Iterative real-time path integral approach to nonequilibrium quantum transport

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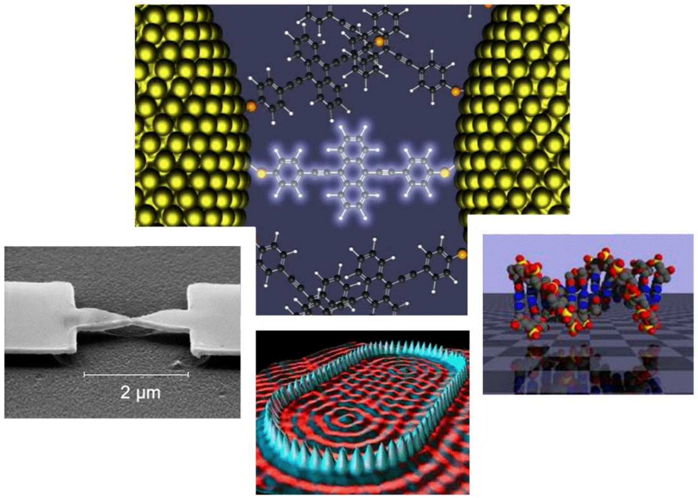

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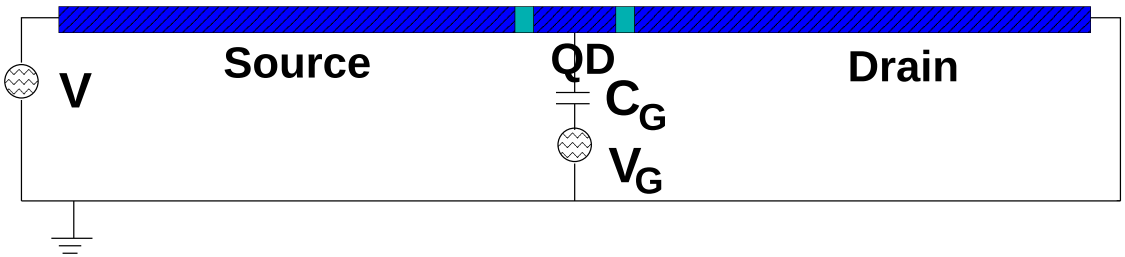
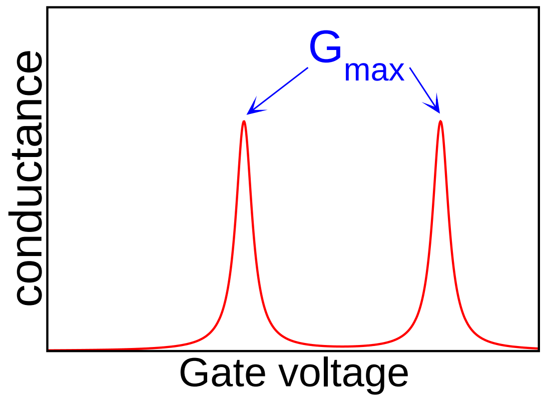
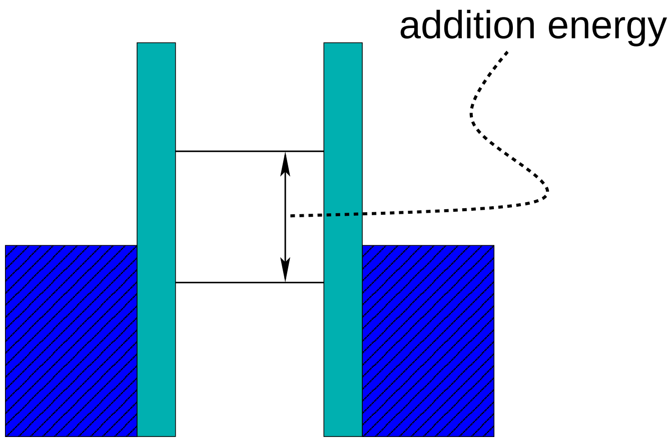
DFG

Transport through a nanoconductor



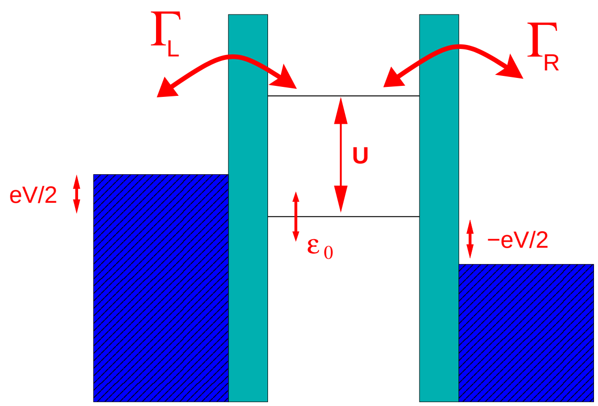


$$\mu(n+1) - \mu(n) \approx \frac{e^2}{2C} + \varepsilon \gg k_B T, eV$$



a)

Linear transport



b)

Nonlinear transport

Motivation

- Quantum transport still challenging for theory:
  - Transport through single molecules
  - Many-body effects, nonequilibrium effects
- Nonequilibrium:
  - Perturbative solutions
  - Real-time QMC increasingly difficult
  - Perturbative RG
  - Generalization of DMRG
  - Functional RG
  - Numerical RG

here: Iterative summation of real-time path integral

Outline

- Anderson model as prototype example
- Nonequilibrium transport:
  Keldysh path-integral for current generating funtion
- Hubbard-Stratonovich transformation $\Longrightarrow$ path summation
- The ISPI scheme: numerically exact results
- Validation: exact analytical and perturbative results
- Regime of small transport voltage
- Regime of large transport voltage
- Recent results
- Summary

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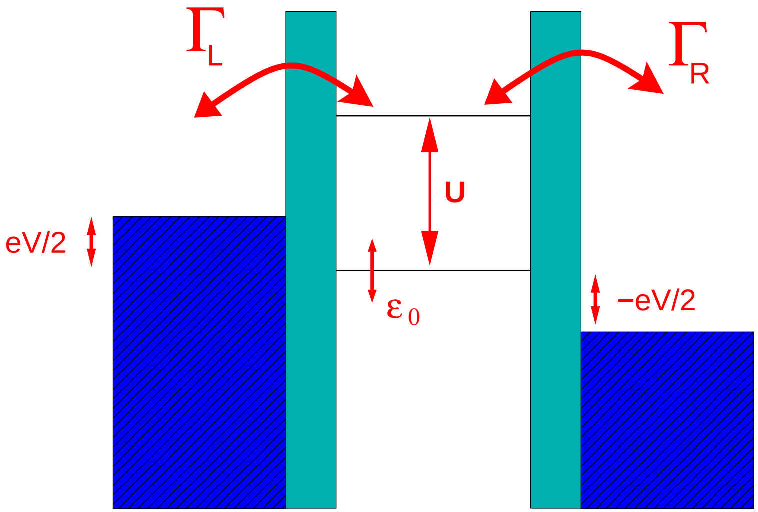
Anderson model as prototype



- single particle energies $E_{0\sigma}$
- on-dot interaction U
  $\Rightarrow$ many-body effects
- finite bias voltage $\mu_{p=L/R} = \pm eV/2$
  $\Rightarrow$ noneq. transport
- single particle energies of leads ϵ_{kp}
- hybridization $\Gamma_p \sim |t_p|^2$

$$
\begin{aligned}
\mathcal{H} &= H_{dot} + H_{leads} + H_T \\
&= \sum_{\sigma} E_{0\sigma}\hat{n}_\sigma + U\hat{n}_\uparrow\hat{n}_\downarrow + \sum_{kp\sigma}(\epsilon_{kp} - \mu_p)c^\dagger_{kp\sigma}c_{kp\sigma} \\
&\quad - \sum_{kp\sigma} t_p c^\dagger_{kp\sigma} d_\sigma + H.c.
\end{aligned}
$$

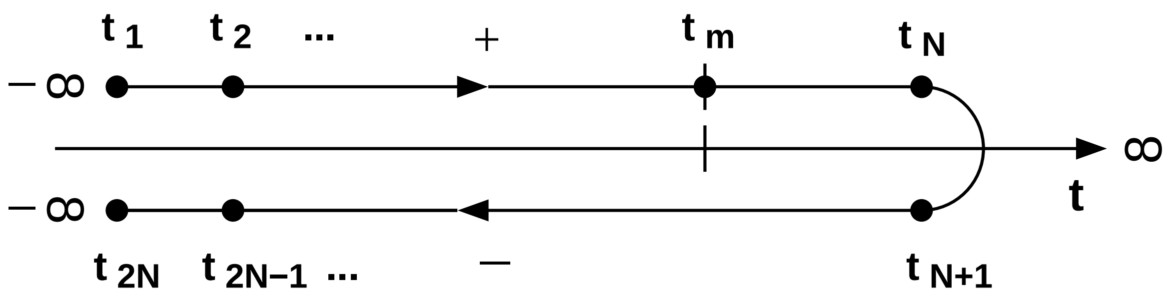
$\hat{n}_\sigma = d^\dagger_\sigma d_\sigma$ dot operators, $c_{kp\sigma}$ lead operators

Nonequilibrium current

- Observable: symmetrized current $I = (I_L - I_R)/2$
  with $I_p(t) = -e\dot{N}_p$

$$I(t) = -\frac{ie}{2}\sum_{kp\sigma}\left[p t_p \langle c^\dagger_{kp\sigma} d_\sigma \rangle_t - p t^*_p \langle d^\dagger_\sigma c_{kp\sigma}\rangle_t\right]$$

- Nonequilibrium current: Keldysh formalism:



- extend real time axis ⇒ Green function: Keldysh matrix

$$G^{\alpha\beta}_{ij}(t_\alpha, t'_\beta) = -i\langle \mathcal{T}_C[\psi_i(t_\alpha)\psi^\dagger_j(t'_\beta)]\rangle$$

Keldysh path integral & generating function

- calculate expectation value $I(t_m)$ via

$$I(t_m) = -i\frac{\partial}{\partial\eta}\ln Z[\eta]\Big|_{\eta=0}$$

from a generating function $\ln Z[\eta]$

- Construct path integral for

$$Z[\eta] = \int \mathcal{D}\left[\prod_\sigma \bar{d}_\sigma, d_\sigma, \bar{c}_{kp\sigma}, c_{kp\sigma}\right] e^{iS[\bar{d}_\sigma, d_\sigma, \bar{c}_{kp\sigma}, c_{kp\sigma}]}$$

with Grassmann fields $d, \bar{d}, c, \bar{c}$ and action

$$S = S_{dot} + S_{leads} + S_T + S_\eta$$

Keldysh path integral & generating function

Action $S = S_{dot} + S_{leads} + S_T + S_\eta$

with

$$
\begin{aligned}
S_{dot} &= S_{dot,0} + S_U \\
&= \int_C dt \left[\sum_\sigma \bar{d}_\sigma \left(i\partial_t - \epsilon_{0\sigma} \right) d_\sigma + \frac{U}{2} (n_\uparrow - n_\downarrow)^2 \right] \\
S_{leads} &= \int_C dt \sum_{kp\sigma} \bar{c}_{kp\sigma} (i\partial_t - \epsilon_{kp} + \mu_p) c_{kp\sigma} \\
S_T &= \int_C dt \sum_{kp\sigma} t_p \bar{c}_{kp\sigma} d_\sigma + h.c. \\
S_\eta &= \frac{ie\eta}{2} \sum_{kp\sigma} p (t_p \bar{c}_{kp\sigma} d_\sigma - t_p^* \bar{d}_\sigma c_{kp\sigma})(t_m)
\end{aligned}
$$

For pedagocial reasons: noninteracting case $U = 0$

- Hamiltonian is quadratic $\Rightarrow$ Gaussian integrals

$$Z_{ni}[\eta] = \prod_{\sigma} \det \left[-iG_{0\sigma}^{-1}(t,t') + \eta \Sigma^J(t,t') \right]$$

with dot GF in presence of the leads

$$\Gamma_L = \Gamma_R = \Gamma/2$$

$$\begin{aligned} G_{0\sigma}(\omega) &= \left[(\omega - \epsilon_{0\sigma})\tau_z - \gamma_L(\omega) - \gamma_R(\omega) \right]^{-1} \\ &= \frac{1}{\Gamma^2 + (\omega - \epsilon_{0\sigma})^2} \begin{pmatrix} \omega - \epsilon_{0\sigma} + i\Gamma(F-1) & i\Gamma F \\ i\Gamma(F-2) & -\omega + \epsilon_{0\sigma} + i\Gamma(F-1) \end{pmatrix} \end{aligned}$$

$$F = f(\omega + eV/2) + f(\omega - eV/2)$$

and source term

$$\Sigma^J(t,t') = \frac{e}{2} \left[\gamma_L(t,t') - \gamma_R(t,t') \right] \left[\delta(t - t_m) - \delta(t' - t_m) \right]$$

Interacting case $U \neq 0$: Hubbard-Stratonovich

- Next: decouple quartic term: Hubbard-Stratonovich trafo

$$e^{\pm i\delta_t U(\hat{n}_\uparrow - \hat{n}_\downarrow)^2/2} = \frac{1}{2}\sum_{s^\pm=\pm} e^{-\delta_t \lambda_\pm s^\pm (\hat{n}_\uparrow - \hat{n}_\downarrow)}$$

- observe that $n_\uparrow - n_\downarrow = 0, \pm 1$
- solution to this equation (in general, not unique):

$$\lambda_\pm = \lambda' \pm i\lambda''$$

with $\delta_t \lambda' = \sinh^{-1}\sqrt{\sin(\delta_t U/2)}, \;\; \delta_t \lambda'' = \sin^{-1}\sqrt{\sin(\delta_t U/2)}$

$\Rightarrow$ Integrate out all fermionic degrees of freedom

Interacting case $U \neq 0$: Hubbard-Stratonovich

- Integrate out all fermions, price: introduce HS Ising fields $s_k^{\pm}$:

$$Z[\eta] = \sum_{\{s\}} \prod_{\sigma} \det G_{\sigma}^{-1}[\{s\}, \eta]$$

where now the path summation extends over all possible Ising fields

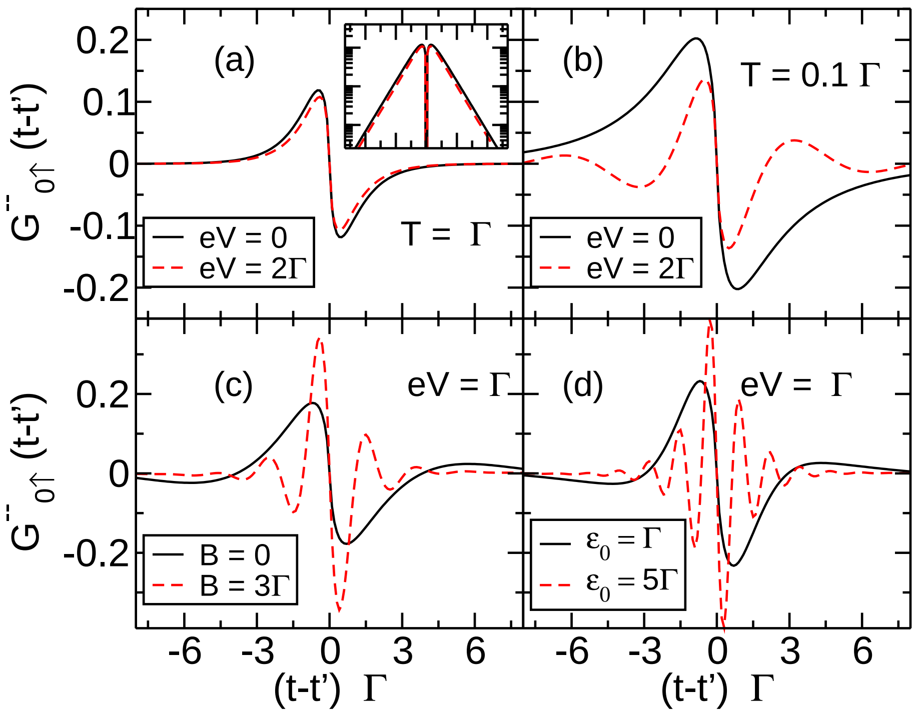
$$\{s\} = (s_1 = \pm 1, s_2 = \pm 1, \ldots, s_N = \pm 1, \ldots, s_{2N} = \pm 1)$$

- Time-discrete full GF takes the form

$$\left(G_{\sigma}^{-1}\right)_{kl}^{\alpha\beta}[\{s\}, \eta] = \left(G_{0\sigma}^{-1}\right)_{kl}^{\alpha\beta} + i\eta\Sigma_{kl}^{J,\alpha\beta} - i\delta_t \delta_{kl} \lambda_{\alpha} s_k^{\alpha} \delta_{\alpha\beta}$$

ISPI now computes this path sum in an exact way!

Iterative Summation of real-time Path Integrals ISPI



- central: each Keldysh component of $G_{0\sigma,kl}$ decays exponentially at finite T for $|k-l| \to \infty$
- $\Rightarrow$ time scale τ_c of correlations exists: $\tau_c^{-1} \sim \max(k_B T, eV)$
- $D_{kl} \simeq 0$ for $|k-l| > \tau_c \equiv K\delta_t$ (convenient: $D_\sigma = G_{0\sigma} G_\sigma^{-1}$)
- Discrete GF assume band matrix structure
- width of band $\sim$ memory K

Iterative Summation of real-time Path Integrals ISPI

Band structure of discrete GF (again, $D_\sigma = G_{0\sigma} G_\sigma^{-1}$):

$$D \equiv D_{(1,N_K)} = \begin{pmatrix} \boxed{D^{11}} & \boxed{D^{12}} & 0 & 0 & \dots & 0 \\ \boxed{D^{21}} & \boxed{D^{22}} & \boxed{D^{23}} & 0 & \dots & \vdots \\ 0 & \boxed{D^{32}} & \boxed{D^{33}} & \boxed{D^{34}} & \dots & \vdots \\ 0 & 0 & \boxed{D^{43}} & \boxed{D^{44}} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \boxed{D^{N_K-1 N_K}} \\ 0 & \dots & \dots & 0 & \boxed{D^{N_K N_K-1}} & \boxed{D^{N_K N_K}} \end{pmatrix}$$

All blocks have size $K \times K$; $N_K = N/K$

Iterative Summation of real-time Path Integrals ISPI

We have to calculate the generating funtion

$$Z[\eta] = \sum_{\{s\}} \prod_\sigma \det G_\sigma^{-1}[\{s\},\eta]$$

Goal: Calculate determinant iteratively, using Schur form:

- general matrix (a,d: square blocks, b,c: rect. blocks)

$$D = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

- Gaussian elimination:

$$\tilde{D} = LD = \begin{pmatrix} I_n & 0 \\ -ca^{-1} & I_m \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a & b \\ 0 & d - ca^{-1}b \end{pmatrix}$$

$$\det(D) = \det(a)\det(d - ca^{-1}b)$$

Iterative Summation of real-time Path Integrals ISPI

Let's apply this to the full GF:

$$D \equiv D_{(1,N_K)} = \left(\begin{array}{c|ccccc} \boxed{D^{11}} & \boxed{D^{12}} & 0 & 0 & \ldots & 0 \\ \hline \boxed{D^{21}} & \boxed{D^{22}} & \boxed{D^{23}} & 0 & \ldots & \vdots \\ 0 & \boxed{D^{32}} & \boxed{D^{33}} & \boxed{D^{34}} & \ldots & \vdots \\ \vdots & 0 & \ldots & \ldots & \ldots & \ldots \end{array}\right)$$

After the first step of the iteration:

$$\begin{aligned} Z[\eta] &= \sum_{s_1^\pm,\ldots,s_N^\pm} \det\left\{D^{11}[s_1^\pm,\ldots,s_K^\pm]\right\} \\ &\times \det\Big\{D_{(2,N_K)}[s_{K+1}^\pm,\ldots,s_N^\pm] - D^{21}[s_{K+1}^\pm,\ldots,s_{2K}^\pm] \\ &\times \left[D^{11}[s_1^\pm,\ldots,s_K^\pm]\right]^{-1} D^{12}[s_{K+1}^\pm,\ldots,s_{2K}^\pm]\Big\} \end{aligned}$$

Iterative Summation of real-time Path Integrals ISPI

- repeat this, finally:

$$Z[\eta] = \sum_{s_1^\pm,\ldots,s_N^\pm} \det\left\{D^{11}[s_1^\pm,\ldots,s_K^\pm]\right\} \prod_{l=1}^{N_K-1} \det\left\{D^{l+1,l+1}[s_{lK+1}^\pm,\ldots,s_{(l+1)K}^\pm]\right.$$
$$\left. - D^{l+1,l}[s_{lK+1}^\pm,\ldots,s_{(l+1)K}^\pm]\left[D^{l,l}[s_{(l-1)K+1}^\pm,\ldots,s_{lK}^\pm]\right]^{-1} D^{l,l+1}[s_{lK+1}^\pm,\ldots,s_{(l+1)K}^\pm]\right\}$$

- reorder and disentangle $\Rightarrow$ iterative scheme:

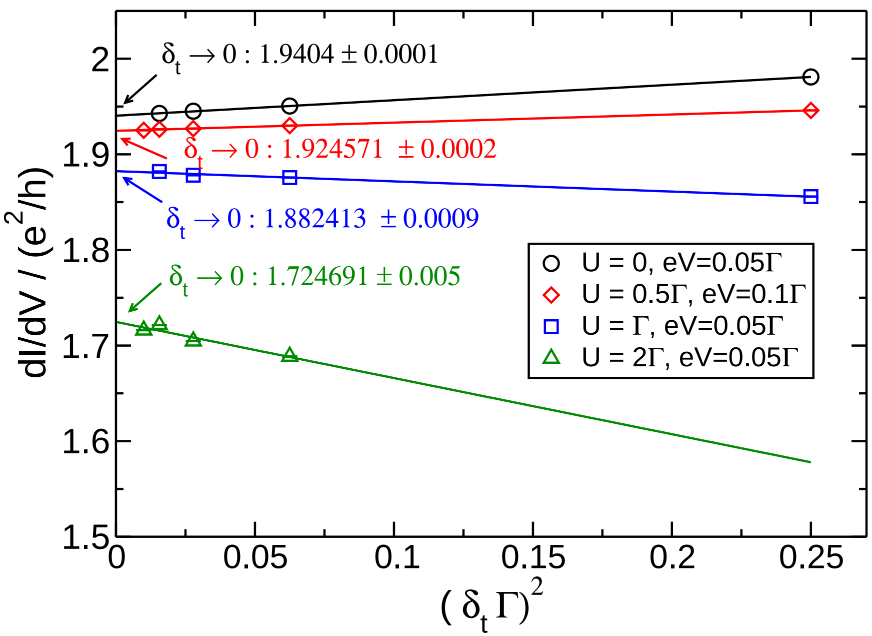
$$Z_{l+1}[s_{lK+1}^\pm,\ldots,s_{(l+1)K}^\pm] = \sum_{s_{(l-1)K+1}^\pm,\ldots,s_{lK}^\pm} \Lambda_l[s_{(l-1)K+1}^\pm,\ldots,s_{lK}^\pm,s_{lK+1}^\pm,\ldots,s_{(l+1)K}^\pm] \times Z_l[s_{(l-1)K+1}^\pm,\ldots,s_{lK}^\pm]$$

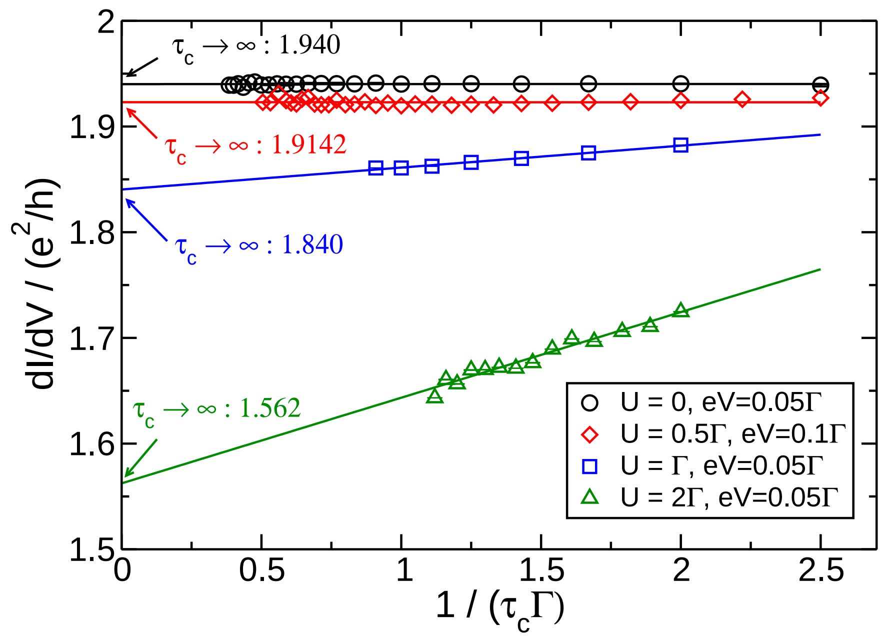
- final step:

$$Z[\eta] = \sum_{s_{N-K+1}^\pm,\ldots,s_N^\pm} Z_{N_K}[s_{N-K+1}^\pm,\ldots,s_N^\pm]$$

ISPI: convergence & extrapolation

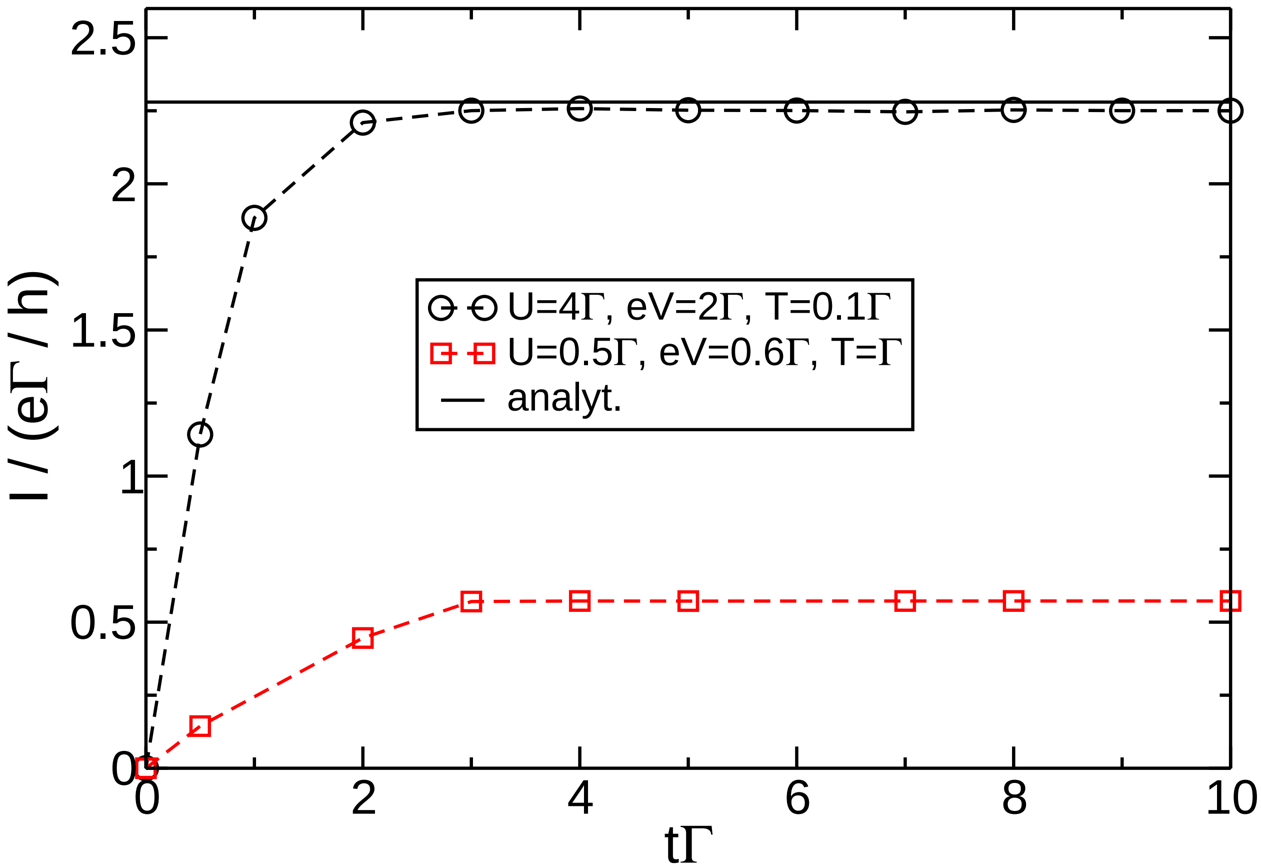
- still two numerical errors:
  1. finite time discretization $t = N\delta_t$: Trotter $\sim \mathcal{O}(\delta_t^2)$
  2. finite memory $\tau_c = K\delta_t$
- naive convergence $\delta_t \to 0$ and $K \to \infty$ not possible!
- But extrapolation:





gives exact result $I = I(\delta_t \to 0, \tau_c \to \infty)$

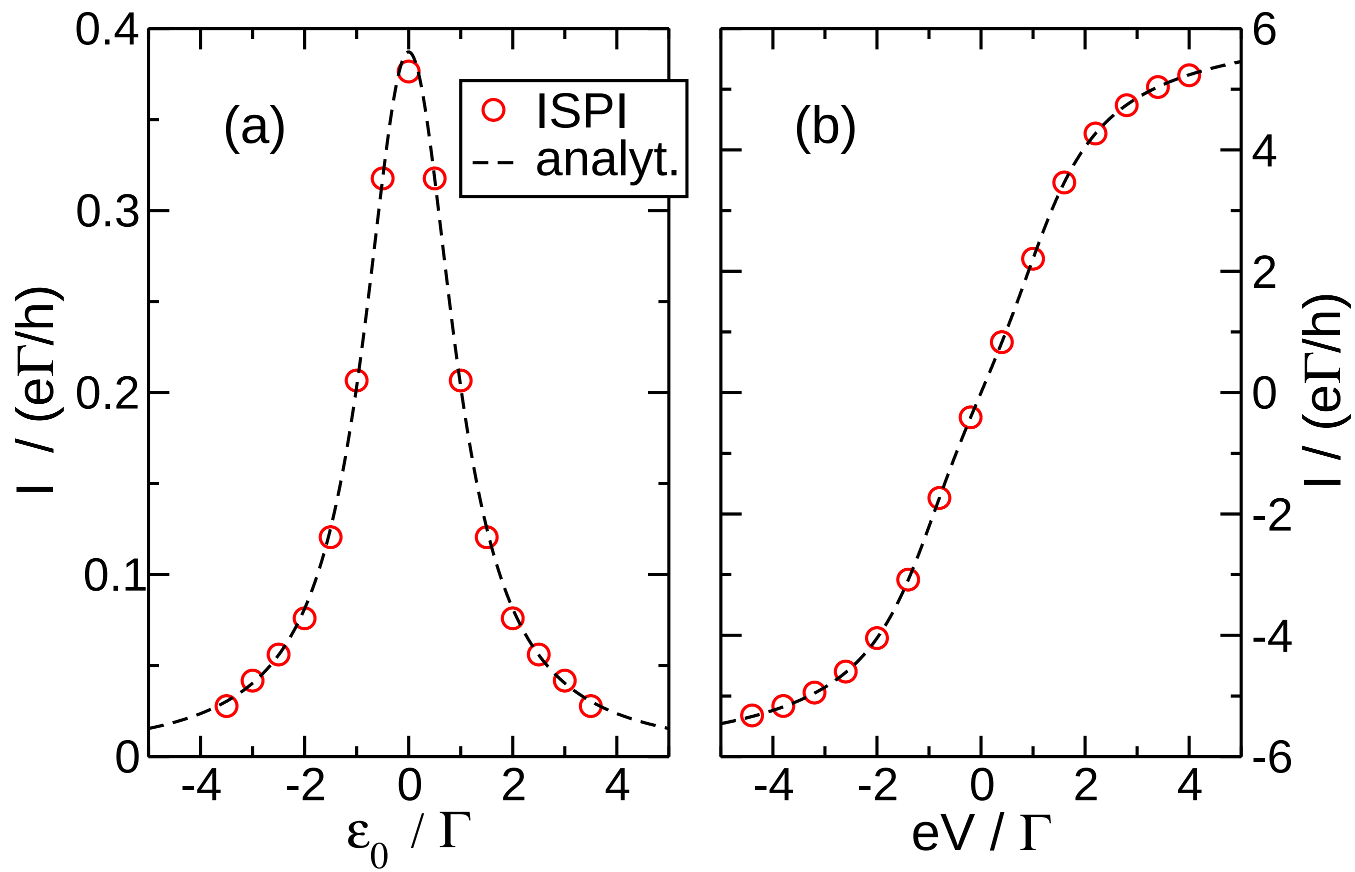
Results: time-dependent current



$\epsilon_0 = B = 0$

- after initial transient behavior, current saturates
- agreement with nonequilibrium Kondo theory of Rosch *et al.* which is valid for $eV \gg T_K (= 0.29\Gamma)$

ISPI vs. analytics: $U = 0$

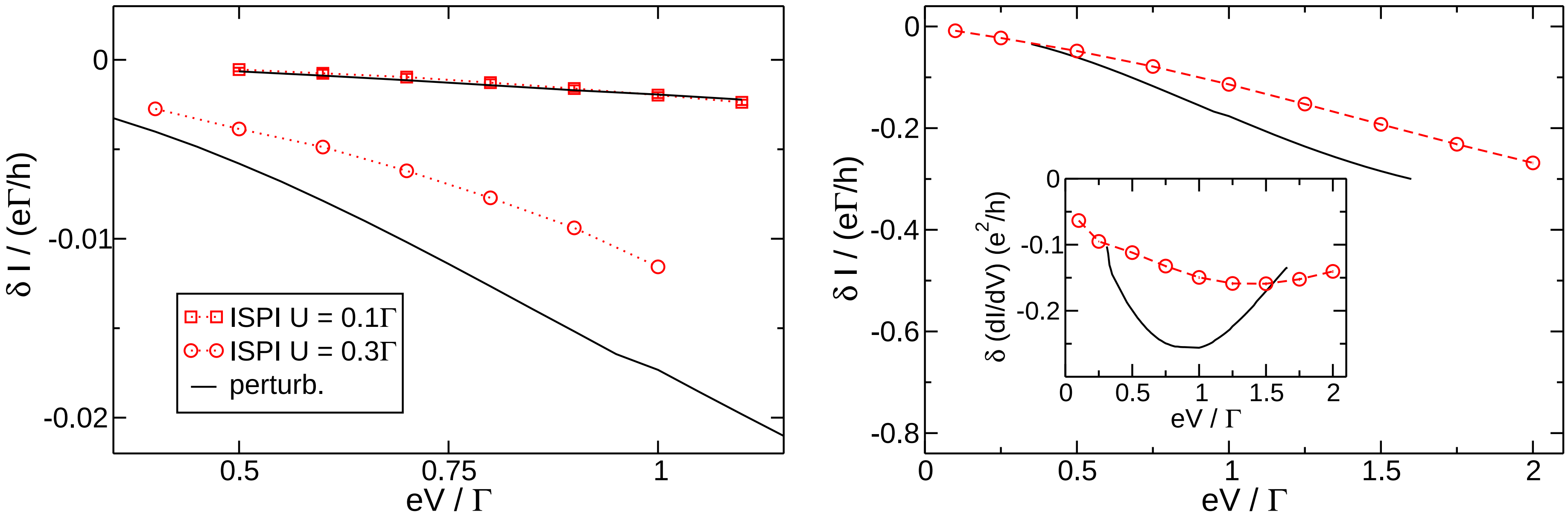


$T = 0.1\Gamma, B = 0$, (a) $eV = 0.2\Gamma$, (b) $\epsilon_0 = 0$

- warm-up check: $U = 0$
- complete agreement
- current conservation also checked!

ISPI vs. analytics: small U

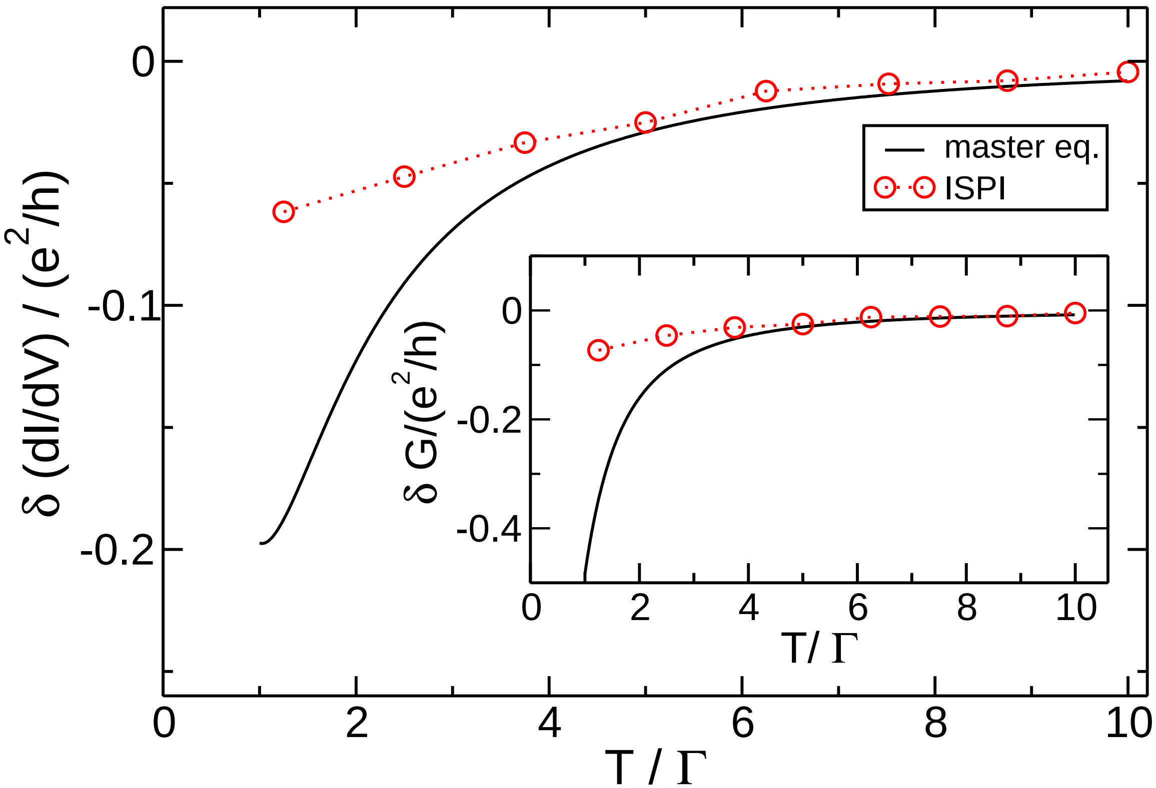
interaction corrections $\delta A \equiv A(U) - A(U=0)$



$U = 0.1\Gamma, 0.3\Gamma$ $\qquad$ $U = \Gamma \qquad T = 0.1\Gamma$

- perturbation theory in U:
  - interaction self-energy up to $\mathcal{O}(U^2)$
  - possible only at the e-h-symmetric point $\epsilon_0 = B = 0$

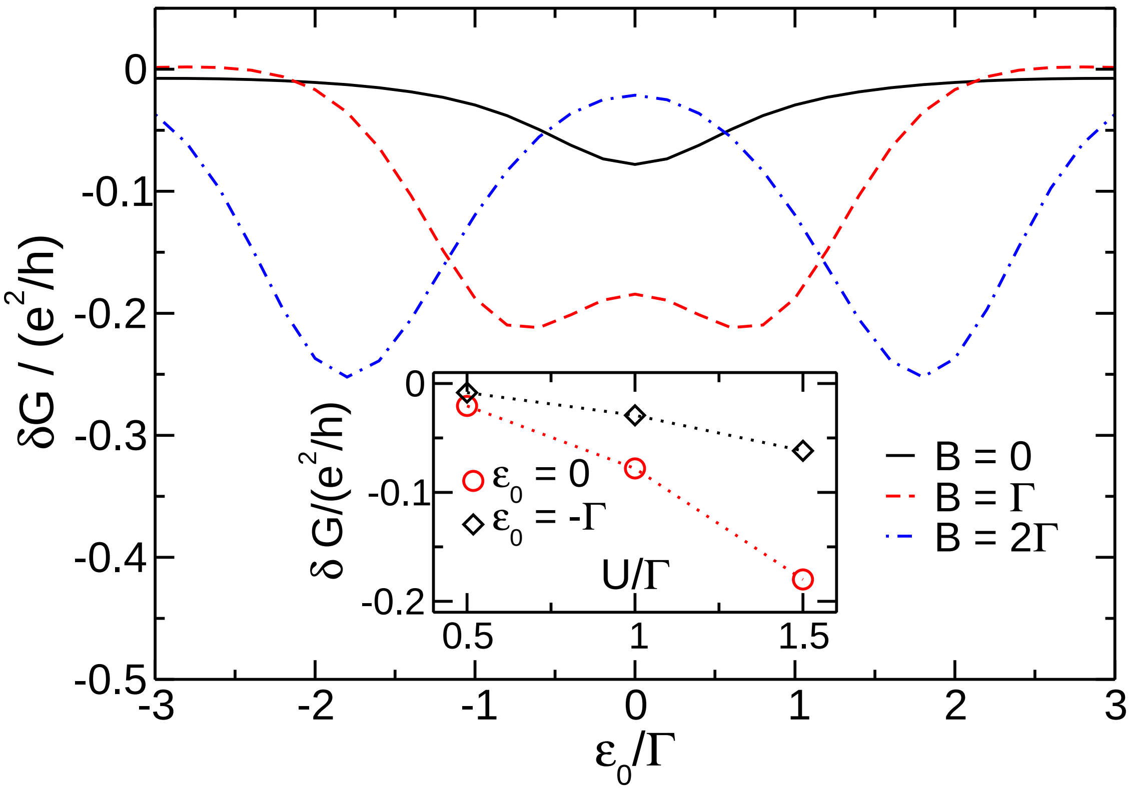
ISPI vs. analytics: sequential regime $T \gg \Gamma$



$U = \Gamma, eV = 3\Gamma, \epsilon_0 = B = 0$

- comparison with simple rate equation vaild at $T \gg \Gamma$
- agreement for $T \gtrsim 4\Gamma$
- coherence effects important for $T < \Gamma$

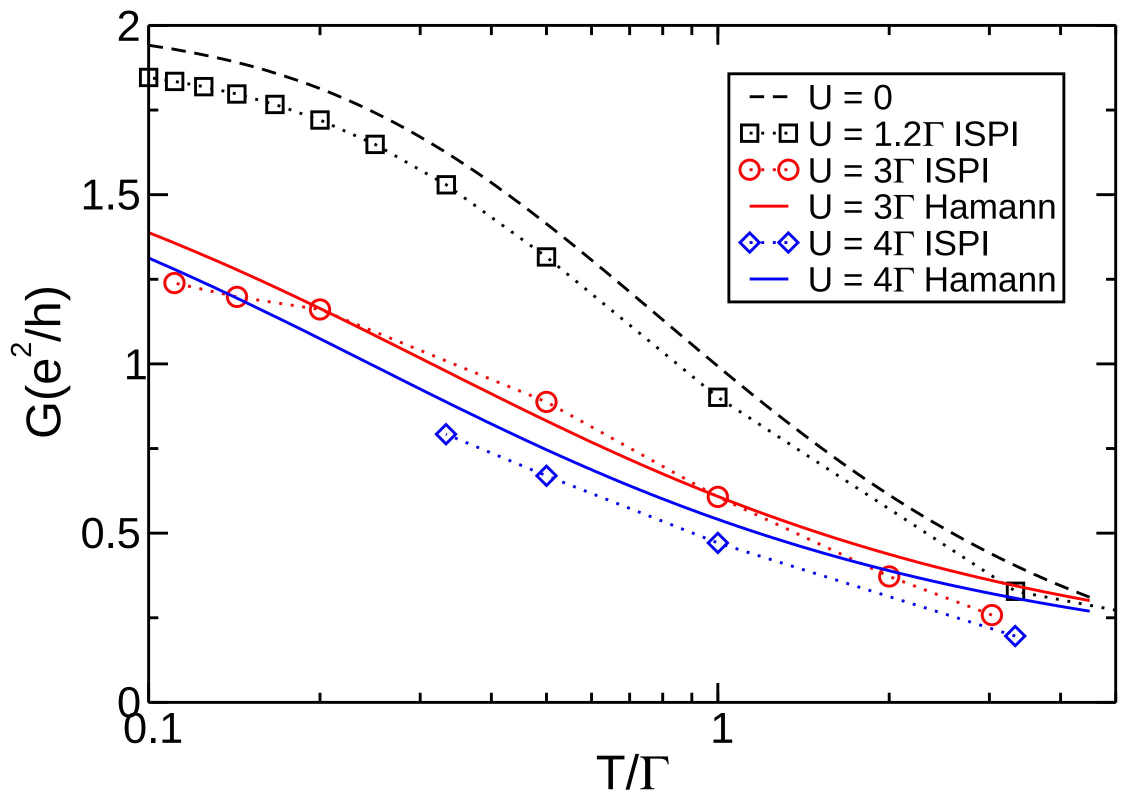
Small bias regime $eV \leq \Gamma$



$U = \Gamma, T = 0.1\Gamma$, inset: $B = 0$

- B-field splits conductance peak: $\Delta\epsilon_0 \approx 2B$
- interaction corrections most pronounced on resonance

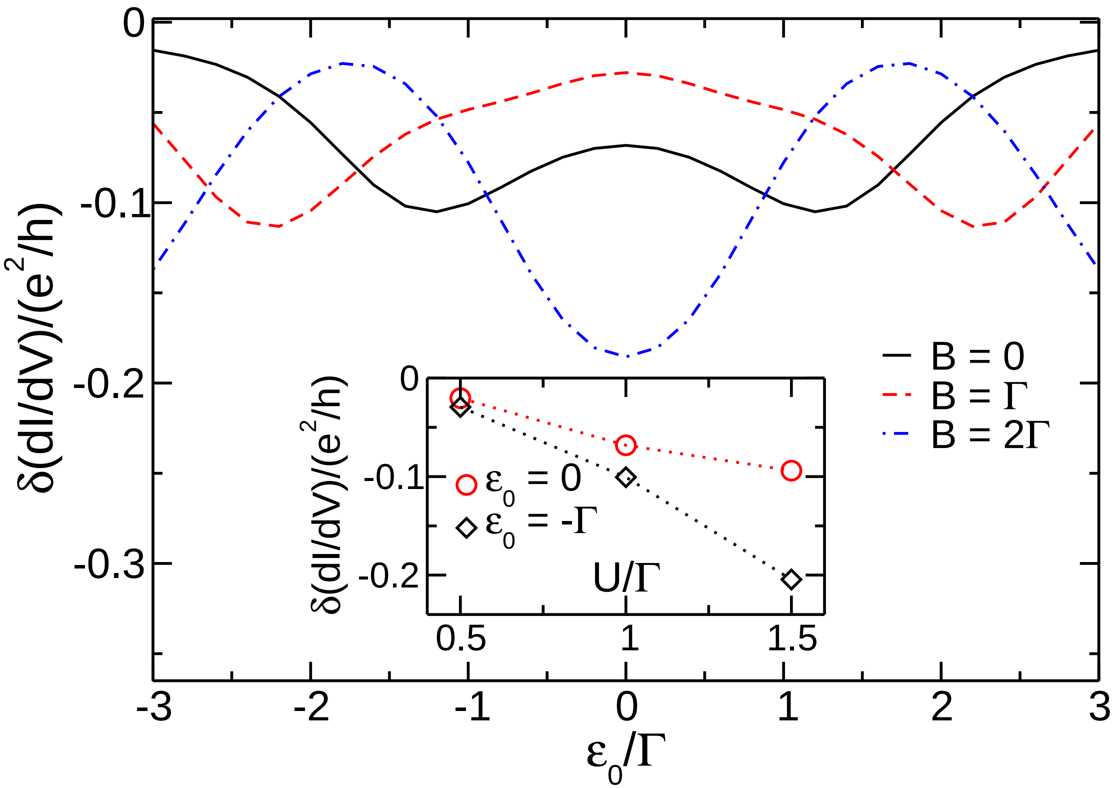
Linear conductance peak



$\epsilon_0 = B = 0\Gamma$

- temperature dependence for $T_K \lesssim T$
- agreement with formula of Hamann, PR (1967) which agrees with NRG results of Costi *et al.* (1994)
- until now: no convergent results for $T \to 0, V \to 0$!

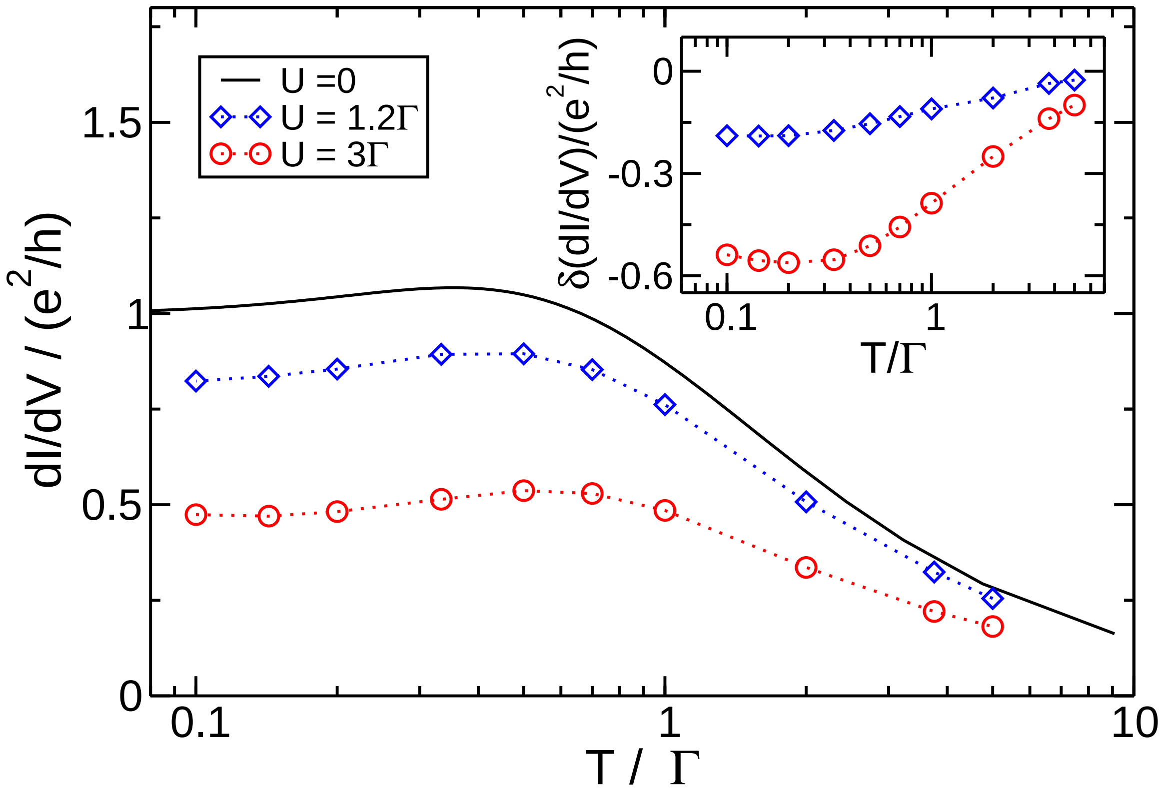
Large bias regime $eV > \Gamma$



$U = \Gamma, eV = 3\Gamma, T = 0.1\Gamma$, inset: $B = 0$

- Splitting of conductance peak at large V for $B = 0$: $\Delta\epsilon_0 \approx eV/2$
- four peak structure at finite B-field
- interaction corrections most pronounced on resonance

Result: nonlinear differential conductance

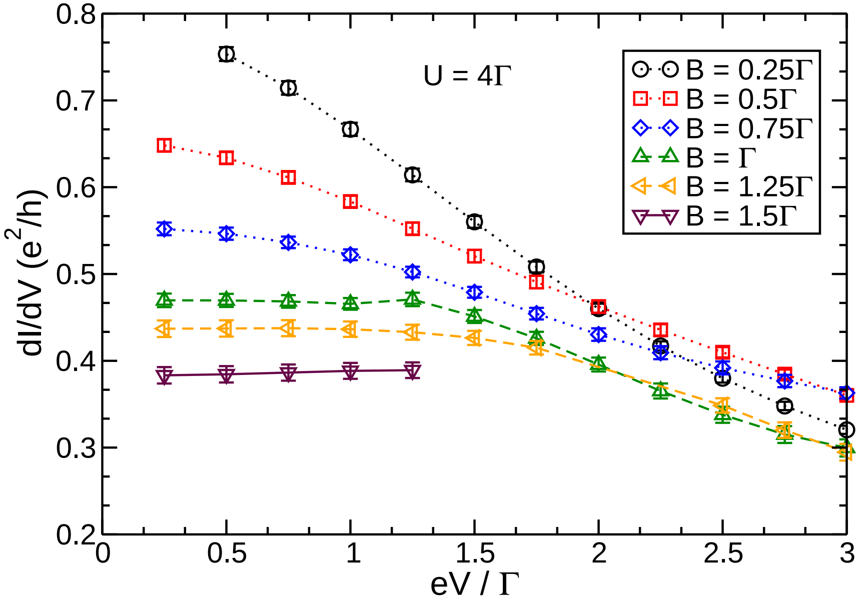


$eV = 2\Gamma, \epsilon_0 = B = 0$

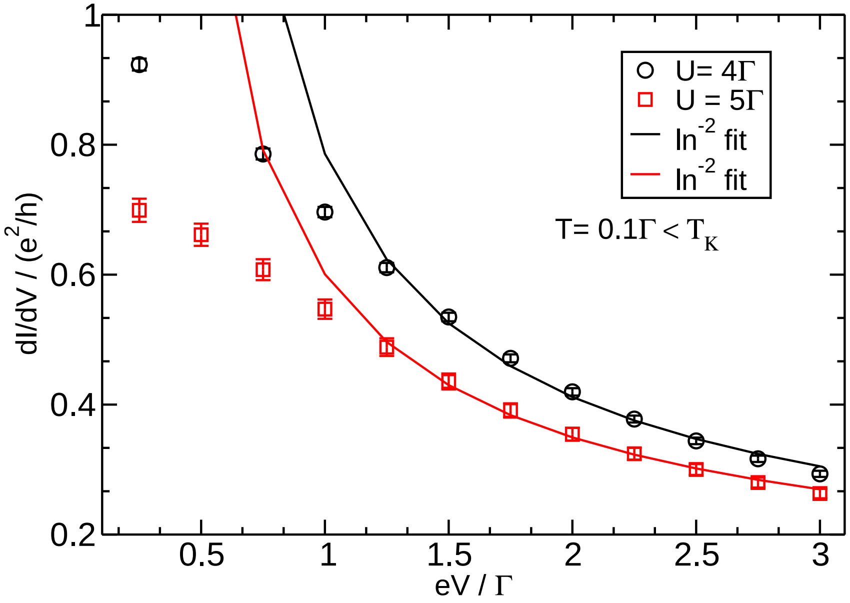
- increase with lowering T
- increasing interaction suppresses conductance
- conductance decreases when bias voltage is raised

Current studies: preliminary results

- nonequilibrium Kondo regime: $eV \approx T_K$
- influence of magnetic field: $T_K \lesssim B$
- calculate spectral function out of equilibrium: splitting of Kondo resonance



$T = 0.1\Gamma, \epsilon_0 = 0$



$\epsilon_0 = B = 0$

Relation to bosonic QUAPI*

similar:

- idea of iterative evaluation of real-time path sum

major difference:

- fermions $\Rightarrow$ Grassmann fields in the functional integrals
- QUAPI: “dipole” coupling $H_{SB} = X \sum_j c_j x_j$
  $\Rightarrow$ use eigenvalues of X to evaluate Feynman-Vernon influence functional
- while here: tunnel coupling $H_T = \sum_j (c_j d^\dagger + c_j^\dagger d)$
  no simultaneous eigenbasis of d and $d^\dagger$ exists!
  $\rightarrow$ QUAPI scheme not applicable!

*Makri, Makarov (1995), M.T. *et al.* (1995-2008)

Conclusions

- Iterative Summation of real-time Path Integrals ISPI
- novel method to study quantum transport at nonequilibrium
- based on exact evaluation of real-time path integrals
- numerically exact, generic, no sign problem
- example of Anderson model
- thorough checks
  $\Rightarrow$ ISPI works in wide regime of parameters!
- does not yet converge for $eV \to 0, T \to 0$
- fancy property:
  the more nonequilibrium, the better ISPI works

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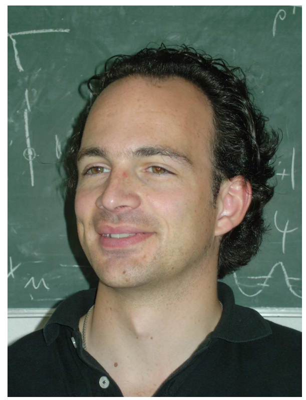

Jens Eckel