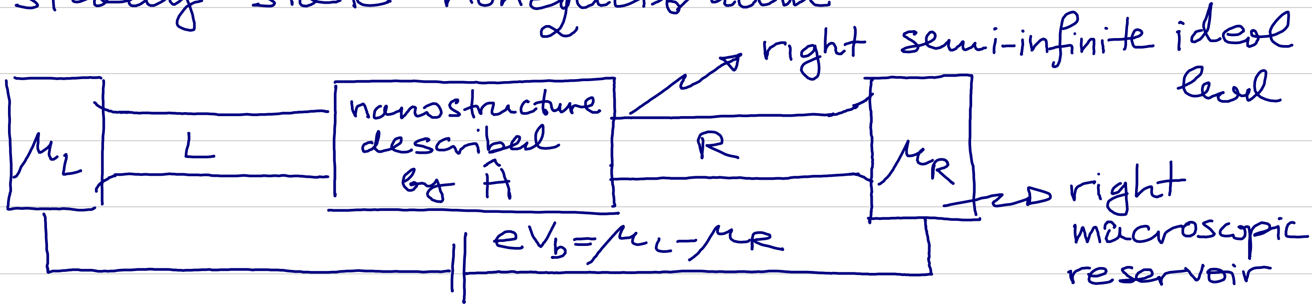
LECTURE 10: Quantum transport via Keldysh or nonequlibrium Green function (NEGF) formalism

1° NEGF-based expression for density matrix in steady-state nonequlibrium



$$\hat{\rho}_{eq} = -\frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{Im}\, \hat{G}^r f(E)\, dE = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{A} f(E)\, dE$$

$$\hat{A} = i(\hat{G}^r - \hat{G}^a)$$

$\hookrightarrow$ spectral function

$$\hat{G}^r = (E - \hat{H} - \hat{\Sigma}_L^r - \hat{\Sigma}_R^r)^{-1}$$

$$\hat{G}^a = [\hat{G}^r]^\dagger$$

$$[\hat{G}^r]^{-1} = E - \hat{H} - \hat{\Sigma}_L^r - \hat{\Sigma}_R^r \Rightarrow [\hat{G}^a]^{-1} = E - \hat{H} - [\hat{\Sigma}_L^r]^\dagger - [\hat{\Sigma}_R^r]^\dagger$$

$$\hat{G}^r \cdot \Big/ \ [\hat{G}^r]^{-1} - [\hat{G}^a]^{-1} = i\hat{\Gamma}_L + i\hat{\Gamma}_R \ \Big/ \cdot \hat{G}^a$$

$$\hat{\Gamma}_L = i(\hat{\Sigma}_L^r - [\hat{\Sigma}_L^r]^\dagger) = \hat{\Gamma}_L^\dagger$$

$$\hat{\Gamma}_R = i(\hat{\Sigma}_R^r - [\hat{\Sigma}_R^r]^\dagger) = \hat{\Gamma}_R^\dagger$$

$$\left.\begin{aligned} \hat{I}\hat{G}^a - \hat{G}^r \cdot \hat{I} &= i\hat{G}^r\hat{\Gamma}_L\hat{G}^a + i\hat{G}^r\hat{\Gamma}_R\hat{G}^a \\ \hat{A} = i(\hat{G}^r - \hat{G}^a) &= \underbrace{\hat{G}^r\hat{\Gamma}_L\hat{G}^a}_{\hat{A}_L} + \underbrace{\hat{G}^r\hat{\Gamma}_R\hat{G}^a}_{\hat{A}_R} \end{aligned}\right\}$$

$\Rightarrow$ ANSATZ: out of equilibrium, states described by the spectral function due to the left lead $\hat{A}_L$ are filled according to $f_L(E) \equiv f(E-\mu_L)$ and equivalently for the right lead using $\hat{A}_R$ and $f_R(E)$:

$$\hat{\rho}_{neq} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\hat{A}_L(E) f_L(E) + \hat{A}_R f_R(E) \right] dE$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \hat{G}^r \underbrace{\left(i f_L \hat{\Gamma}_L + i f_R \hat{\Gamma}_R \right)}_{\text{lesser self-energy due to semi-infinite leads}} \hat{G}^a$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \hat{G}^<(E)\, dE$$

$\Rightarrow$ lesser Green function for quantum-coherent transport in two-terminal geometry where inelastic scattering of electrons from other quasiparticles (electrons, phonons, magnons, ...) is ABSENT

$$\hat{G}^r = \left(E - \hat{H} - \hat{\Sigma}^r_L - \hat{\Sigma}^r_R \right)^{-1}$$ $\Rightarrow$ gives density of states

$$\underbrace{G^< = \hat{G}^r \hat{\Sigma}^< \hat{G}^a}_{\text{Keldysh integral equation}}$$ $\Rightarrow$ describes how those states are occupied in nonequilibrium

$\langle \hat{O} \rangle = \mathrm{Tr}\left[\hat{\rho}_{neq} \hat{O} \right]$ $\Rightarrow$ expectation value of any quantity in steady (i.e., time-independent) nonequilibrium

2° Splitting $\hat{\rho}_{neq}$ into "equilibrium" and "current-driven" contribution for theoretical analysis or numerical integration

$$\underbrace{\hat{G}^< + \hat{G}^r\hat{\Gamma}_L\hat{G}^a f_R - i\hat{G}^r\hat{\Gamma}_L\hat{G}^a f_R}$$

$$\Rightarrow \hat{G}^< = i\,\hat{G}^r\underbrace{(\hat{\Gamma}_L + \hat{\Gamma}_R)}\hat{G}^a f_R + i\,\hat{G}^r\hat{\Gamma}_L\hat{G}^a(f_L - f_R)$$

$$\hat{\Gamma}_L + \hat{\Gamma}_R = i\left([\hat{G}^a]^{-1} - [\hat{G}^r]^{-1}\right)$$

$$\hat{G}^< = i\,(\hat{G}^r - \hat{G}^a)f_R + i\,\hat{G}^r\hat{\Gamma}_L\hat{G}^a(f_L - f_R)$$

FIRST TERM

$$\hat{\rho}_{neq} = \frac{1}{2\pi i}\int dE\,\hat{G}^< = -\frac{1}{\pi}\int_{-\infty}^{\infty} dE\,\mathrm{Im}\,\hat{G}^r f(E-\mu_R)$$

$$+\frac{1}{2\pi}\int_{-\infty}^{\infty} dE\,\hat{G}^r\hat{\Gamma}_L\hat{G}^a\underbrace{[f(E-\mu_L) - f(E-\mu_R)]}$$

SECOND TERM

→ true current-driven part of $\hat{\rho}_{neq}$ is $\hat{\rho}_{CD} = \hat{\rho}_{neq} - \hat{\rho}_{eq}$

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HOW TO CONSTRUCT THE PROPER GAUGE-INVARIANT DENSITY MATRIX IN STEADY-STATE NONEQUILIBRIUM: APPLICATIONS TO SPIN-TRANSFER AND SPIN-ORBIT TORQUES

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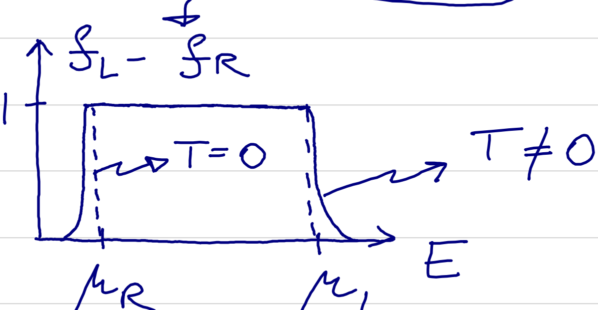
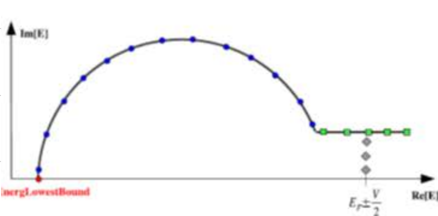


→ computational algorithms for integration of two terms in $\hat{\rho}_{neq}$

integration contour moved into the complex plane to avoid spiky integrand directly along Re[E], but this violates current conservation

adaptive integration of the second term directly along Re[E] axis



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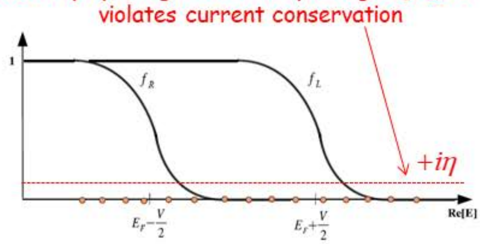
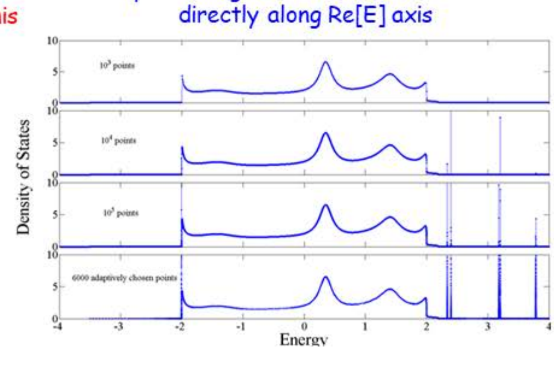
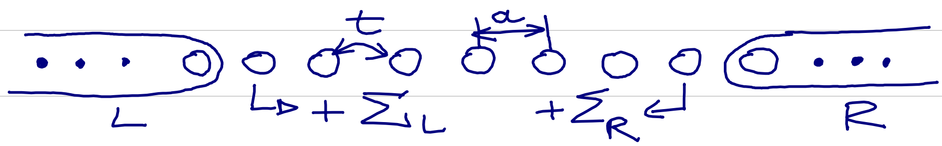


SECOND TERM



2° NEGF-based expression for Landauer-Büttiker formula and the scattering matrix



$\rightarrow$ in 1D tight-binding chain $\Sigma_L = \Sigma_R = -te^{ika}$

$$\Gamma_R = i(\Sigma_R - \Sigma_L) = 2t\sin ka = \underbrace{\frac{\hbar v}{a}}$$

electron escape rate into the right lead and right reservoir at $+\infty$

$\hat I_R = \frac{2_s e}{\hbar}\hat\Gamma_R$ looks like operator of total current in the right lead

$$I_R = \mathrm{Tr}[\hat\rho_{neq}\cdot\hat I_R] = \frac{2_s e}{2\pi}\int_{-\infty}^{\infty} dE\,\mathrm{Tr}\left[\frac{\hat\Gamma_R}{\hbar}\hat G^r\Gamma_L\hat G^a\right](f_L - f_R)$$

$$I_R = -I_L = I = \frac{2e}{h}\int_{-\infty}^{+\infty} dE\,\mathrm{Tr}[\hat\Gamma_R\hat G^r\hat\Gamma_L\cdot\hat G^a](f_L - f_R)$$

(Caroli, Combescot, Nozieres, Saint-James 1971)

■ Linear-response conductance

$V_b \to 0 \Rightarrow f_L - f_R \approx (-\partial f/\partial E)(\mu_L - \mu_R)$

$$G = \lim_{V_b\to 0} I/V_b = \int_{-\infty}^{+\infty} dE\left(-\frac{\partial f}{\partial E}\right)\underbrace{\mathrm{Tr}[\hat\Gamma_R\hat G^r\hat\Gamma_L\hat G^a]},$$

$\mathrm{Tr}[\hat t\hat t^\dagger]$ where $\hat t = \sqrt{\hat\Gamma_R}\cdot\hat G^r\cdot\sqrt{\hat\Gamma_L}$

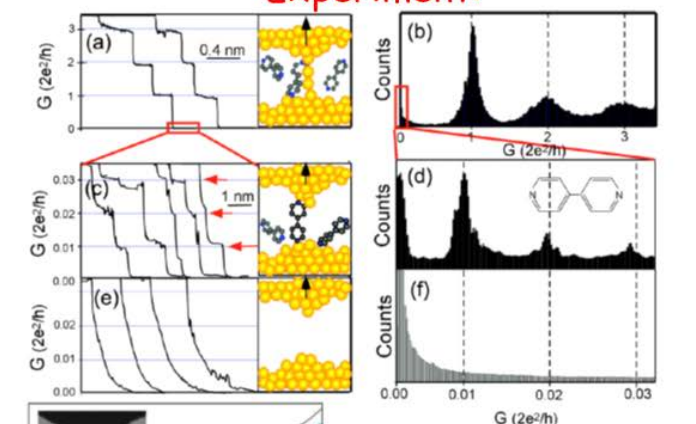
scattering matrix

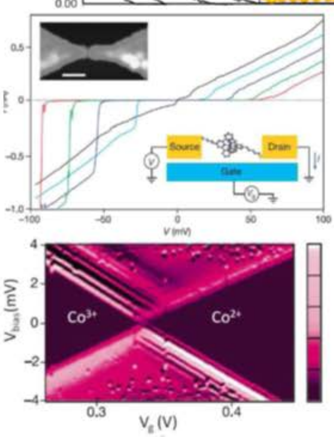
$$\hat S = \begin{pmatrix}\hat S_{LL}\equiv\hat r & \hat S_{LR}\equiv\hat t' \\ \hat S_{RL}\equiv\hat t & S_{RR}\equiv\hat r'\end{pmatrix} = -i\hat I\delta_{pq} + i\sqrt{\hat\Gamma_p}\cdot\hat G^r_{pq}\cdot\sqrt{\hat\Gamma_q}$$

(Fisher-Lee formula)

3° EXAMPLE: Single molecule nanojunction

Experiment:





Coulomb blockade and the Kondo effect in single-atom transistors

Jiwoong Park, Abhay N. Pasupathy, Jonas I. Goldsmith, Connie Chang, Yuval Yaish, Jason R. Petta, Marie Rinkoski, James P. Sethna, Héctor D. Abruña, Paul L. McEuen & Daniel C. Ralph

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Advances and challenges in single-molecule electron transport

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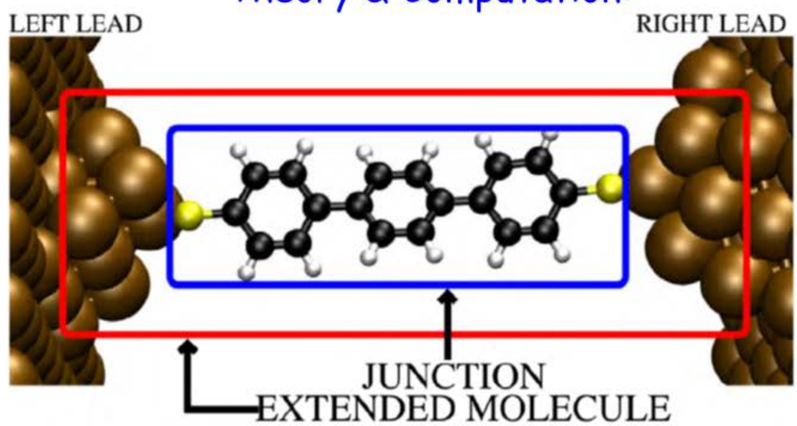
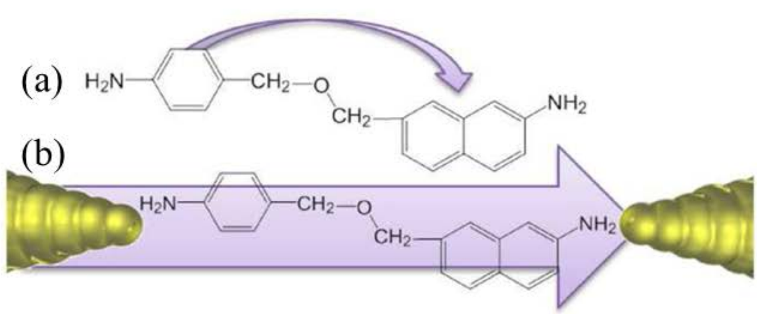
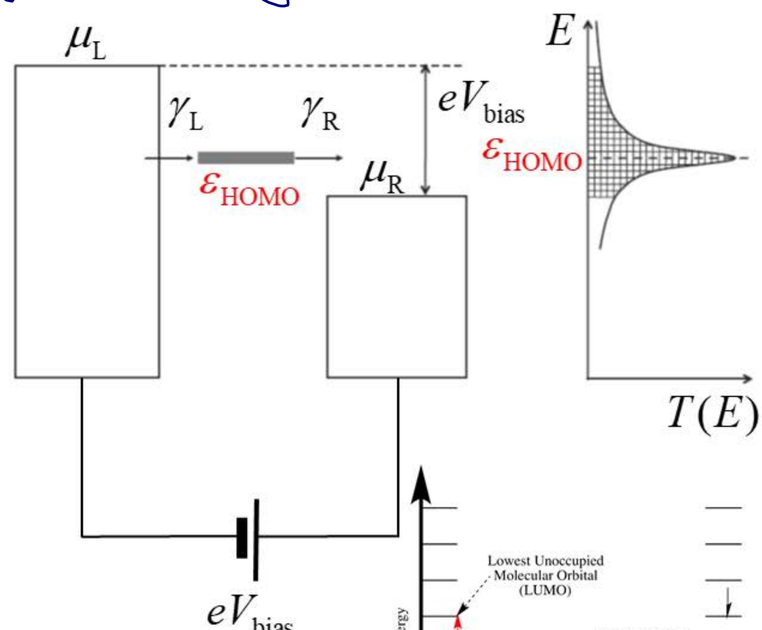
Theory & Computation:

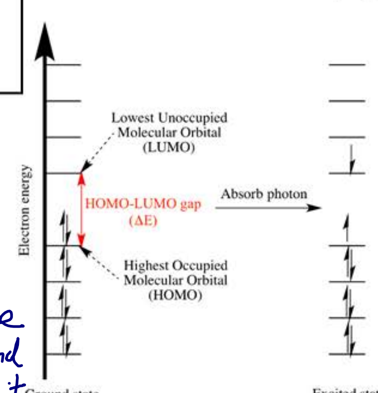


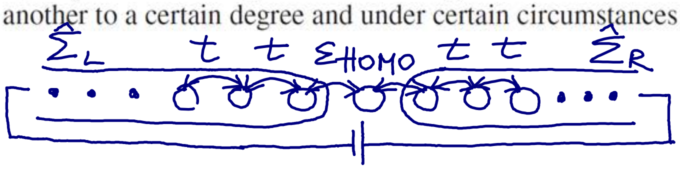
Formulate simplest 1D tight-binding model:



Schematic representations of charge transfer and charge transport processes. (a) In the charge transfer example, an electron tunnels from the benzene donor to the acceptor naphthalene via the intervening bridge. (b) When the molecule is connected to macroscopic electrodes a junction is formed and injected charges move, for instance, from the left-hand electrode to the right-hand electrode via the molecule. These two scenarios are very different; however, they both involve quantum tunneling and can be related to one another to a certain degree and under certain circumstances







$$\hat{H} = \varepsilon_{HOMO} |0\rangle\langle 0|$$

$$\left.\begin{array}{l}\hat{\Sigma}_L = -i\gamma_L/2 \\ \hat{\Sigma}_R = -i\gamma_R/2\end{array}\right\} \text{wide band limit}$$

$\Rightarrow$ if HOMO & LUMO originate from d-orbitals, which are intrinsically localized in space, one can expect weak coupling to metallic electrode

$$\gamma_{L,R} \ll |\varepsilon_{HOMO,LUMO} - E_F|$$

$$\hat{G}^r = [E - \hat{H} - \hat{\Sigma}_L - \hat{\Sigma}_R]^{-1} = [E - \varepsilon_{HOMO} - i(\gamma_L + \gamma_R)]^{-1}$$

$$\hat{\Gamma}_L = \gamma_L, \quad \hat{\Gamma}_R = \gamma_R, \quad \gamma = \gamma_L + \gamma_R$$

$$D(E) = -\frac{1}{\pi} \operatorname{Im} \hat{G}^r = \frac{1}{2\pi} \frac{\gamma}{(E-\gamma)^2 + (\gamma/2)^2}$$

$$I(V_{bias}) = \frac{2se}{h} \int_{-\infty}^{+\infty} \underbrace{\mathrm{Tr}[\gamma_R \hat{G}^r \gamma_L \hat{G}^a]}_{\text{real number so Tr is redundant}} (f_L - f_R)\, dE$$

$$= \frac{2se}{h} \int_{-\infty}^{+\infty} \underbrace{\frac{\gamma_L \gamma_R}{\gamma_L + \gamma_R} D(E)}_{T(E, V_{bias}) \text{ is transmission function}} \cdot (f_L - f_R)\, dE$$

$$\equiv \frac{\gamma_L \gamma_R}{(E - \gamma_L - \gamma_R)^2 + [(\gamma_L + \gamma_R)/2]^2}$$

Lorentzian function centered at ε_{HOMO} whose brodening is determined by by the sum $\gamma_L + \gamma_R$, so current is then integral of all the resonances entering into the bias window $\mu_L - \mu_R$

$\Rightarrow$ in the linear-response limit at zero temperature: $G = \frac{2e^2}{h} T(E_F)$

FIRST refinement:

$\varepsilon_{HOMO} = \varepsilon_{HOMO}(n_0)$

$$n_0 = [S_{neq}]_{00} = \left[\frac{1}{2\pi i} \int \hat{G}^<(E)\, dE\right]_{00}$$

$$= \int_{-\infty}^{+\infty} D(E) \frac{\gamma_L f_L + \gamma_R f_R}{\gamma_L + \gamma_R}$$

SECOND refinement:

many-body Coulomb interaction effect beyond DFT can downshift ε_{HOMO} and enlarge ΔE

4° Inelastic processes and/or dephasing in the scattering region $\Rightarrow$ switch from Landauer–Büttiker to Meir–Wingreen formula

$\rightarrow$ during passage through the scattering region, an electron of energy E_{in} can excite lattice vibration (i.e., phonon), or excitation of localized spins (i.e., magnon) if the scattering region is magnetic material, so that it will be absorbed by the right electrode at energy $E_{out} = E_{in} - \hbar\omega$

$\rightarrow$ intuitively $\Rightarrow$ add inelastic contribution to level width:

$$\hat{H} = \left(\varepsilon_0 - i\gamma_L/2 - i\gamma_R/2 + i\gamma_{inelastic}\right)|0\rangle\langle 0|$$

$\rightarrow$ rigorously $\Rightarrow$ use additional self-energies in NEGF:

$$\hat{\Sigma}^r = \hat{\Sigma}^r_L + \hat{\Sigma}^r_R + \hat{\Sigma}^r_{e-e} + \hat{\Sigma}^r_{e-ph} + \hat{\Sigma}^r_{e-m}$$

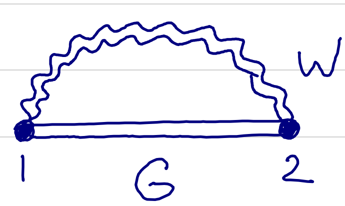
$$\hat{\Sigma}^< = \hat{\Sigma}^<_L + \hat{\Sigma}^<_R + \hat{\Sigma}^<_{e-e} + \hat{\Sigma}^<_{e-ph} + \hat{\Sigma}^<_{e-m}$$

$\hookrightarrow$ quantifies rate at which electrons come in

$\hat{\Sigma}^> \rightarrow$ quantifies rate at which they come out

$$\check{\Sigma} = \begin{pmatrix} \hat{\Sigma}^< + \hat{\Sigma}^r & \hat{\Sigma}^> \\ \hat{\Sigma}^< & \hat{\Sigma}^> - \hat{\Sigma}^r \end{pmatrix}$$

can be evaluated using Feynman diagrammatic perturbation theory, such as:

$\check{\Sigma} =$ 

$$\hat{G}^r = \Big(E - \hat{H} - \hat{\Sigma}^r_L - \hat{\Sigma}^r_R - \overbrace{\hat{\Sigma}^r_{e-e} - \hat{\Sigma}^r_{e-ph} - \hat{\Sigma}^r_{e-m}}^{\hat{\Sigma}^r_{int}}\Big)^{-1}$$

$$\hat{G}^< = \hat{G}^r \Big(\hat{\Sigma}^<_L + \hat{\Sigma}^<_R + \underbrace{\hat{\Sigma}^<_{e-e} + \hat{\Sigma}^<_{e-ph} + \hat{\Sigma}^<_{e-m}}_{\hat{\Sigma}^<_{int}}\Big)\hat{G}^a$$

$$\hat{G}^> = \hat{G}^r \Big(\hat{\Sigma}^>_L + \hat{\Sigma}^>_R + \hat{\Sigma}^>_{e-e} + \hat{\Sigma}^>_{e-ph} + \hat{\Sigma}^>_{e-m}\Big)\hat{G}^a$$

$$\boxed{I_p = \frac{2_s e}{h}\int dE\, \mathrm{Tr}\Big[\hat{\Sigma}^<_p(E)\hat{G}^>(E) - \hat{\Sigma}^>_p \hat{G}^<(E)\Big]}$$

↳ Meir-Wingreen formula (1992)

$\hat{\Sigma}^<_p(E)\hat{G}^>(E)$: describes current flowing from lead p into the scattering region because it is proportional to $\hat{G}^<(E)$, which quantifies empty states in the scattering region, and $\hat{\Sigma}^<_p$ which quantifies filled states in leap p

$\hat{\Sigma}^>_p \hat{G}^<(E)$: describes current flowing from the scattering region into lead p

$$I_p = I_p^{el} + I_p^{inel}$$

$$I_p^{el} = \frac{2_s e}{h}\int dE\, \mathrm{Tr}\big[\hat{\Gamma}_2 \hat{G}^r \hat{\Gamma}_p \hat{G}^a\big](f_p - f_2)$$

it looks like NEGF-based expression of Caroli et al. for non-interacting electrons but here $\hat{G}^r$ includes $\hat{\Sigma}^r_{int}$

$$I_p^{inel} = \frac{2_s e}{h}\int dE\, \mathrm{Tr}\Big[\hat{G}^r \hat{\Sigma}^>_{int}\hat{G}^a \hat{\Sigma}^<_p - \hat{G}^r \Sigma^<_{int}\hat{G}^a \hat{\Sigma}^>_p\Big]$$

■ EXAMPLE: Interacting self-energies for momentum-conserving and momentum relaxing phenomenological dephasing

momentum-conserving

$$\hat{\Sigma}^r_{int}(E) = d_p\, G^r(E)$$
$$\hat{\Sigma}^<_{int}(E) = d_p\, G^<(E)$$

momentum-relaxing

$$\hat{\Sigma}^r(E) = \mathrm{diag}\left[d_m \hat{G}^r(E)\right]$$
$$\hat{\Sigma}^r(E) = \mathrm{diag}\left[d_m \hat{G}^<(E)\right]$$

$$\hat{G}^r_{out}(E) = \left[E - \hat{H} - \hat{\Sigma}^r_L(E) - \hat{\Sigma}^r_R - d_p \hat{G}^r_{in}(E)\right]$$

$\|\hat{G}^r_{in}(E) - \hat{G}_{out}(E)\| < \delta \Rightarrow$ exit self-consistent iterative loop

then compute lesser GF

$$\hat{G}^<(E) = \hat{G}^r(E)\left[i f_L(E)\hat{\Gamma}_L(E) + i f_R(E)\hat{\Gamma}_R(E) + d_p \hat{G}^<(E)\right]\hat{G}^a(E)$$

↳ no need for iterations since SciPy and MATLAB have function to solve Sylvester equation of linear algebra: $\hat{A}\hat{X} + \hat{X}\hat{B} + \hat{C} = 0$

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Nonequilibrium Green's function based models for dephasing in quantum transport

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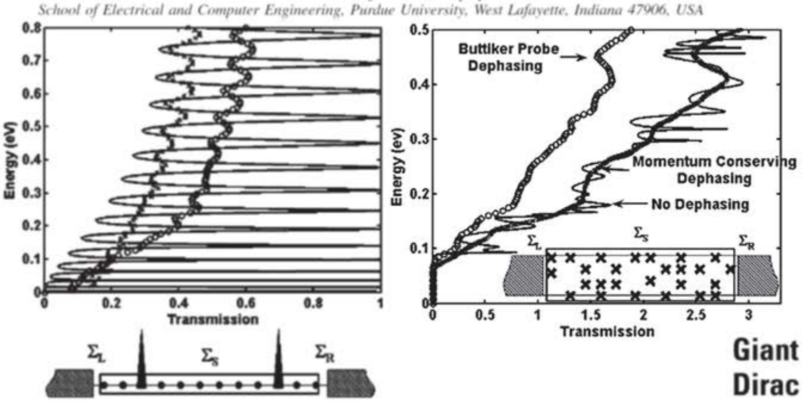

PHYSICAL REVIEW B 85, 155414 (2012)

Quantum coherence and its dephasing in the giant spin Hall effect and nonlocal voltage generated by magnetotransport through multiterminal graphene bars

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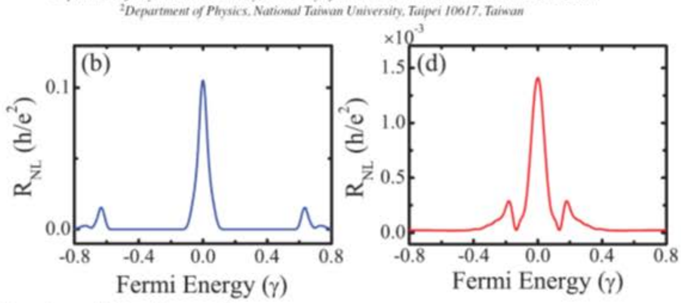

Giant Nonlocality Near the Dirac Point in Graphene

15 APRIL 2011 VOL 332 SCIENCE

D. A. Abanin,[1,2] S. V. Morozov,[3,4] L. A. Ponomarenko,[3] R. V. Gorbachev,[3] A. S. Mayorov,[3] M. I. Katsnelson,[5] K. Watanabe,[6] T. Taniguchi,[6] K. S. Novoselov,[3] L. S. Levitov,[5*] A. K. Geim[3*]