Transport properties: conductance and thermopower

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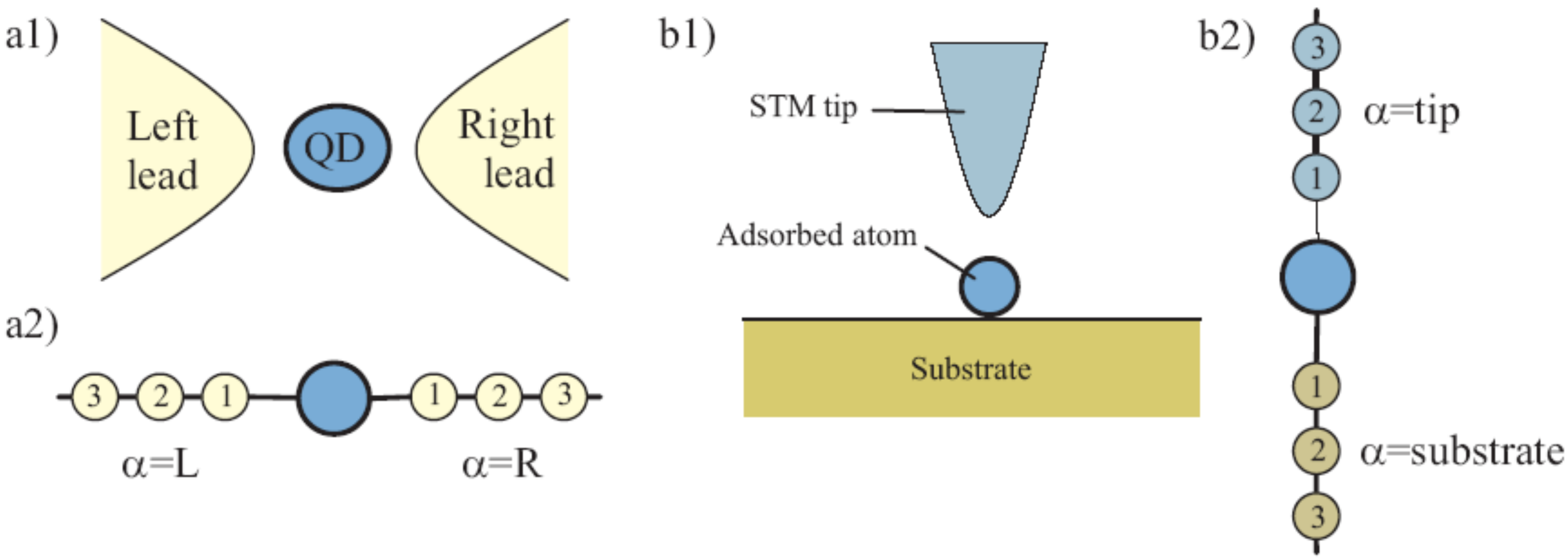
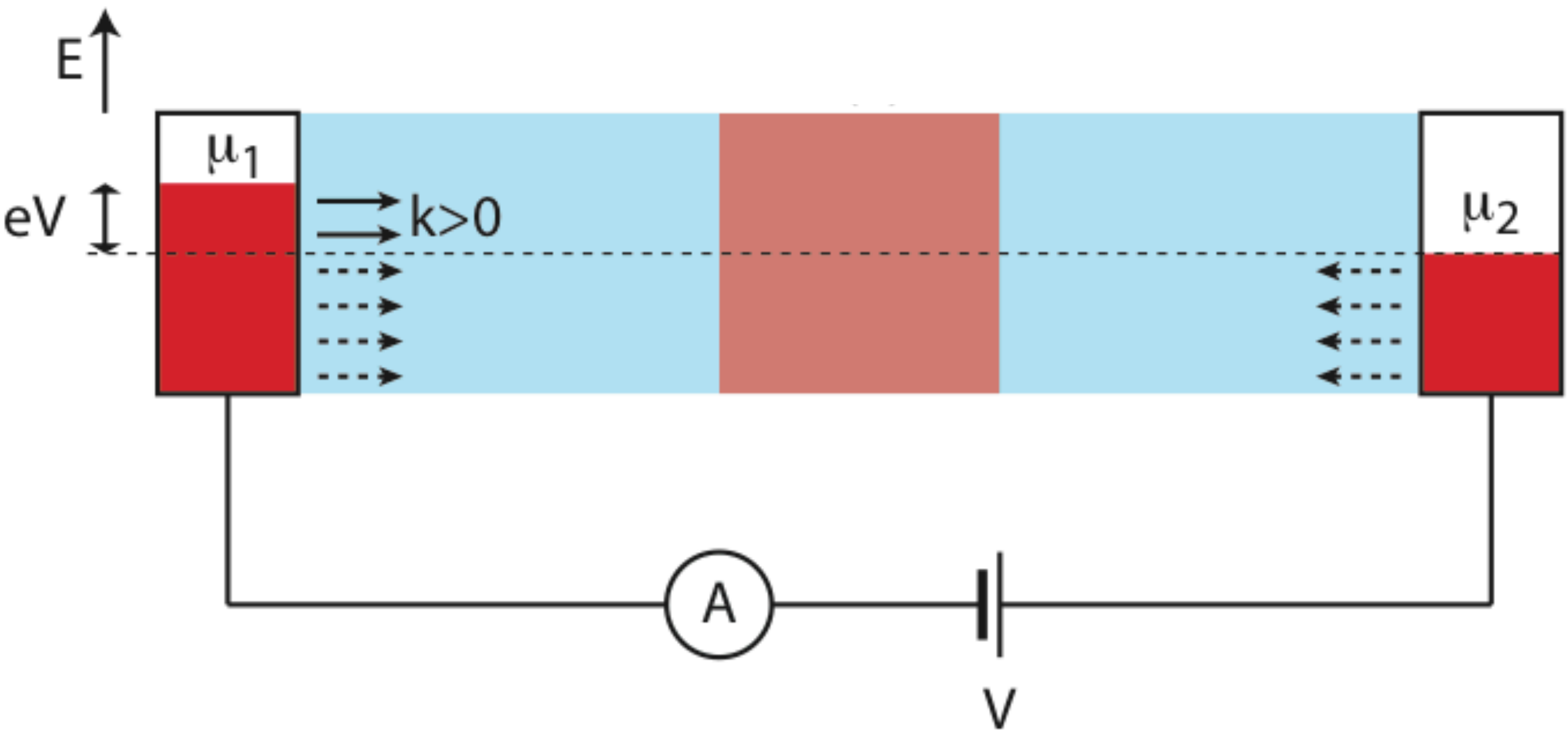
Transport in nanostructures



Landauer formalism



Density of states per unit length: $g(E) = \frac{2}{h}\sqrt{\frac{2m_e}{E}}$

(Includes factor 2 for spin)

$$E = \frac{\hbar^2}{2m_e}k^2 \qquad v = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{1}{\hbar}\frac{\mathrm{d}E}{\mathrm{d}k} = \frac{\hbar k}{m_e} = \sqrt{\frac{2E}{m_e}}$$

$$g(E) = \frac{4}{hv}$$

$$I = jS = qv(\rho S)$$

↓

$$I = \int_{\mu_2}^{\mu_1} qv(E)\frac{1}{2}g(E)T(E)\mathrm{d}E$$

For T(E)=1 (ballistic conductor):

$$I = \int_{\mu_2}^{\mu_1} qv(E)\frac{1}{2}\left(\frac{4}{hv(E)}\right)\mathrm{d}E = \frac{2q}{h}(\mu_1 - \mu_2) = \frac{2e^2}{h}V$$

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

$$G_0 = \frac{2e^2}{h} = \frac{e^2}{\pi\hbar} \approx [12.9\,\mathrm{k}\Omega]^{-1}$$

In general, at T=0:

$$G = \frac{2e^2}{h}T(\mu)$$

Multi-channel leads:

$$G = \frac{2e^2}{h}\sum_n T_n(\mu)$$

resistance $= \frac{h}{2e^2}\frac{1}{T} = \frac{h}{2e^2}\left(1 + \frac{1-T}{T}\right) = \frac{h}{2e^2} + \frac{h}{2e^2}\frac{R}{T}$

↑ quantized contact resistance

Scattering theory

$$S^\mu = \begin{pmatrix} S^\mu_{LL} & S^\mu_{RL} \\ S^\mu_{LR} & S^\mu_{RR} \end{pmatrix} = \begin{pmatrix} r^\mu_L & t^\mu_R \\ t^\mu_L & r^\mu_R \end{pmatrix}$$

$$G(T=0) = G_0 \tfrac{1}{2} \sum_\mu |S^\mu_{RL}|^2 \qquad G_0 = \frac{2e^2}{h}$$

quasiparticle phase shifts

$$\exp(i\theta\tau^y) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \qquad U S^\mu U^\dagger = \begin{pmatrix} e^{2i\delta^{a\mu}_{\mathrm{qp}}} & 0 \\ 0 & e^{2i\delta^{b\mu}_{\mathrm{qp}}} \end{pmatrix}$$

$$G = G_0 \sin^2(2\theta) \tfrac{1}{2} \sum_\mu \sin^2(\delta^{a\mu}_{\mathrm{qp}} - \delta^{b\mu}_{\mathrm{qp}})$$

$$G = G_0 \tfrac{1}{2} \sum_\mu \sin^2(\delta^{\mathrm{even},\mu}_{\mathrm{qp}} - \delta^{\mathrm{odd},\mu}_{\mathrm{qp}})$$

Spin symmetry, single effective channel:

$$G = G_0 \sin^2 \delta_{\mathrm{qp}}$$

Keldysh approach

$$H = \sum_{k,\alpha=\{L,R\},\sigma} \epsilon_{k\mu} c^\dagger_{k\alpha\mu} c_{k\alpha\mu} + H_{\rm int}(\{d^\dagger_{n\mu}\},\{d_{n\mu}\}) + \sum_{n,k,\alpha=\{L,R\},\mu} \left(V^{\alpha\mu}_{k,n} c^\dagger_{k\alpha\mu} d_{n\mu} + \text{h.c.} \right)$$

$$I = \frac{ie}{2h} \int d\epsilon \sum_\mu \left(\mathrm{Tr}\left\{ \left[f_L(\epsilon)\boldsymbol{\Gamma}^{L\mu} - f_R(\epsilon)\boldsymbol{\Gamma}^{R\mu} \right] \left(\mathbf{G}^{r\mu} - \mathbf{G}^{a\mu} \right) \right\} + \mathrm{Tr}\left\{ \left(\boldsymbol{\Gamma}^{L\mu} - \boldsymbol{\Gamma}^{R\mu} \right) \mathbf{G}^{<\mu} \right\} \right)$$

Relection symmetric problems:

$$G(T=0) = -G_0 \sum_\mu \mathrm{Tr}\left[\boldsymbol{\Gamma}^\mu \mathrm{Im}\, \mathbf{G}^{r\mu}(\epsilon = 0) \right]$$

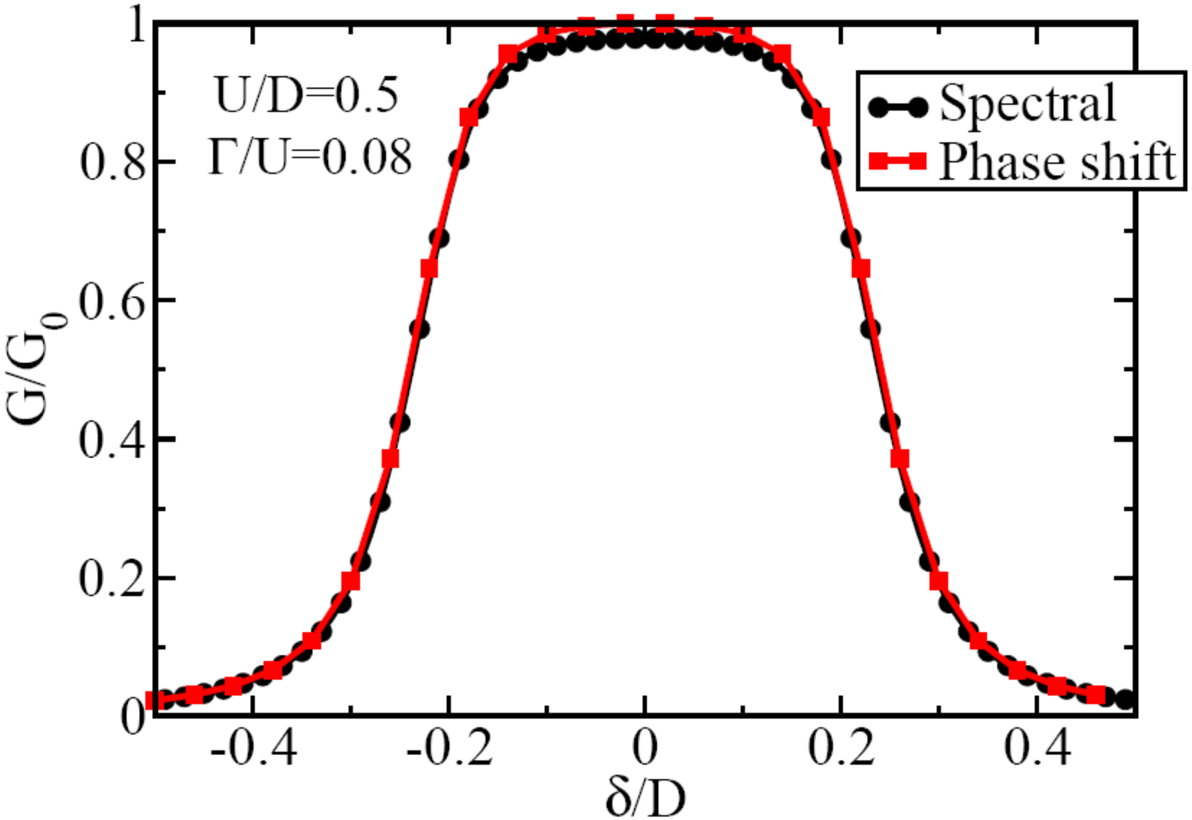
One impurity: $G = G_0 \pi \Gamma A(\epsilon = 0)$

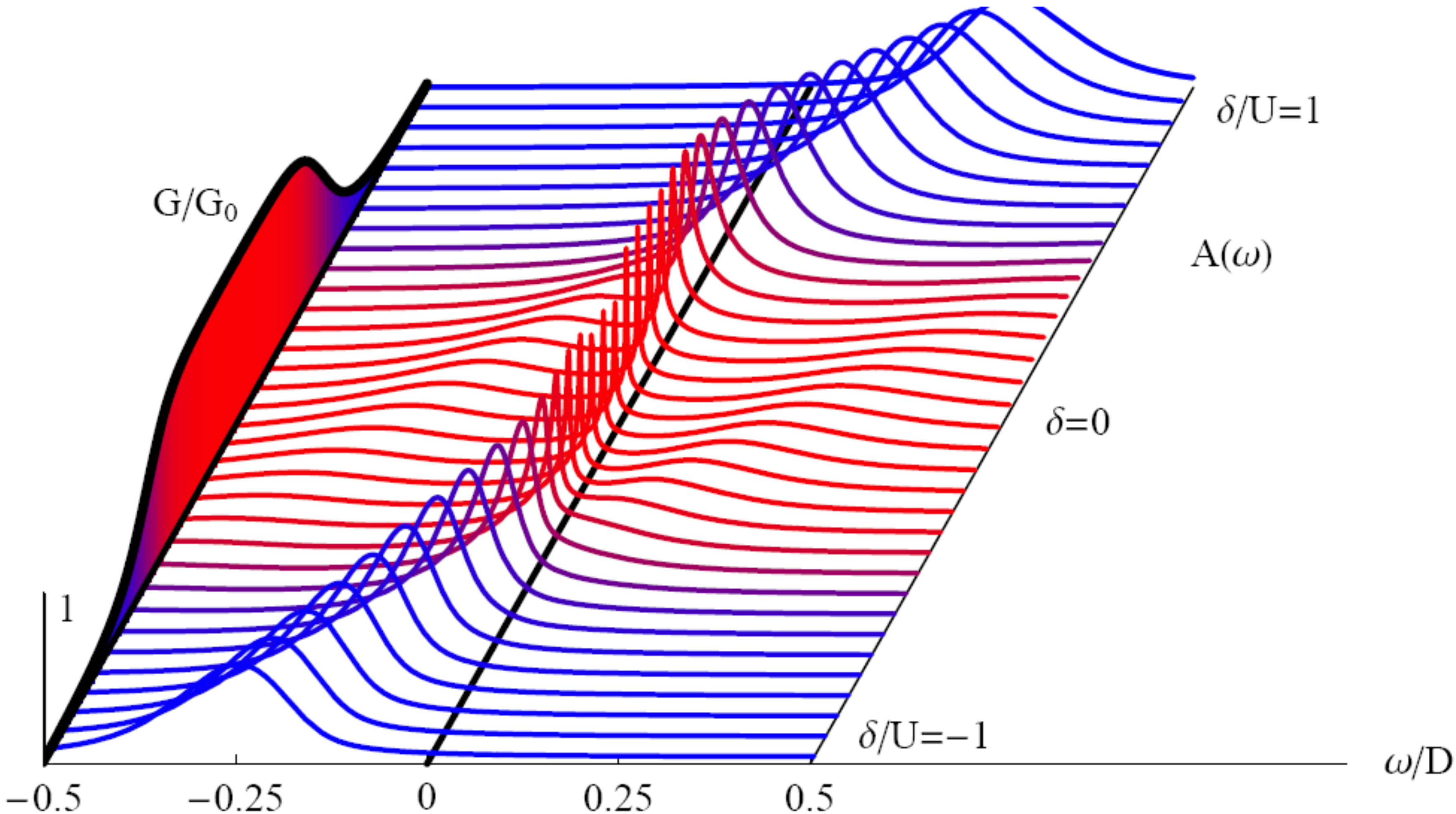
Also known as the Meir-Wingreen formula

Conductance of quantum dot (SIAM)

$$G = G_0 \pi \Gamma A(\epsilon = 0) \qquad G = G_0 \tfrac{1}{2} \sum_\mu \sin^2(\delta_{\mathrm{qp}}^{\mathrm{even},\mu} - \delta_{\mathrm{qp}}^{\mathrm{odd},\mu})$$

$$G_0 = \frac{2e^2}{h} = \frac{e^2}{\pi\hbar} \approx [12.9\,\mathrm{k}\Omega]^{-1}$$



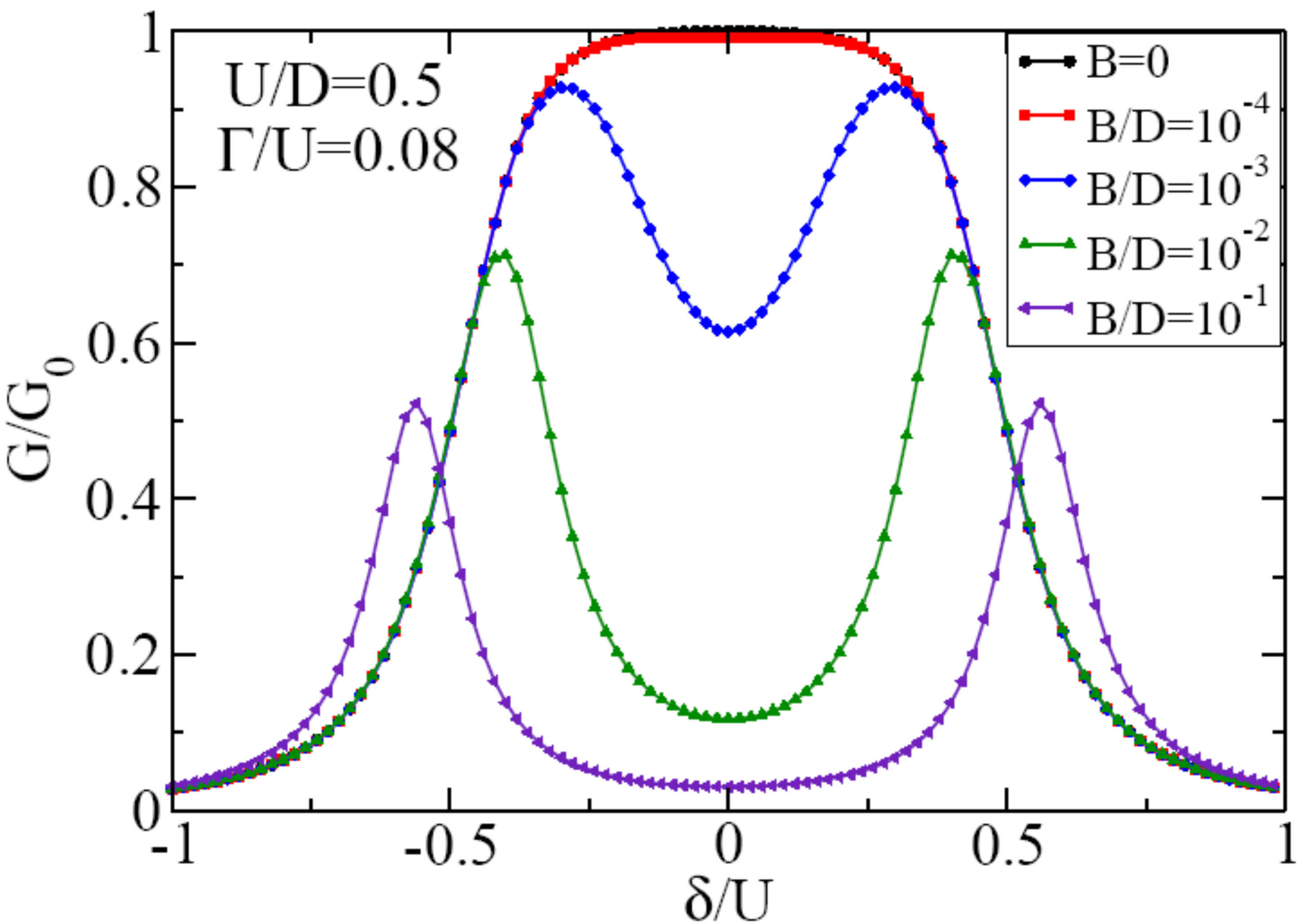

G/G0
δ/U=1
A(ω)
δ=0
δ/U=−1
1
ω/D
−0.5
−0.25
0
0.25
0.5

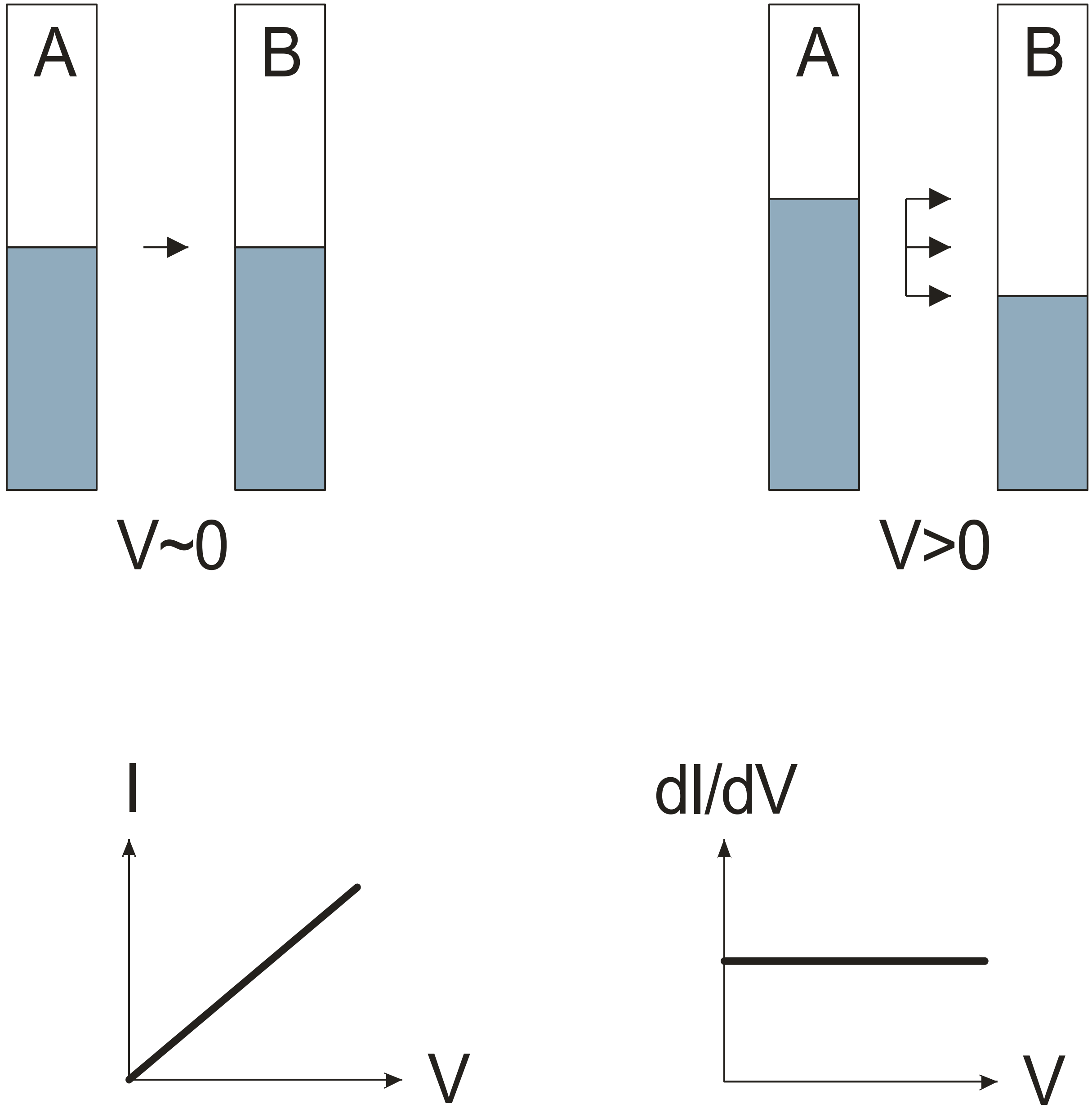
Finite temperatures

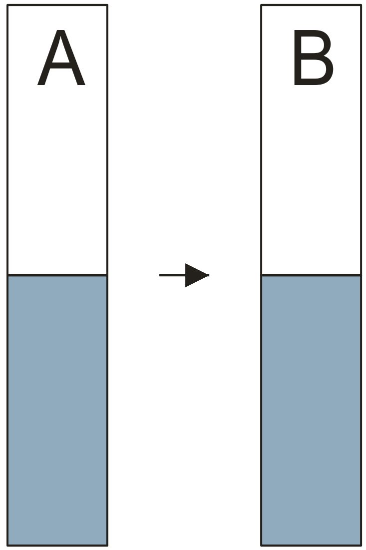
$$G(T) = G_0 \pi \Gamma \int_{-\infty}^{\infty} \mathrm{d}\omega \Big(-\frac{\partial f}{\partial \omega} \Big) A(\omega, T)$$

$$f(\omega) = \frac{1}{1 + e^{\beta \omega}}$$

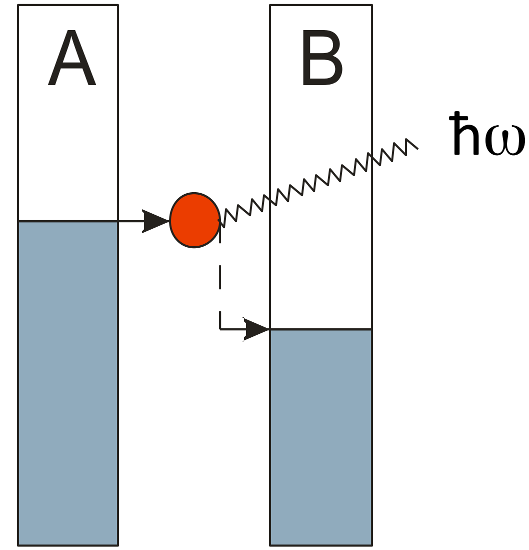
Effect of the magnetic field




A
B
V~0
A
B
V>0
I
V
dI/dV
V

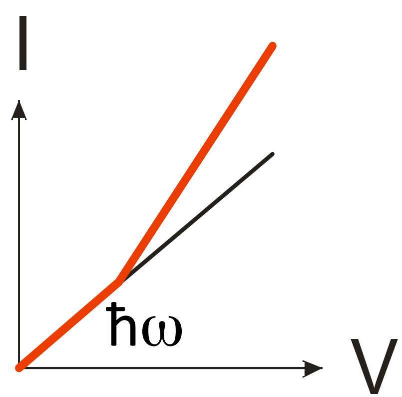


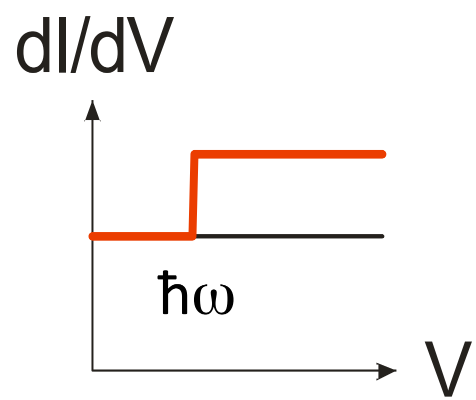
V~0



eV>ħω

Inelastic scattering





Information about internal degrees of freedom!

Linear response theory for calculating the conductance of nanostructures

$$I = e\dot{N}_L \qquad N_L = \sum_k c_k^\dagger c_k \qquad \dot{N}_L = \frac{i}{\hbar}[H, N_L]$$

$$\dot{N}_L = \sum_k V_k \left(-ic_k^\dagger d + id^\dagger c_k\right) = V\left(-if_0^\dagger d + id^\dagger f_0\right)$$

$$H' = -N_L V_L - N_R V_R = eV(N_L - N_R)/2$$

$$\phi_{BA}(t) = \frac{1}{i\hbar}\mathrm{Tr}\left([\rho, A]B(t)\right)$$

$$\chi_{BA}(\omega) = \frac{1}{i\hbar}\int_0^\infty dt e^{-\delta t + i\omega t}\mathrm{Tr}\left([\rho, A]B(t)\right)$$

Kubo (1957)

$$\sigma_{\mu\nu} = \lim_{\omega \to 0} \langle\langle N_\nu; \dot{N}_\mu \rangle\rangle_\omega$$

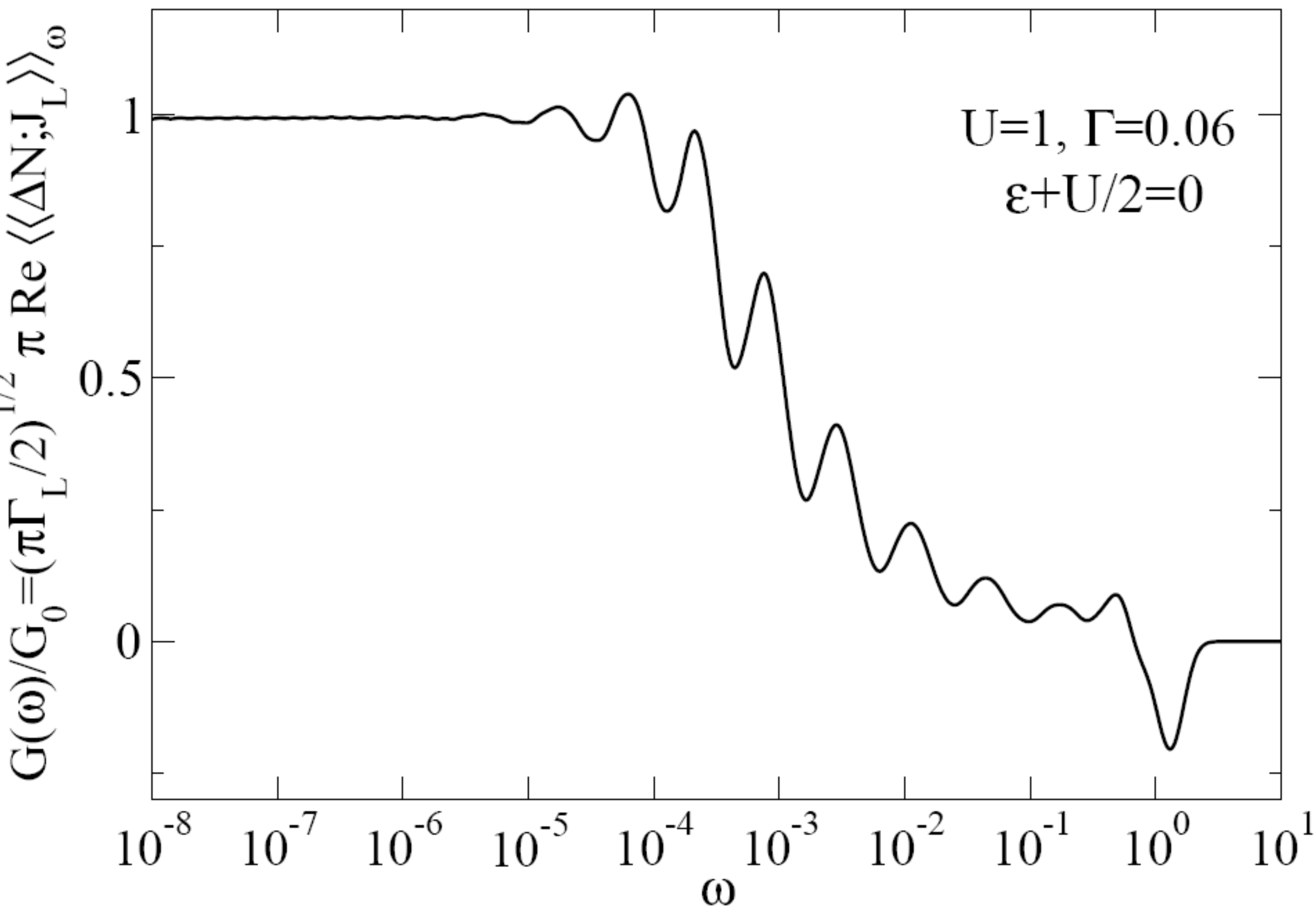
Standard approach: $$K_{\mu\nu}(\omega) = \langle\langle \dot{N}_\nu; \dot{N}_\mu \rangle\rangle_\omega$$

$$\sigma_{\mu\nu} = \lim_{\omega \to 0} \frac{K''_{\mu\nu}(\omega)}{\omega}$$

Difficulty: the slope is difficult to calculate reliably!

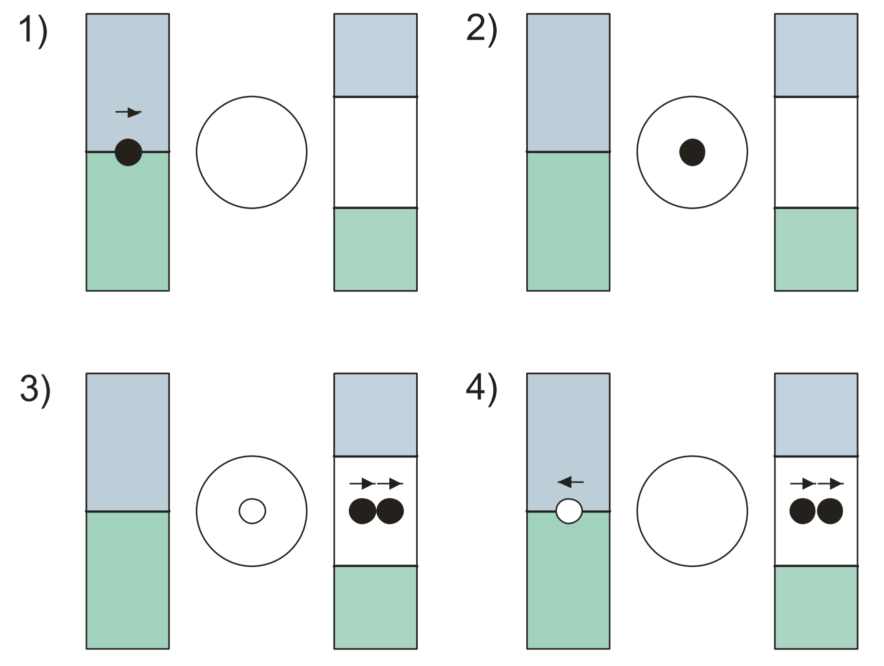
Solution: we can work with the global operator N_ν itself!

Test case: single-impurity Anderson model



Proposed application: conductance of a S-QD-N structure

- Open problem:
  the transition from $G=4e^2/h$ to $G=2e^2/h$ conductance as the gap closes



Anyone interested?

Transport integrals, thermopower

$$\mu_\alpha = \frac{1}{2}\left(\mu_{\alpha\uparrow} + \mu_{\alpha\downarrow}\right)$$

$$\mu = \frac{1}{2}(\mu_L + \mu_R)$$

$$eV = \mu_L - \mu_R$$

$$eV_s = (\mu_{L\uparrow} - \mu_{L\downarrow}) - (\mu_{R\uparrow} - \mu_{R\downarrow})$$

$$T = \frac{1}{2}(T_L + T_R)$$

$$\Delta T = T_L - T_R$$

$$I = I_\uparrow + I_\downarrow$$

$$I = \frac{e}{h}\left[(\mathcal{I}_{1\uparrow} + \mathcal{I}_{1\downarrow})\frac{\Delta T}{T} + (\mathcal{I}_{0\uparrow} + \mathcal{I}_{0\downarrow})eV + \frac{1}{2}\left(\mathcal{I}_{0\uparrow} - \mathcal{I}_{0\downarrow}\right)eV_s\right]$$

$$I_s = I_\uparrow - I_\downarrow$$

$$I_s = \frac{e}{h}\left[(\mathcal{I}_{1\uparrow} - \mathcal{I}_{1\downarrow})\frac{\Delta T}{T} + (\mathcal{I}_{0\uparrow} - \mathcal{I}_{0\downarrow})eV + \frac{1}{2}\left(\mathcal{I}_{0\uparrow} + \mathcal{I}_{0\downarrow}\right)eV_s\right]$$

$$\mathcal{I}_{n\sigma} = \int \mathrm{d}\omega\, \omega^n [-f'(\omega)]\mathcal{T}_\sigma(\omega)$$

B=0

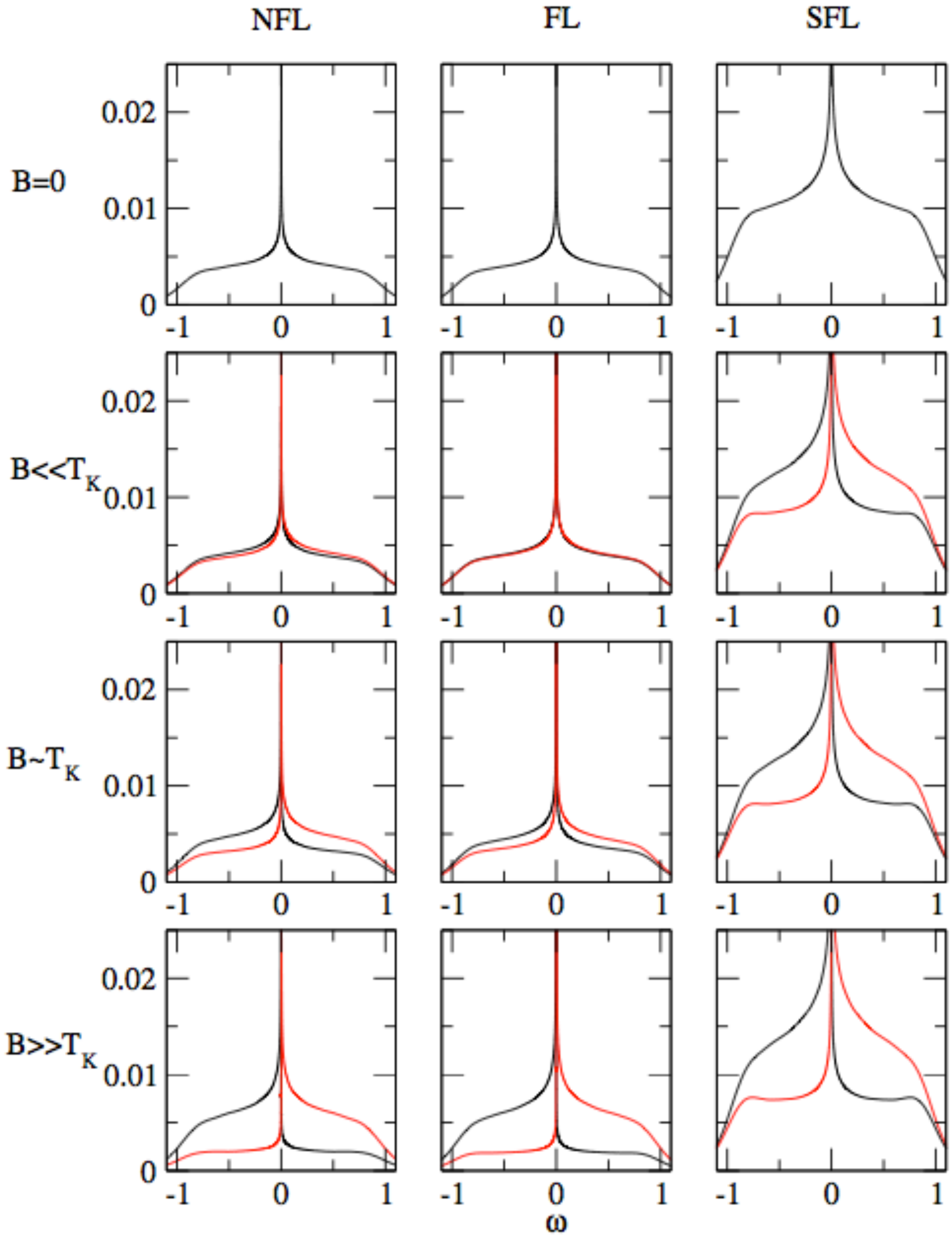
$$S = -\frac{eV}{\Delta T}\bigg|_{I=0} = \frac{1}{T}\frac{\mathcal{I}_1}{\mathcal{I}_0}$$

(charge) Seebeck coefficient

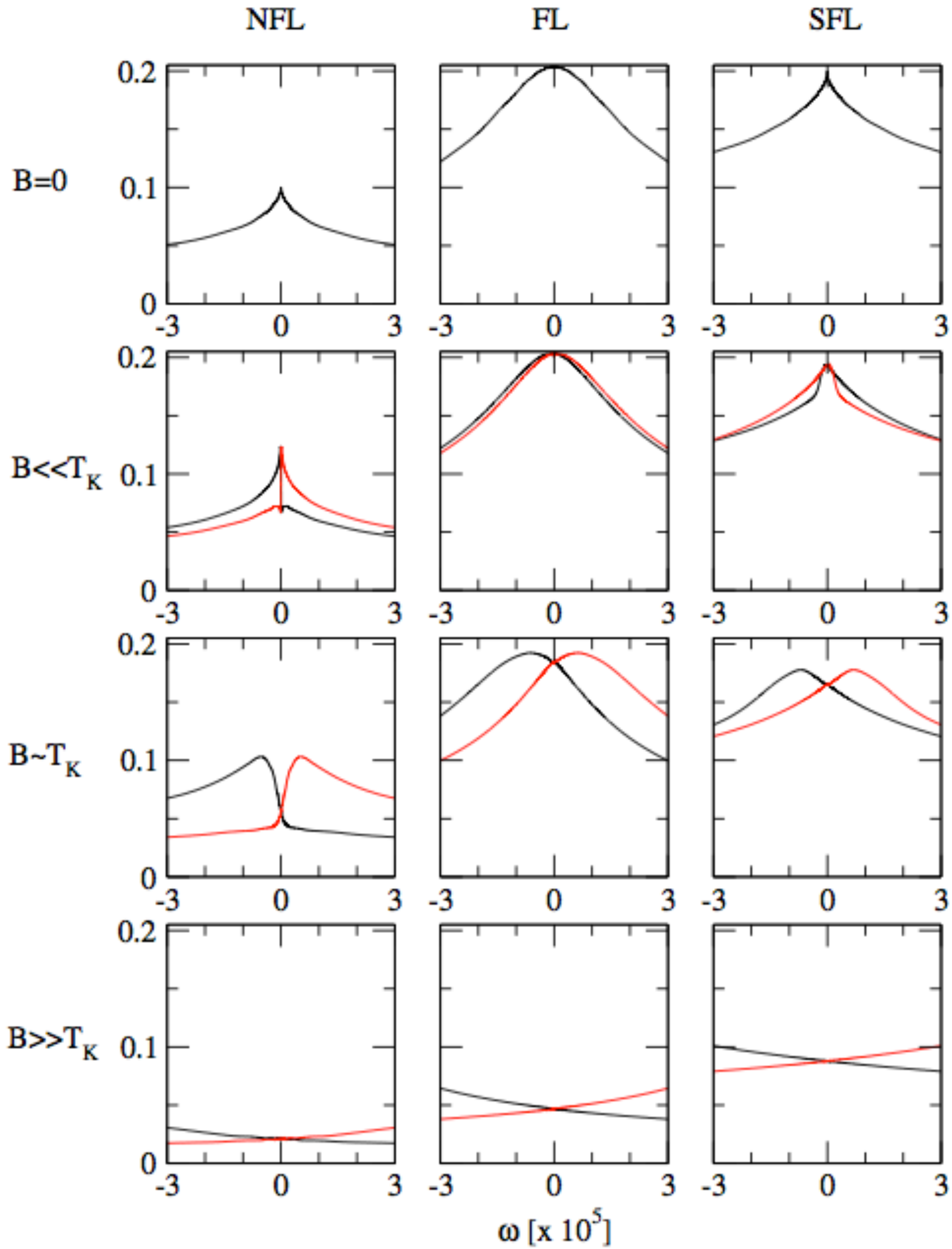
δ=0 (particle-hole symmetric point)

$$S_s = -\frac{eV_s}{\Delta T}\bigg|_{I_s=0} = \frac{2}{T}\frac{\mathcal{I}_1}{\mathcal{I}_0}$$

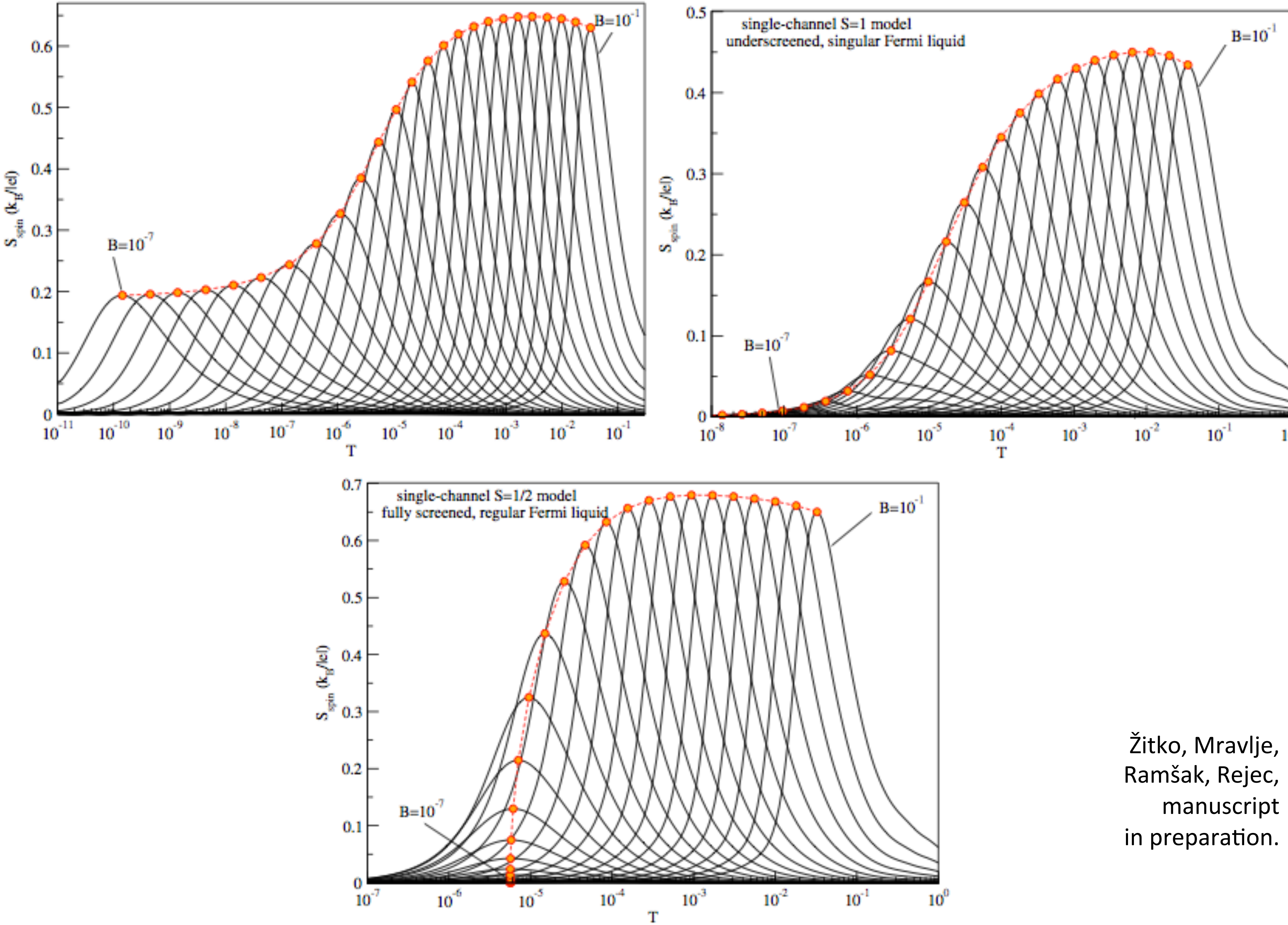
spin Seebeck coefficient



NFL
FL
SFL
B=0
B<<T_K
B~T_K
B>>T_K
0.02
0.01
0
-1
1
ω



NFL
FL
SFL
B=0
B<<T_K
B~T_K
B>>T_K
0.2
0.1
0
-3
3
ω [x 10^5]



Žitko, Mravlje, Ramšak, Rejec, manuscript in preparation.

Spin thermopower is a sensitive probe of the response of the system in magnetic field.