_\alpha(\vec{r})|^2$$

where $f_0(E) \equiv \left[1 + \exp(\frac{E}{k_B T})\right]^{-1}$ → *average occupancy of a state*

- @ eigenstate basis, we can write:

$$\varrho(\alpha,\beta) = f_\alpha \delta_{\alpha\beta} \ ; n(\vec{r}) = \sum_\alpha \sum_\beta \varrho(\alpha,\beta)\, \phi_\alpha(\vec{r})\phi_\alpha^*(\vec{r})$$

→ Can be generalized to (density ← diagonal elements of DM):

$$\varrho(\vec{r},\vec{r}') = \sum_\alpha f_0(\varepsilon_\alpha - \mu)\, \phi_\alpha(\vec{r})\phi_\alpha^*(\vec{r}')$$

real space basis

unitary transformation

eigenstate basis

or

$$[\varrho] = \sum_\alpha f_0(\varepsilon_\alpha - \mu)\, \{\phi_\alpha\}\{\phi_\beta\}^+$$

Density matrix @ Equilibrium

∴ A powerful concept: The *density matrix ϱ at equilibrium* can be written as the *Fermi function of the Hamiltonian matrix*

$$\varrho(\vec{r},\vec{r}') = \sum_\alpha f_0(\varepsilon_\alpha - \mu)\, \phi_\alpha(\vec{r})\phi_\alpha^*(\vec{r}')$$

$$\Updownarrow$$

$$\boxed{[\varrho] = f_0([H] - \mu[\mathbb{I}])}$$

or

$$n = \text{diag}\, f_0([H] - \mu[\mathbb{I}])$$

- @ eigenstate basis (representation)

$$[\varrho] = \begin{bmatrix} f_0(\varepsilon_1 - \mu) & 0 & 0 & \\ 0 & f_0(\varepsilon_2 - \mu) & 0 & \cdots \\ 0 & 0 & f_0(\varepsilon_\alpha - \mu) & \\ & \cdots & & \cdots \end{bmatrix}$$

- Total # of electrons: $N = Trace[\rho] = \sum_\alpha f_0(\varepsilon_\alpha - \mu)$

Spectral function ↔ Correlation function

- Density matrix ↔ Spectral function (@ Equilibrium):

$$[\varrho] = f_0([H] - \mu[\mathbb{I}])$$
$$= \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E-\mu)\delta([E\mathbb{I} - H])$$
$$= \int_{-\infty}^{\infty} \frac{dE}{2\pi} f_0(E-\mu)[A(E)]$$
$$\equiv \int_{-\infty}^{\infty} \frac{dE}{2\pi} [G^n(E)]_{eq}$$

- Electron correlation function:

$$N = \int_{-\infty}^{\infty} dE\, f_0(E-\mu) D(E)$$

∴

$$[G^n(E)]_{eq} = [A(E)] f_0(E-\mu)$$

$$G^n \equiv -iG^<$$

GFs: Powerful tool for open systems

- Spectral representation (eigenvalue expansion) of GFs:

$$G_{ij}(E) = \sum_n \frac{\phi_i^{(n)} * \phi_j^{(n)}}{E + i0^+ - \varepsilon_n}$$

- GFs @ eigenstate basis

$$[G(E)] = \begin{bmatrix} \frac{1}{E-\varepsilon_1+i0^+} & 0 & \cdots \\ 0 & \frac{1}{E-\varepsilon_2+i0^+} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix}$$

- cf. self energy & source

$$\Sigma_{ij}(E) = \sum_n \frac{[\tau]_{in}[\tau^+]_{nj}}{E + i0^+ - \varepsilon_n}$$

$$S_i(E) = \sum_n [\tau]_{in}\{\phi_R\}_n$$

GFs: Powerful tool for open systems

Q. Why do we want to work with

$$[\varrho] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} [G^n(E)]_{eq}$$

a continuous independent energy variable E

where, in equilibrium,

$$[G^n(E)]_{eq} = [A(E)] f_0(E-\mu)$$

rather than

$$[\varrho] = f_0(E-\mu)\delta([E\mathbb{I} - H])$$

a discrete set of eigenstates

?

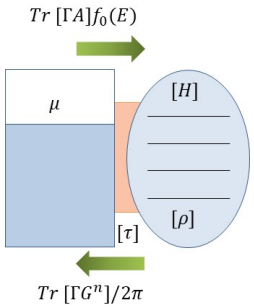
A. If we deal with $\hat{\boldsymbol{H}}_{\boldsymbol{tot}} = \hat{\boldsymbol{H}}_{\boldsymbol{S}} + \hat{\boldsymbol{H}}_{\boldsymbol{R}} + \hat{\boldsymbol{H}}_{\boldsymbol{int}}$ i.e.

$$\hat{\boldsymbol{H}}_{\boldsymbol{tot}} = \hat{\boldsymbol{H}}_{\boldsymbol{S}} \otimes \mathbb{I}_{\boldsymbol{R}} + \mathbb{I}_{\boldsymbol{S}} \otimes \hat{\boldsymbol{H}}_{\boldsymbol{R}} + \hat{\boldsymbol{H}}_{\boldsymbol{int}}$$

or

$$\bar{H} = \begin{bmatrix} H_S & H_{SR} \\ H_{RS} & H_R \end{bmatrix}$$

dimension → ∞, because dimension of $H_R \to \infty$!



GFs for open systems → Self-energy matrix

cf. Datta Ch. 8.2

- We want to calculate:

$$G \equiv \begin{bmatrix} G_S & G_{SR} \\ G_{RS} & G_R \end{bmatrix} = \begin{bmatrix} (E+i0^+)\mathbb{I}_S - H_S & -\tau \\ -\tau^+ & (E+i0^+)\mathbb{I}_R - H_R \end{bmatrix}^{-1}$$

cf. Matrix algebra:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1}$$

then,

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}$$

so that

$$Aa + Bc = I \;\&\; Ca + Dc = 0$$

$$\to c = -D^{-1}Ca$$

$$\therefore a = (A - BD^{-1}C)^{-1} \;\&$$

$$d = (D - CA^{-1}B)^{-1}$$

Self-energy matrix

- We want to calculate:

$$G \equiv \begin{bmatrix} G_s & G_{sR} \\ G_{Rs} & G_R \end{bmatrix} = \begin{bmatrix} (E+i0^+)\mathbb{I}_s - H_s & -\tau \\ -\tau^+ & (E+i0^+)\mathbb{I}_R - H_R \end{bmatrix}^{-1}$$

- Then, using $a = (A - BD^{-1}C)^{-1}$:

$$G_s(E) = \{(E+i0^+)\mathbb{I}_s - H_s - \tau G_R(E)\,\tau^+\}^{-1}$$

- Self-energy matrix: $\boxed{\Sigma_s(E) = \tau \quad G_R(E)\ \tau^+}$

$(s \times s) \quad (s \times r)\ (r \times r)\ (r \times s)$

- Power of the GF method: We can evaluate the $(s \times s)$ subsection of G exactly from

$$G_s(E) = \{(E+i0^+)\mathbb{I}_s - H_s - \Sigma_s(E)\}^{-1}$$

Self–energy matrix & Broadening matrix

- Self-energy matrix:

$$[\Sigma(E)] = [\tau][G_R]\,[\tau]^+$$

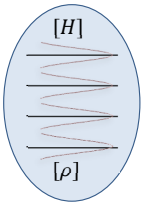
- $\Sigma(E)$: can be written as:

$$H + \Sigma(E) = [H + \Sigma_H(E)] - \frac{i\Gamma(E)}{2}$$

1. Hermitian component of Σ :

$$\Sigma_H(E) = \frac{1}{2}[\Sigma(E) + \Sigma^+(E)]$$

→ shift of energy levels - "renormalization"



2. Anti-Hermitian component of Σ :

$$\Gamma(E) = i[\Sigma(E) - \Sigma^+(E)]$$

→ broadening of energy levels - "lifetime"

Dyson's equation

For the system with dimension $(s \times s)$,

- (retarded) Green's function:

$$G_s(E) = \{(E + i0^+)\mathbb{I}_s - H_s - \Sigma_s(E)\}^{-1}$$

- Self-energy:

$$\Sigma_s(E) = \tau\, G_R(E)\, \tau^+$$

- Dyson equation:

$$\boxed{G_s = \left[G_0{}^{-1} - \Sigma\right]^{-1}} \text{ or } \boxed{\Sigma = G_0{}^{-1} - G_s{}^{-1}} \text{ or } \boxed{G_s = G_0 + G_0\, \Sigma\, G_s}$$

cf. Useful mathematical identity:

$$\boxed{\mathbf{A} \equiv \mathrm{i}[\mathbf{G} - \mathbf{G}^+] = \mathbf{G\Gamma G}^+ = \mathbf{G}^+\mathbf{\Gamma G}}$$

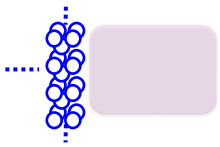
Proof:

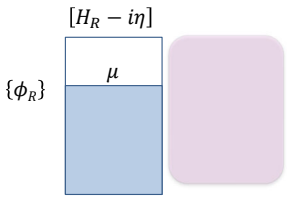
$$(\mathbf{G}^+)^{-1} - (\mathbf{G})^{-1} = -\mathbf{\Sigma}^+ + \mathbf{\Sigma} = -i\mathbf{\Gamma}$$

$$\mathbf{G}(\cdots)\mathbf{G}^+ = \mathbf{G} - \mathbf{G}^+ = -i\mathbf{G\Gamma G}^+ \quad \Rightarrow \quad \mathbf{A} = \mathbf{G\Gamma G}^+$$

$$\mathbf{G}^+(\cdots)\mathbf{G} = \mathbf{G} - \mathbf{G}^+ = -i\mathbf{G}^+\mathbf{\Gamma G} \quad \Rightarrow \quad \mathbf{A} = \mathbf{G}^+\mathbf{\Gamma G}$$

Physical picture: Electrode-only





cf. Datta Ch. 8.1

Consider first disconnected electrode & channel → EOM for the isolated electrode:

$$[E\mathbb{I}_R - H_R]\{\phi_R\} = \{0\} \text{ (electron in the bulk electrode)}$$

Modify the equation to:

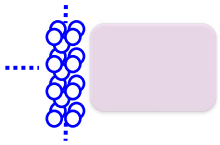
$$[E\mathbb{I}_R - H_R + i\eta]\{\phi_R\} = \{S_R\}$$

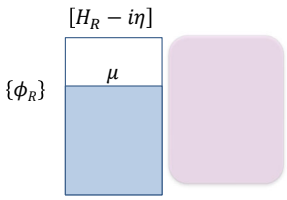
Here,

- $i[\eta] = i0^+[\mathbb{I}_R]$: extraction of electrons from the electrode
- $[S_R]$: reinjection of electrons from external sources

→ maintain the electrode at a constant electrochemical potential μ

Electrode + α → Implications





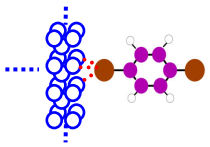
$$[E\mathbb{I}_R - H_R + i\eta\mathbb{I}_R]\{\phi_R\} = \{S_R\}$$

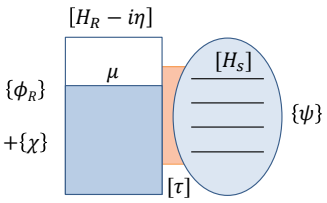
→ Implications:

- N.B. 1: Change on the viewpoint of "energy"
  - $\{\phi_R\}$ is non-zero for all energies (with peaks around the eigenenergies of $[H_R]$)

  → E: an independent variable representing the energy of excitation (probe) from the external source $\{S\}$
- N.B. 2: Breaking of "time" reversal symmetry
  - $i0^+\mathbb{I}_R$: non-Hermitian

Electrode + Channel





- Coupling channel to the electrode:

"spilling over" of ϕ_R → (1) a wavefuntion $\{\psi\}$ in the channel & (2) scattered waves $\{\chi\}$:

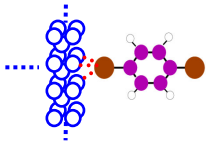
$$\begin{bmatrix} E\mathbb{I}_R - H_R + i0^+\mathbb{I}_R & -\tau^+ \\ -\tau & E\mathbb{I} - H_s \end{bmatrix} \begin{Bmatrix} \phi_R + \chi \\ \psi \end{Bmatrix} = \begin{Bmatrix} S_R \\ 0 \end{Bmatrix}$$

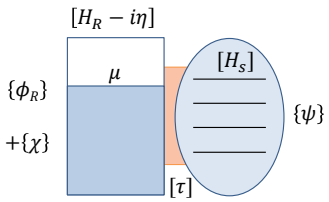
- NB: dimension of matrix blocks:

$$\begin{bmatrix} (R \times R) & (R \times s) \\ (s \times R) & (s \times s) \end{bmatrix} \begin{Bmatrix} (R \times 1) \\ (s \times 1) \end{Bmatrix} = \begin{Bmatrix} (R \times 1) \\ (s \times 1) \end{Bmatrix}$$

$$R \gg s$$

Electrode + Channel





- Coupling channel to the electrode:

"spilling over" of ϕ_R → (1) a wavefuntion $\{\psi\}$ in the channel & (2) scattered waves $\{\chi\}$:

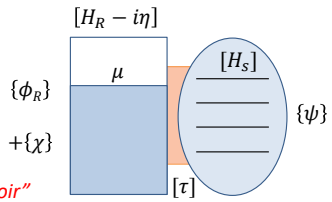
$$\begin{bmatrix} E\mathbb{I}_R - H_R + i0^+\mathbb{I}_R & -\tau^+ \\ -\tau & E\mathbb{I} - H_s \end{bmatrix} \begin{Bmatrix} \phi_R + \chi \\ \psi \end{Bmatrix} = \begin{Bmatrix} S_R \\ 0 \end{Bmatrix}$$

- Then, we can rewrite these equations:

$$[E\mathbb{I}_R - H_R + i\eta]\{\chi\} - [\tau^+]\{\psi\} = \{0\} \quad \cdots ①$$

$$[E\mathbb{I} - H_s]\{\psi\} - [\tau]\{\chi\} = [\tau]\{\phi_R\} \quad \cdots ②$$

Electrode + Channel (cont'd)



From ①,

$$\{\chi\} = [G_R]\,[\tau]^+\,\{\psi\}$$

where

$$[G_R] \equiv [E\mathbb{I}_R - H_R + i\eta\mathbb{I}_R]^{-1} \cdots ③$$

"reservoir" Retarded GF

Substituting ③ into ②, we obtain

$$[E\mathbb{I} - H_s - \Sigma]\{\psi\} = \{S\}$$

or

$$\{\psi\} = [G]\{S\};\ [G] = [E\mathbb{I} - H_s - \Sigma]^{-1}$$

where

$$\underset{(s\times s)}{[\Sigma]} = \underset{(s\times R)}{[\tau]}\ \underset{(R\times R)}{[G_R]}\ \underset{(R\times s)}{[\tau]^+}$$

Self-energy : modification of the channel due to the coupling with electrode

&

$$\underset{(s\times 1)}{\{S\}} = \underset{(s\times R)}{[\tau]}\ \underset{(R\times 1)}{\{\phi_R\}}$$

Source : excitation from the electrode

N.B.
- $R \gg s$ → $[G_R]$ & $\{\phi_R\}$ represents a property of isolated electrode
- In standard NEGF code, one-way construction (no feedback loop)

Electrode + Channel (cont'd)

From ①,

$$\{\chi\} = [G_R]\,[\tau]^+\,\{\psi\}$$

where

$$[G_R] \equiv [E\mathbb{I}_R - H_R + i\eta\mathbb{I}_R]^{-1} \cdots ③$$

Substituting ③ into ②, we obtain

$$[E\mathbb{I} - H_s - \Sigma]\{\psi\} = \{S\}$$

or

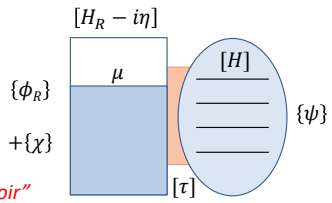
$$\{\psi\} = [G]\{S\};\ [G] = [E\mathbb{I} - H_s - \Sigma]^{-1}$$

where

$$[\Sigma] = [\tau]\ [G_R]\ [\tau]^+$$
$$(s\times s)\ \ (s\times r)\ (r\times r)\ (r\times s)$$

&

$$\{S\} = [\tau]\ \{\phi_R\}$$
$$(s\times 1)\ \ (s\times r)\ (r\times 1)$$



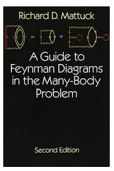
"reservoir"
Retarded GF

Self-energy : modification of the channel due to the coupling with electrode

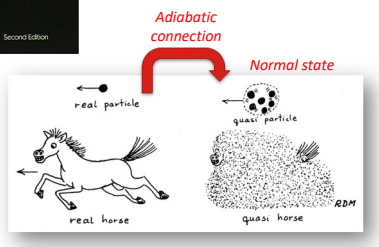
Source : excitation from the electrode

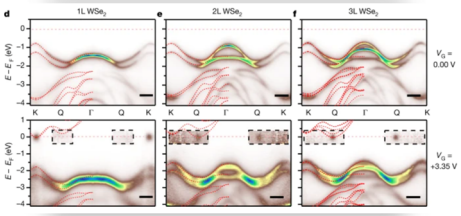
Q.
- *Size of <u>reduced</u> dimension r?*
- *How to accurately <u>model</u> $[G_R]$ & $\{\phi_R\}$ without $s \rightarrow R$ feedback effect?*

cf. "Quasi-particles"



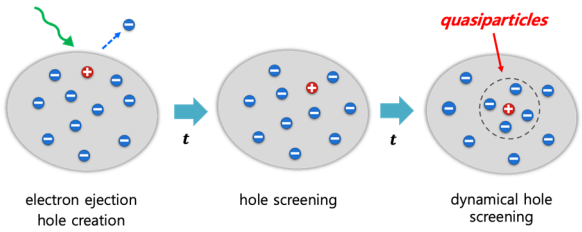
Landau Fermi liquid theory (1956~57)





P. Ngueyn et al., Nature **572**, 220 (2019)

cf. RMM, Reining, & DMC Ch. 7



- Dinamical matrix ϵ
- Dinamically screened Coulomb interaction (Fourier transform)

$$W(\boldsymbol{r},\boldsymbol{r}',t) = \int d\boldsymbol{r}''\,\frac{\epsilon^{-1}(\boldsymbol{r},\boldsymbol{r}'',t)}{|\boldsymbol{r}''-\boldsymbol{r}'|}$$

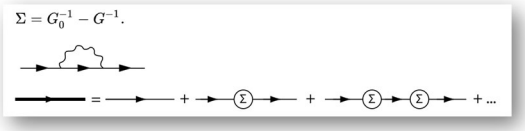
or (Fourier transform)

$$W_{\boldsymbol{G},\boldsymbol{G}'}(\boldsymbol{q};\omega) = \epsilon_{\boldsymbol{G},\boldsymbol{G}'}(\boldsymbol{q},\omega)v_C(\boldsymbol{q}+\boldsymbol{G}')$$

Self energy and Green's functions

- Self energy ← GW approximation:

$$\Sigma = iGW$$

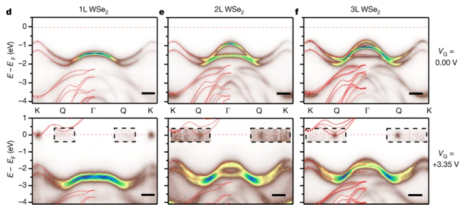


- Assuming the system is homogeneous:

$$A_{\boldsymbol{k}}(E) = -2\mathrm{Im}\, G_{\boldsymbol{k}}(E) \approx \frac{Z_{\boldsymbol{k}}}{E - (\varepsilon_{\boldsymbol{k}}' + i\Gamma_{\boldsymbol{k}})}$$

quasi-particle weight (pointing to $Z_{\boldsymbol{k}}$)

Inverse lifetime (pointing to $\Gamma_{\boldsymbol{k}}$)



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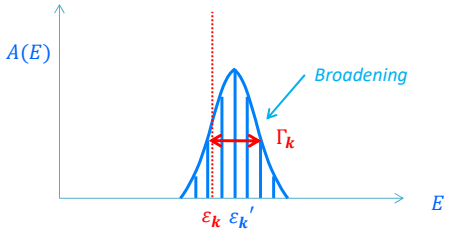


Supplemental Notes

Physical significance of GFs: Time-domain picture

cf. Datta Ch. 8.3

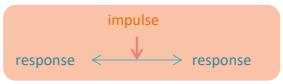
- Remind:

$$2\pi\delta([E\mathbb{I}-H]) = i\{[(E+i\delta)\mathbb{I}-H]^{-1}-[(E-i\delta)\mathbb{I}-H]^{-1}\}$$

$$\mathbf{A}(E) = i[\mathbf{G}(E)-\mathbf{G}^{+}(E)]$$

- $\mathbf{G}(E)$ @ eigenstate basis:

$$[G(E)] = \begin{bmatrix} \frac{1}{E-\varepsilon_1+i0^+} & 0 & \cdots \\ 0 & \frac{1}{E-\varepsilon_2+i0^+} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix}$$



Impulse response of the Schrödinger equation

- Consider the Fourier transform of $G(E)$:

$$[\tilde{G}^R(t)] = \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar} e^{-Et/\hbar}\,[G(E)]$$

$$= -\frac{i}{\hbar}\,\Theta(t)\,e^{-0^+t}\begin{bmatrix} e^{-\varepsilon_1 t/\hbar} & 0 & \cdots \\ 0 & e^{-\varepsilon_2 t/\hbar} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix}$$

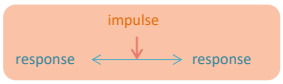
Physical significance of GFs (cont'd)

- Diagonal elements satisfy:

$$\left(i\hbar\frac{\partial}{\partial t}-\varepsilon_\alpha\right)\tilde{G}^R_{\alpha\alpha}(t) = \delta(t)$$

so we can write:

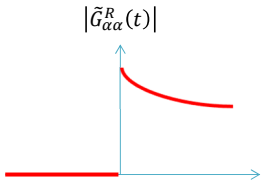
$$\left(i\hbar\frac{\partial}{\partial t}-[H]\right)[\tilde{G}^R(t)] = [I]\delta(t)$$



Impulse response of the Schrödinger equation

→ Interpretation of $\tilde{G}^R(t)$: impulse response of the Schrödinger equation (*"retarded GFs"*)

$$\left(i\hbar\frac{\partial}{\partial t}-[H]\right)[\Psi(t)] = 0$$



- $\tilde{G}^R_{nm}(t)$: n-th component of the wavefunction if the system is given an impulse excitation at its m-th component

Advanced GFs in time domain

- "Advanced" GFs:

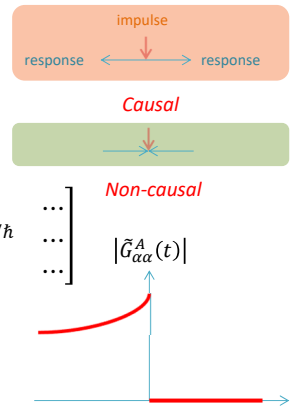
$$\left[\tilde{G}^A(t)\right] = \left[\tilde{G}^R(-t)\right]^*$$

→ satisfies the same equation:

$$\left(i\hbar\frac{\partial}{\partial t} - [H]\right)\left[\tilde{G}^A(t)\right] = [I]\delta(t)$$

but it is zero at all times after $t = 0$:

$$\left[\tilde{G}^R(t)\right] = +\frac{i}{\hbar}\,\Theta(-t)\,e^{+0^+t}\begin{bmatrix} e^{-\varepsilon_1 t/\hbar} & 0 & \cdots \\ 0 & e^{-\varepsilon_2 t/\hbar} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix}$$



← Fourier transform of $\mathbf{G}^+(E)$

∴ Retarded & Advanced GFs in the energy domain:

$\mathbf{G}(E) = [(E + i\delta)\mathbb{I} - \mathbf{H}]^{-1}$ *"retarded GF"*

$\mathbf{G}^+(E) = [(E - i\delta)\mathbb{I} - \mathbf{H}]^{-1}$ *"advanced GF"*

Spectral function in time domain

- Remind:

$$2\pi\delta([E\mathbb{I} - H]) = i\{[(E + i\delta)\mathbb{I} - H]^{-1} - [(E - i\delta)\mathbb{I} - H]^{-1}\}$$

$$\mathbf{A}(E) = i[\mathbf{G}(E) - \mathbf{G}^+(E)]$$

- Spectral function in time domain:

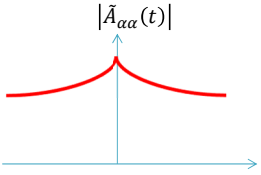
$$\tilde{A}_{\alpha\alpha}(t) = i\left[\tilde{G}^R_{\alpha\alpha}(t) - \tilde{G}^A_{\alpha\alpha}(t)\right]$$

- Since both GFs satisfy the same differential equation:

$$\left(i\hbar\frac{\partial}{\partial t} - [H]\right)\left[\tilde{G}^A(t)\right] = [I]\delta(t)$$

→ $[A(t)]$ satisfies the homogeneous differential equation *without* the impulse excitation:

$$\left(i\hbar\frac{\partial}{\partial t} - [H]\right)[A(t)] = [0]$$



Self-energy: Physical meaning

- Back to the device subset:

$$\left(i\hbar\frac{\partial}{\partial t}-[H]\right)[G(t)]-\int dt'\,[\Sigma(t-t')][G(t')]=[I]\delta(t)$$

convolution

- Let's ignore the E dependence of Σ ("memory effect") and simplify the problem by considering a device with just a single energy level ε :

$$\left(i\hbar\frac{\partial}{\partial t}-\varepsilon-\Sigma\right)[G(t)]=\delta(t)$$

N.B. Will ignore the energy of the self-energy

$$\Rightarrow G(t)=-\frac{i}{\hbar}e^{-i(\varepsilon+\Sigma)t/\hbar}\Theta(t)$$

$$\Rightarrow G(t)=-\frac{i}{\hbar}e^{-i\varepsilon' t/\hbar}e^{-\gamma t/2\hbar}\Theta(t)$$

where

$$\varepsilon'=\varepsilon\underbrace{+\mathrm{Re}\Sigma}_{\text{shift in energy level}} \quad \& \quad \gamma=\underbrace{-2\mathrm{Im}\Sigma}_{\text{finite lifetime}}$$

Self-energy: Physical meaning (cont'd)

- Back to the device subset:

$$\left(i\hbar\frac{\partial}{\partial t}-[H]\right)[G(t)]-\int dt'\,[\Sigma(t-t')][G(t')]=[I]\delta(t)$$

convolution

- Let's ignore the E dependence of Σ ("memory effect") and simplify the problem by considering a device with just a single energy level ε :

$$\left(i\hbar\frac{\partial}{\partial t}-\varepsilon-\Sigma\right)[G(t)]=\delta(t)$$

$$\Rightarrow G(t)=-\frac{i}{\hbar}e^{-i\varepsilon' t/\hbar}e^{-\gamma t/2\hbar}\Theta(t)$$

- Fourier transform

$$\Rightarrow G(E)=(E-\varepsilon'+i\gamma/2)^{-1}$$

$$\Rightarrow \frac{\mathrm{A}(E)}{2\pi}=i\{G(E)-G^{+}(E)\}=\underbrace{\frac{\gamma}{(E-\varepsilon')^2+(\gamma/2)^2}}_{\text{"broadening"}}$$

$$|G(t)|^2=\frac{1}{\hbar^2}e^{-\gamma t/\hbar}\Theta(t)$$

where

$$\frac{1}{\tau}=\frac{\gamma}{\hbar}=-\frac{2\mathrm{Im}\Sigma}{\hbar}$$

N.B. "Uncertainty" relation:

$$\tau\,\gamma=\hbar$$

"inverse lifetime"