Dissipative Effects in the Electronic Transport through DNA molecular wires

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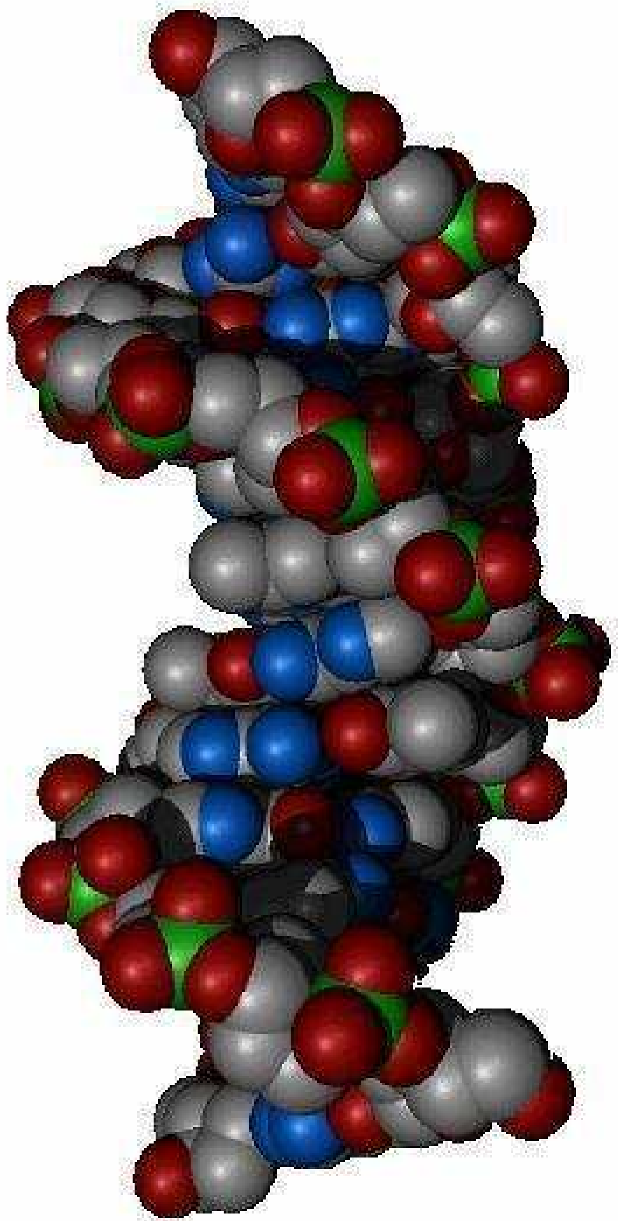
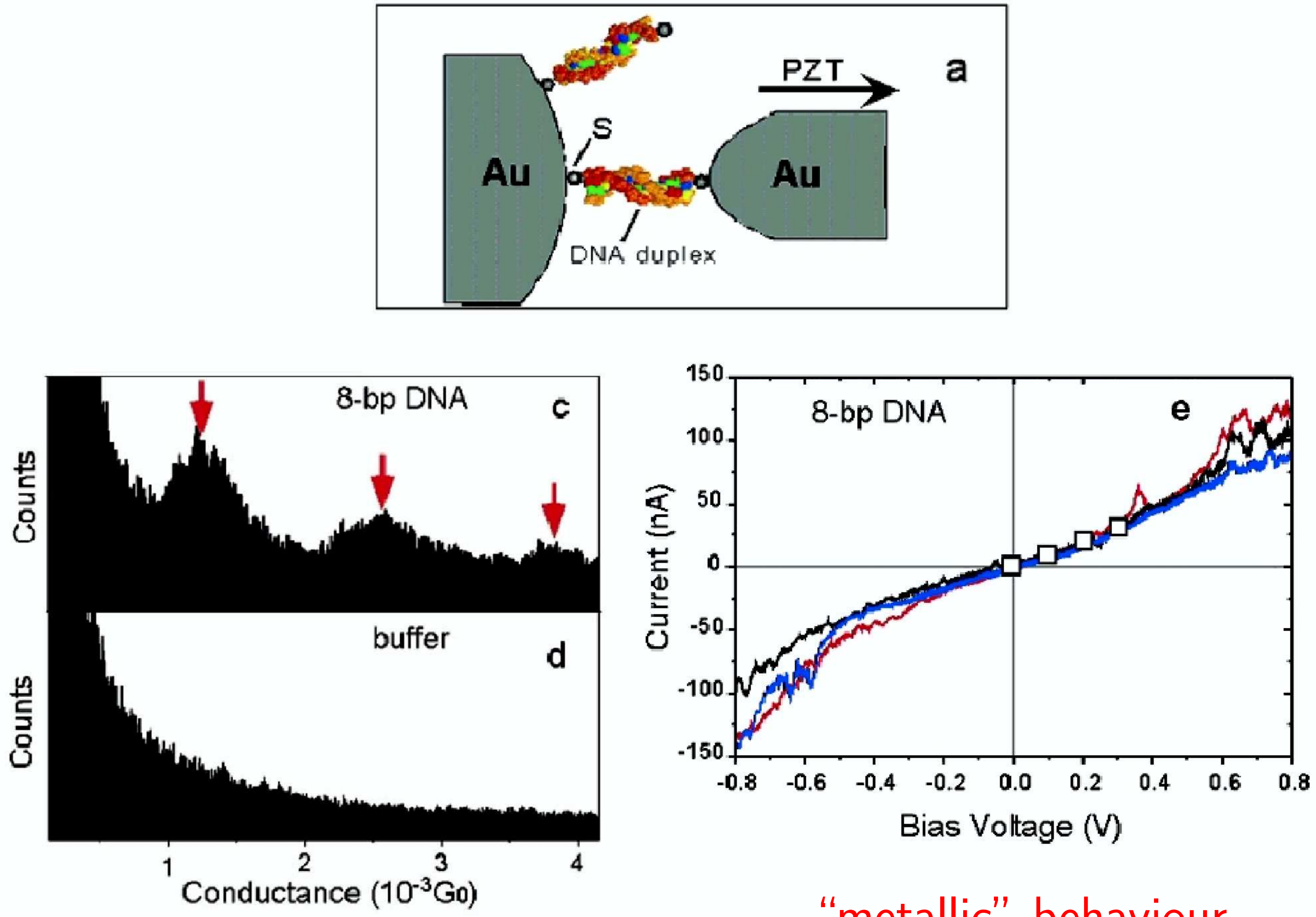


Motivation: Transport in *single* Poly(GC) oligomers in *water*

B. Xu *et al.* Nanoletters **4**, 1105 (2004)



"metallic" behaviour

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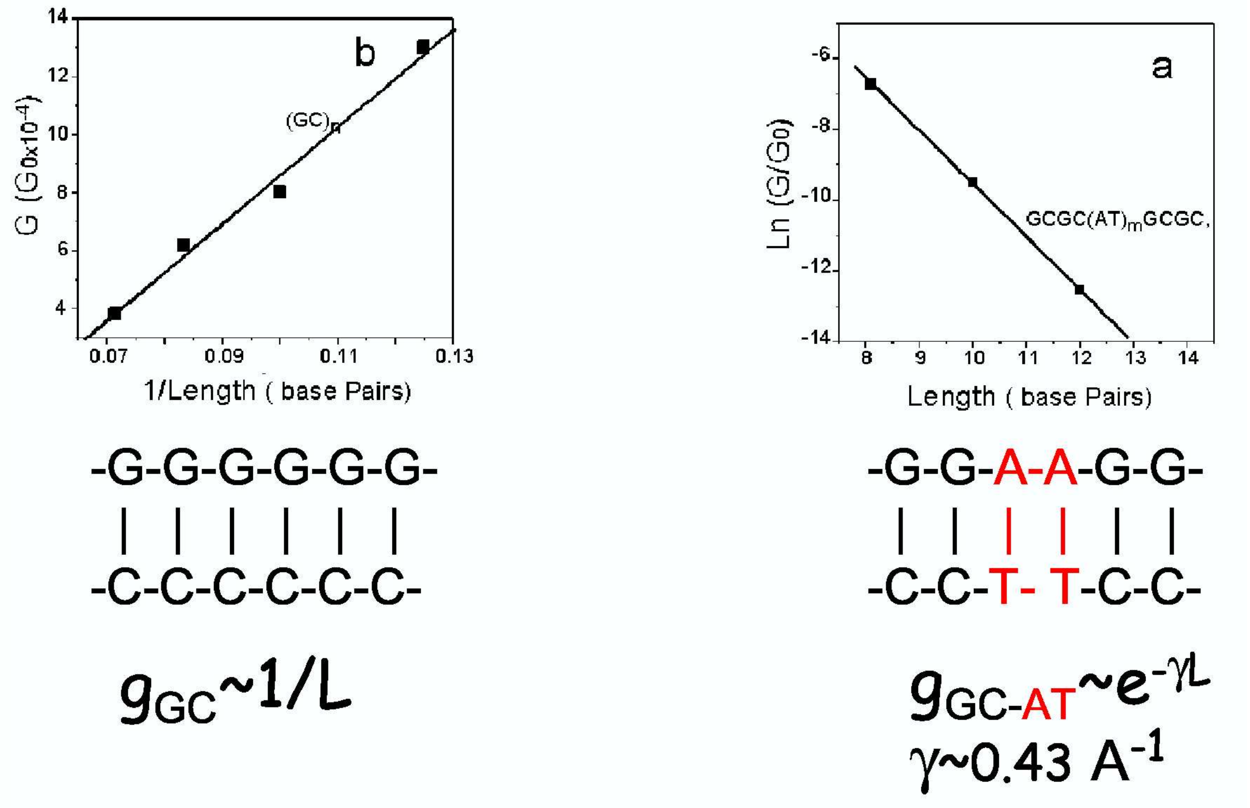
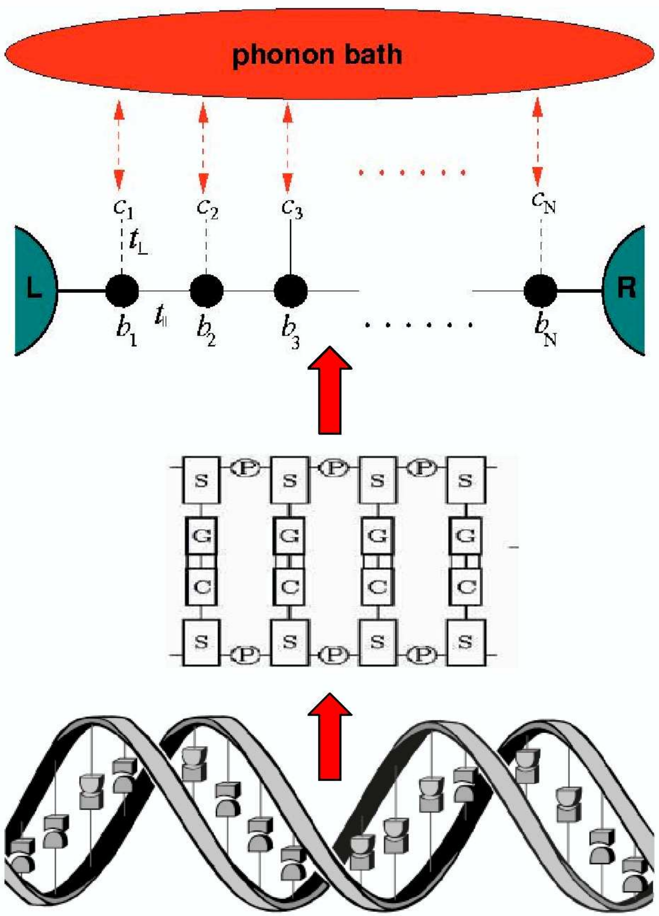


$\Longrightarrow$ *Ab initio* (H. Wang *et al.* (2004)): dry Poly(GC) $\rightsquigarrow e^{-\gamma L}, \gamma \sim 1.5$ Å^{-1}

Algebraic behavior induced by the environment ?

A minimal model for a DNA wire in water

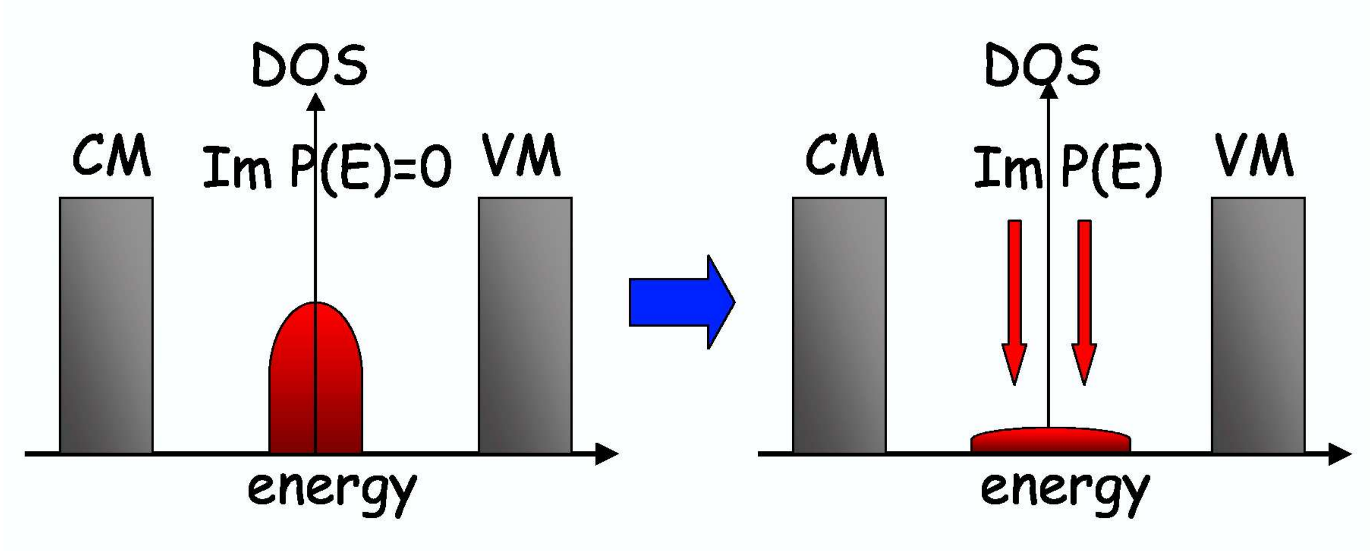


$$\begin{aligned}\mathcal{H} &= \overbrace{\sum_j \epsilon_{b,j} b_j^\dagger b_j - t_{||} \sum_{<i,j>} \left(b_i^\dagger b_j + \mathrm{H.c.}\right)}^{\text{HOMO(LUMO)}} \\ &+ \underbrace{\sum_j \epsilon_j c_j^\dagger c_j}_{\text{side chain}} - \underbrace{t_\perp \sum_j \left(b_j^\dagger c_j + \mathrm{H.c.}\right)}_{\text{HOMO(LUMO)}-\text{side chain}} \\ &+ \underbrace{\sum_\alpha \Omega_\alpha B_\alpha^\dagger B_\alpha}_{\text{bath}} + \underbrace{\sum_{\alpha,j} \lambda_\alpha c_j^\dagger c_j \left(B_\alpha + B_\alpha^\dagger\right)}_{\text{bath}-\text{side chain}} \\ &+ \mathcal{H}_{\text{leads}} + \mathcal{H}_{\text{HOMO(LUMO)}-\text{leads}}\end{aligned}$$

Method+Approximations

- Green function techniques
- low-bias, equilibrium regime
- conductance $g = g_0 t(E) = g_0 Tr[G_W^\dagger \Gamma_R G_W \Gamma_L]$

Results (qualitative): Low-bias, strong dissipative limit

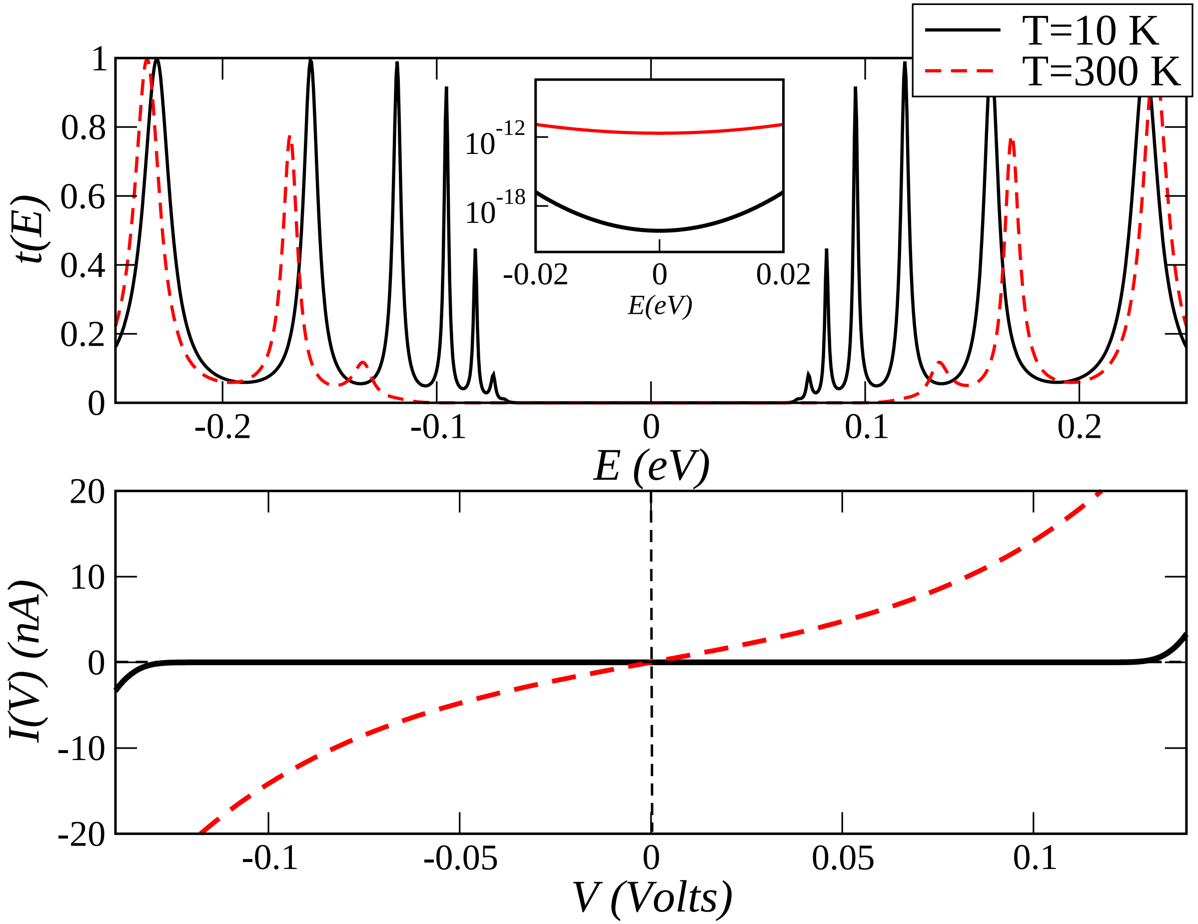


Bath-selfenergy $P(E)$:

Re $P(E)$ $\rightsquigarrow$ k$_{\mathrm{B}}$T-dependent polaronic manifold

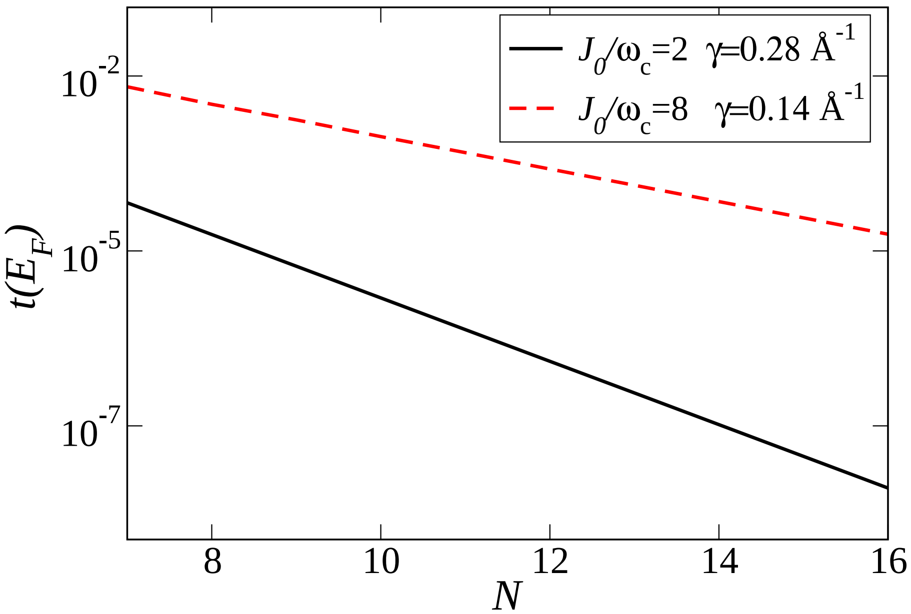
Im $P(E)$ ("friction") $\rightsquigarrow$ incoherent polaron band, pseudo-gap opens

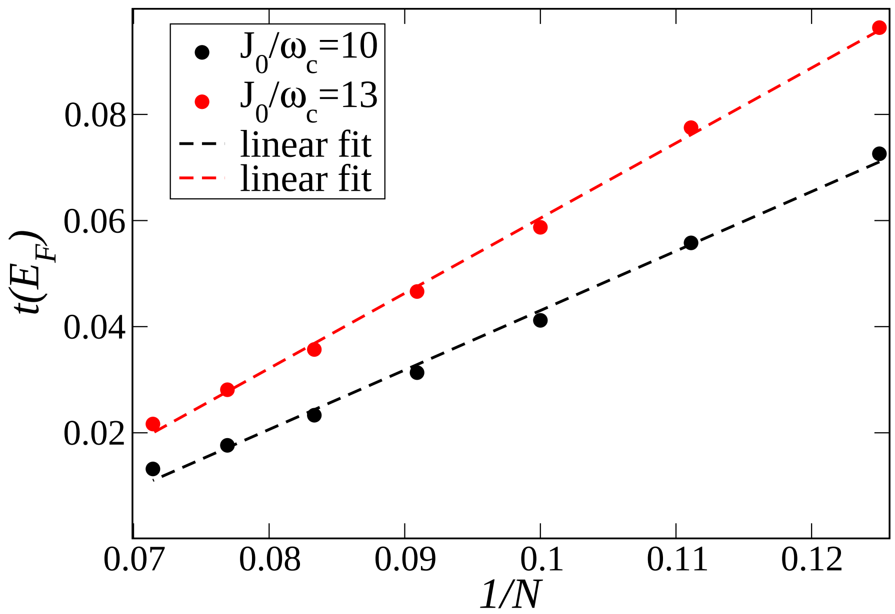
Results: Transmission and low-bias current



Crossover from tunneling (low T) $\rightsquigarrow$ activated (high-T) transport

Results: Scaling of $t(E_F)$ with the chain length $L = Na_{\mathrm{bp}}$ (T=300 K)

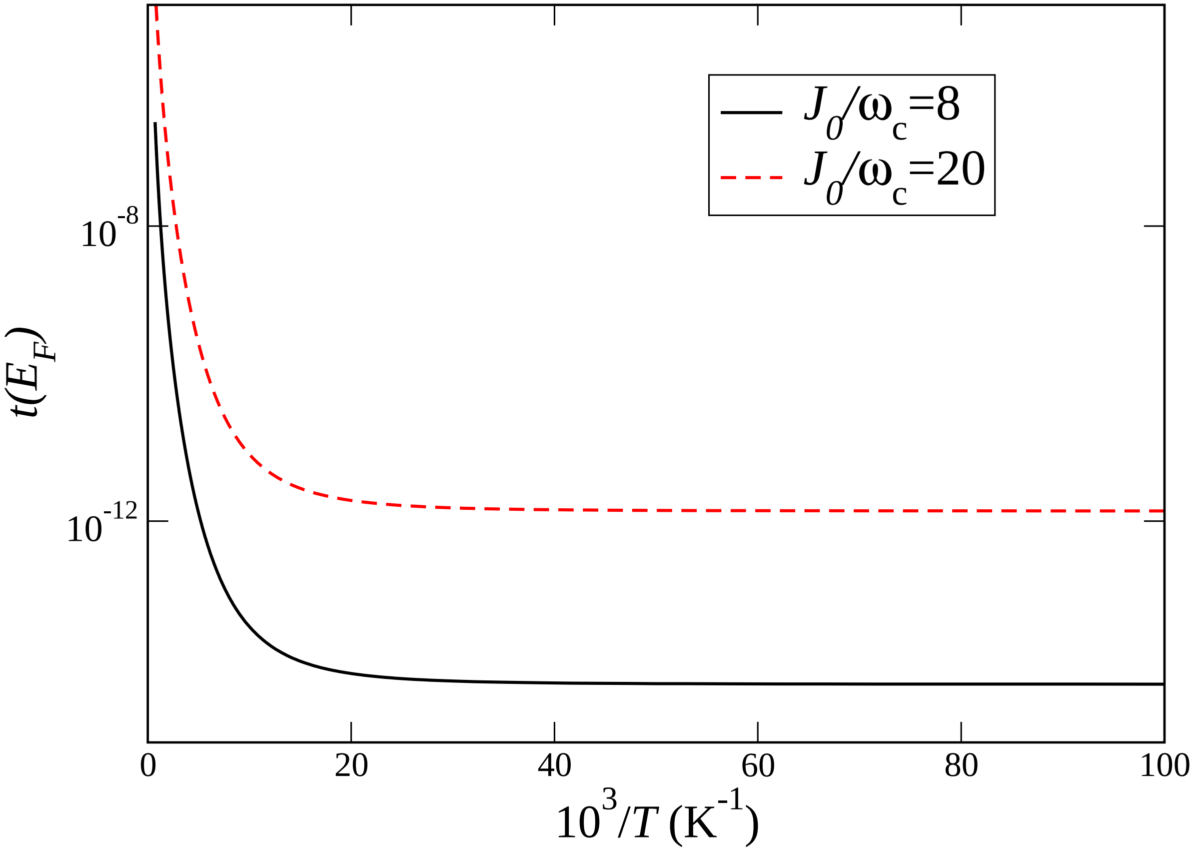




- With increasing coupling to the bath transition from

  weak exponential $(\gamma \ll 1)\ t_F \sim e^{-\gamma L} \Longrightarrow$ algebraic $t_F \sim L^{-\alpha}$

Results: $t(E_F, T)$ (Arrhenius plot)



Activated behaviour: $t(E_F) \sim e^{-const./k_\mathrm{B}T}$

Conclusions + Outlook

- Environment drastically affects charge transport $\rightsquigarrow$

  (i) bath-induced pseudo-gap in the wire electronic spectrum

  (ii) temperature-dependent (incoherent) DOS near $\mathsf{E_F}$

  $\rightsquigarrow$ non-zero low-bias current at high $\mathsf{k_B}T$

  $\rightsquigarrow$ weak exponential or algebraic $L-$dependence

  $\Longrightarrow$ Relation to Xu et al. experiments !?

- Outlook:

  (internal) dynamical degrees of freedom?

  Sequence complexity ? Nonequilibrium transport ?