# Iterative Simulation of Path Integrals (ISPI)


Reinhold Egger

Michael Thorwart, Stephan Weiss, Jens Eckel

# Overview

- Nonequilibrium quantum transport for strongly correlated dots/molecules: no numerically exact methods available until very recently !!
- Of interest: steady-state transport properties under applied bias voltage V
- Numerical path-integral approach: ISPI
- Anderson dot implementation
  - Perturbative (in U) regime
  - High temperature regime: master equation
  - Kondo effect (linear transport & nonequilibrium regime)
- Outlook

***PRB 77, 195316 (2008)***

# Nonequilibrium theories for quantum transport through molecules /dots / quantum impurities

- Analytical methods
  - Perturbation theory in various limits
    *Fujii & Ueda, PRB 2003; Egger & Gogolin, PRB 2008*
  - Exact approaches (interacting resonant level model)
    *Doyon, PRL 2007; Mehta & Andrei, PRL 2006; Boulat & Saleur, PRB 2008*
  - Approximate interpolation schemes *Aligia, PRB 2006*
  - Perturbative RG *Rosch, Paaske, Kroha & Wölfle, PRL 2003*
- Numerically exact methods ?
  - Real-time QMC simulations (but: sign problem)
    *Egger et al., PRE 2000; Mühlbacher & Rabani, PRL 2008*
  - Renormalization group based approaches: Wegner´s flow equation approach, functional RG, numerical RG, DMRG *Kehrein, PRL 2005; Jakobs, Meden & Schoeller, PRL 2007; Anders, PRL 2008*
  - **This talk: ISPI**

# ISPI scheme: Anderson dot

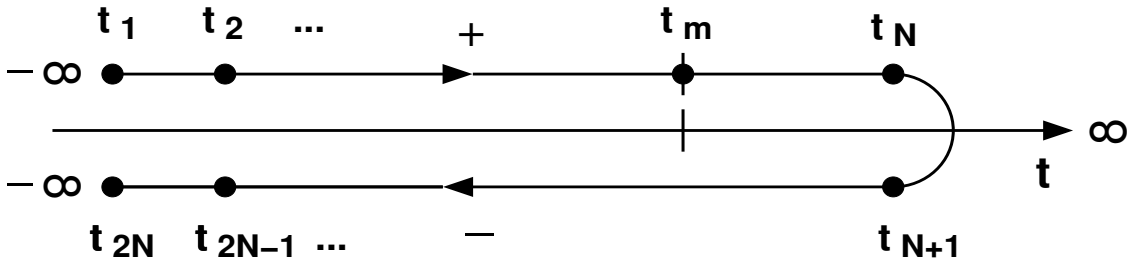
- Consider Anderson model as prototype example (scheme is completely general!)

$$H = H_{dot} + H_{tunnel} + H_{leads}$$

$$H_{dot} = \sum_{\sigma=\pm} \underbrace{(\varepsilon_0 + \sigma B)}_{=\varepsilon_{0,\sigma}} n_\sigma - \frac{U}{2}(n_\uparrow - n_\downarrow)^2$$

- Free parameters (for simplicity: symmetric case)
  - Charging energy U>0, magnetic field scale B, dot level $\varepsilon_0$
  - Hybridization $\Gamma_L = \Gamma_R = \Gamma/2$ between dot and leads
  - Applied voltage V, temperature T
- Observable of main interest: current I(V)
  - ✓ Current conservation is explicitly verified in our scheme

# Keldysh approach to noneq. current




- Obtain current from generating functional with suitable source term

$$I(t_m) = -i \frac{\partial}{\partial \eta} \ln Z(\eta = 0)$$

- Directly computed via path integral on the (discretized) Keldysh contour, follows as function of measurement time $t_m$
- Stationary steady-state current is long time limit

# Hubbard Stratonovich transformation

- Time-discretized representation of partition function with 2N time slices, $t = N\delta_t$
- Trotter breakup of short-time propagator

$$e^{\mp i\delta_t (H_{dot}+H_{tunnel})} = e^{\mp i\delta_t H_{tunnel}/2} e^{\mp i\delta_t H_{dot}} e^{\mp i\delta_t H_{tunnel}/2} + O\left(\delta_t^2\right)$$

- Decouple the interaction: discrete HS transformation on each time slice

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

$$\lambda_\pm = \delta_t^{-1} \cosh^{-1} e^{\pm i\delta_t U/2}$$

introduces 2N auxiliary Ising spins $s_i^\alpha = \pm$, living on the upper/lower Keldysh branch $\alpha = \pm$

(NB: other choices for HS decomposition are possible)

# Exact path-integral representation

Generating functional after the integration over noninteracting fermions: Path integral over all $2^{2N}$ Ising spin configurations

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

$$\left(G_{\sigma}^{-1}\right)_{mn}^{\alpha\beta}[\{s\},\eta]=\left(g_{\sigma}^{-1}\right)_{mn}^{\alpha\beta}+i\eta\Sigma_{mn}^{J,\alpha\beta}-i\delta_{\alpha\beta}\delta_{mn}\delta_{t}\lambda_{\alpha}s_{n}^{\alpha}$$

Keldysh Green´s function of interacting dot coupled to leads

# Ingredients

Noninteracting Keldysh Green´s function of dot:

$$g_{\sigma,mn} = \int \frac{d\omega}{2\pi} e^{i\delta_t (m-n)\omega} g_\sigma(\omega)$$

$$g_\sigma(\omega) = \frac{1}{\Gamma^2 + (\omega - \varepsilon_{0,\sigma})^2} \begin{pmatrix} \omega - \varepsilon_{0,\sigma} + i\Gamma(F_\omega - 1) & i\Gamma F_\omega \\ i\Gamma(F_\omega - 2) & -\omega + \varepsilon_{0,\sigma} + i\Gamma(F_\omega - 1) \end{pmatrix}$$

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

… self energy $\Sigma^J$ (from source term) can be given in similar fashion …

# Keldysh approach: initial state

Our formulation assumes factorizing initial conditions for the total density matrix

$$\rho(t=0) = \rho_{dot} \otimes \rho_L \otimes \rho_R$$

- For simplicity: assume initially empty dot
- After t=0, tunneling between dot and leads is switched on (Γ)
- If transient currents are of interest, those assumptions could be lifted
- Here: steady state value at long times!

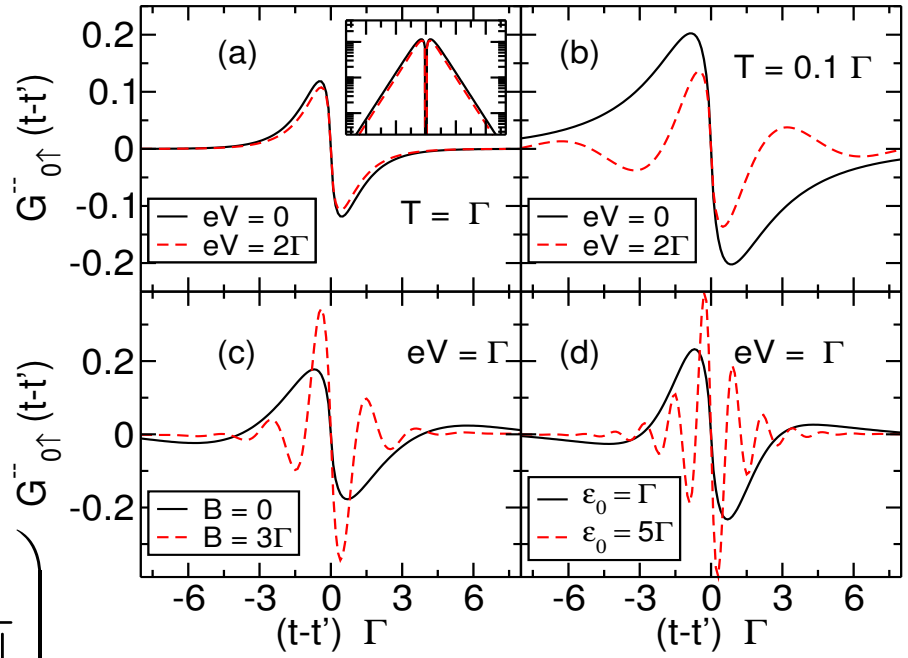
# Iterative scheme

- Computational cost for brute-force exact path summation grows as $2^{2N}$, i.e. exponentially with real time t ↷ impossible in practice
  - Stochastic Monte Carlo evaluation for this path integral suffers from severe sign problem…
- Here: deterministic iterative ISPI scheme
  - ✓ Time correlations in noninteracting Keldysh GF decay exponentially at finite T or V: Truncate after memory time
  - ✓ Full GF is then band matrix, allows for iterative scheme
  - ✓ Numerically exact after Trotter & memory time extrapolation

# Decay of the noninteracting GF

Each component of noninteracting GF decays exponentially with time difference, on memory time scale of order

$$\tau_{mem} \equiv K\delta_t \approx \min\left(\frac{\hbar}{k_B T}, \frac{\hbar}{|eV|}\right)$$




Scheme exact (but useless) for

$$K = N, N \to \infty, \delta_t = t / N \to 0$$

# Finite K truncation

- For finite memory time (i.e. K): approximate GF matrix elements $\left(g_\sigma^{-1}\right)_{mn} = 0$ for $|m-n| \geq K$
- Then $D = \prod_\sigma g_\sigma G_\sigma^{-1}$ is a band matrix in time space, and
$$Z(\eta) = \tilde{N} \sum_{\{s\}} \det D[\{s\}, \eta]$$
- Choose Trotter number $N = KN_K$
- Allows for iterative evaluation…
- Set irrelevant normalization to one

# Band matrix structure

With „elementary“ $K \times K$ blocks $\underline{D^{ll'}}$

(all entries $D_{mn}$ still carry Keldysh and spin structure):

$$\underline{D^{12}} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ D_{2,K+1} & 0 & 0 & \cdots & \cdots \\ \vdots & \vdots & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & 0 & 0 \\ D_{K,K+1} & \vdots & \vdots & D_{K,2K-1} & 0 \end{pmatrix}$$

$$D = \begin{pmatrix} \underline{D^{11}} & \underline{D^{12}} & 0 & \cdots & 0 \\ \underline{D^{21}} & \underline{D^{22}} & \underline{D^{23}} & 0 & \vdots \\ 0 & \underline{D^{32}} & \underline{D^{33}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \underline{D^{N_K-1,N_K}} \\ 0 & \cdots & 0 & \underline{D^{N_K,N_K-1}} & \underline{D^{N_K N_K}} \end{pmatrix}$$

# Spin blocks

- Introduce „spin blocks“ for $l=1,\ldots,N_K$, containing $2K$ Ising spins:

$$S_l = \left\{ s^+_{(l-1)K+1}, s^-_{(l-1)K+1}, \ldots, s^+_{lK}, s^-_{lK} \right\}$$

- Dependence of block matrices on spins:

$$\underline{D^{ll'}} = \underline{D^{ll'}(S_l)}$$

# Iterative solution

- We need determinant of full D
- Use determinant identity (*a,d* are quadratic, *b,c* rectangular block matrices; *a* invertible)

$$\det\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \det(a)\det\left(d - ca^{-1}b\right)$$

Schur complement

- First step: identify $a = \underline{D^{11}(S_1)}$ and perform $S_1$ summation (for *2K* spins, this is still manageable computational problem!)

# Iterative solution

- Now iterate…
- For consistency, we must neglect higher-order terms in the Schur complement, reflecting generated effective couplings with time separations $|m-n| \geq K$

$$\underline{D^{l+2,l+1}}\,\underline{D^{l+1,l}}\left(\underline{D^{l,l}}\right)^{-1}\underline{D^{l,l+1}}\,\underline{D^{l+1,l+2}} \to 0$$

- We then arrive at

$$Z(\eta) = \sum_{\{S\}} \det\left(\underline{D^{11}(S_1)}\right) \times$$

$$\times \prod_{l=1}^{N_K-1} \det\left\{\underline{D^{l+1,l+1}(S_{l+1})} - \underline{D^{l+1,l}(S_{l+1})}\left[\underline{D^{ll}(S_l)}\right]^{-1}\underline{D^{l,l+1}(S_l)}\right\}$$

# Iterative simulation scheme

- Reordering implies ISPI, get generating function as last element of iteration:

$$Z(\eta) = \sum_{S_{N_K}} Z_{N_K}(S_{N_K})$$

$$Z_{l+1}(S_{l+1}) = \sum_{S_l} \Lambda_l[S_{l+1}, S_l] Z_l(S_l)$$

- Propagating „tensor“

$$\Lambda_l(S_{l+1}, S_l) = \det\left(\underline{D^{l+1,l+1}(S_{l+1})} - \underline{D^{l+1,l}(S_{l+1})}\left(\underline{D^{ll}(S_l)}\right)^{-1}\underline{D^{l,l+1}(S_l)}\right)$$

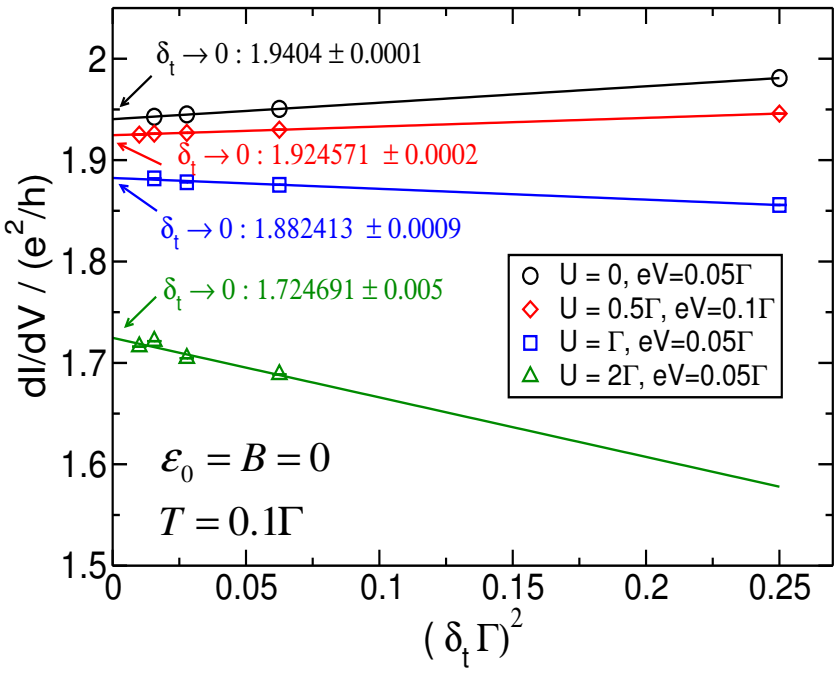
- Initial condition: $Z_1(S_1) = \det \underline{D^{11}(S_1)}$

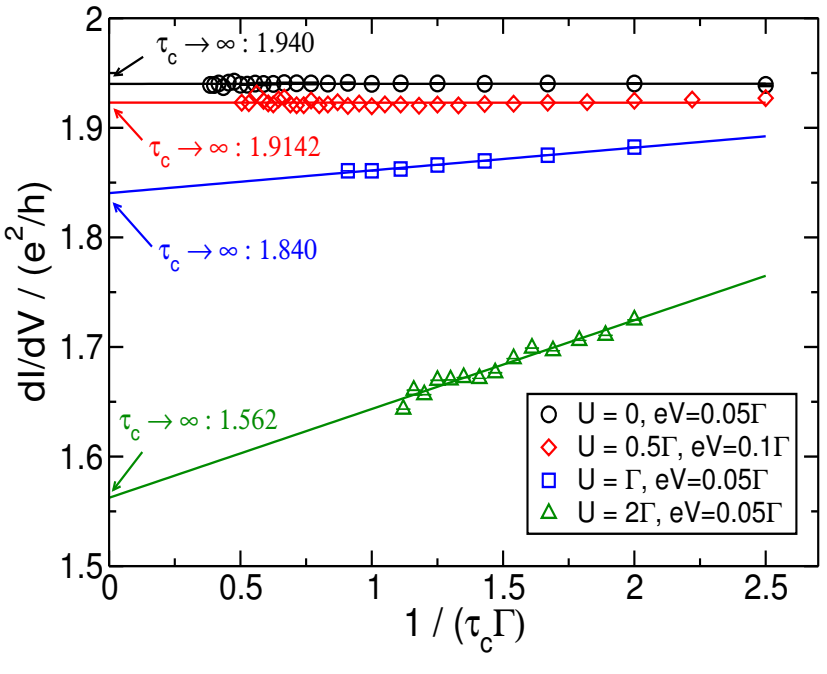
# ISPI: convergence and extrapolation

Eliminate the two remaining errors by extrapolation

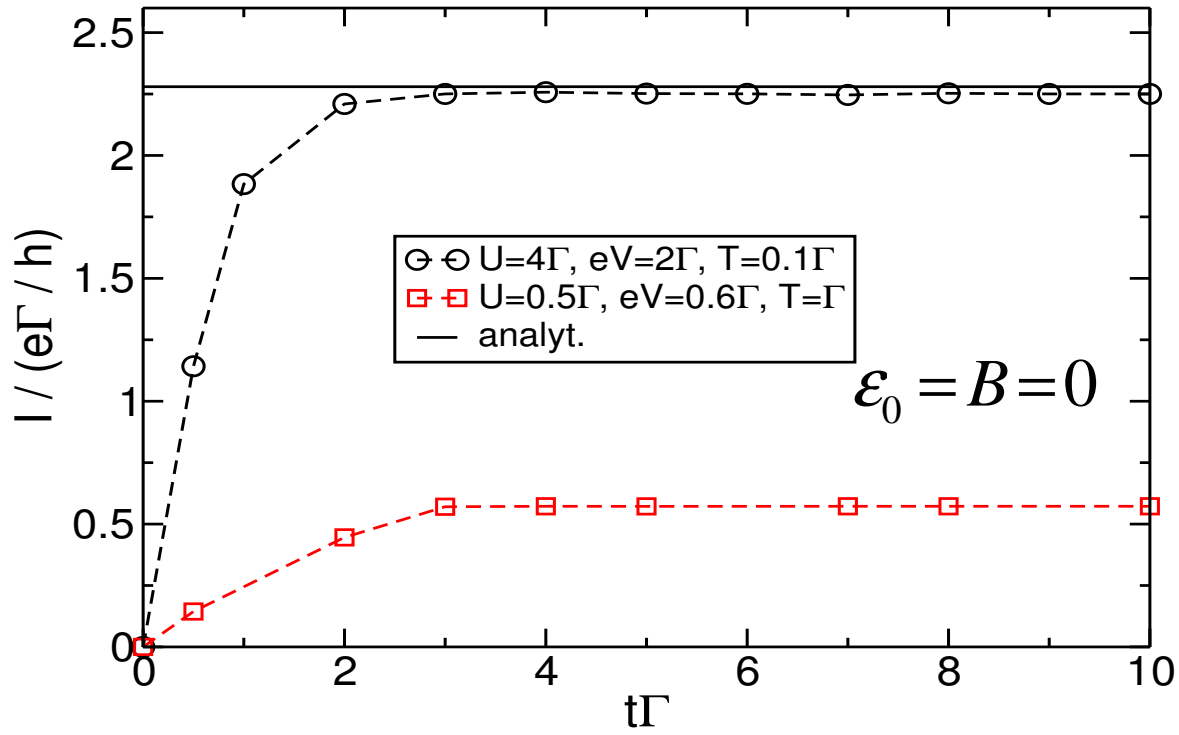
1. Trotter error due to finite N is quadratic in $\delta_t \to 0$
2. Memory time due to finite K

If convergent, numerically exact scheme!



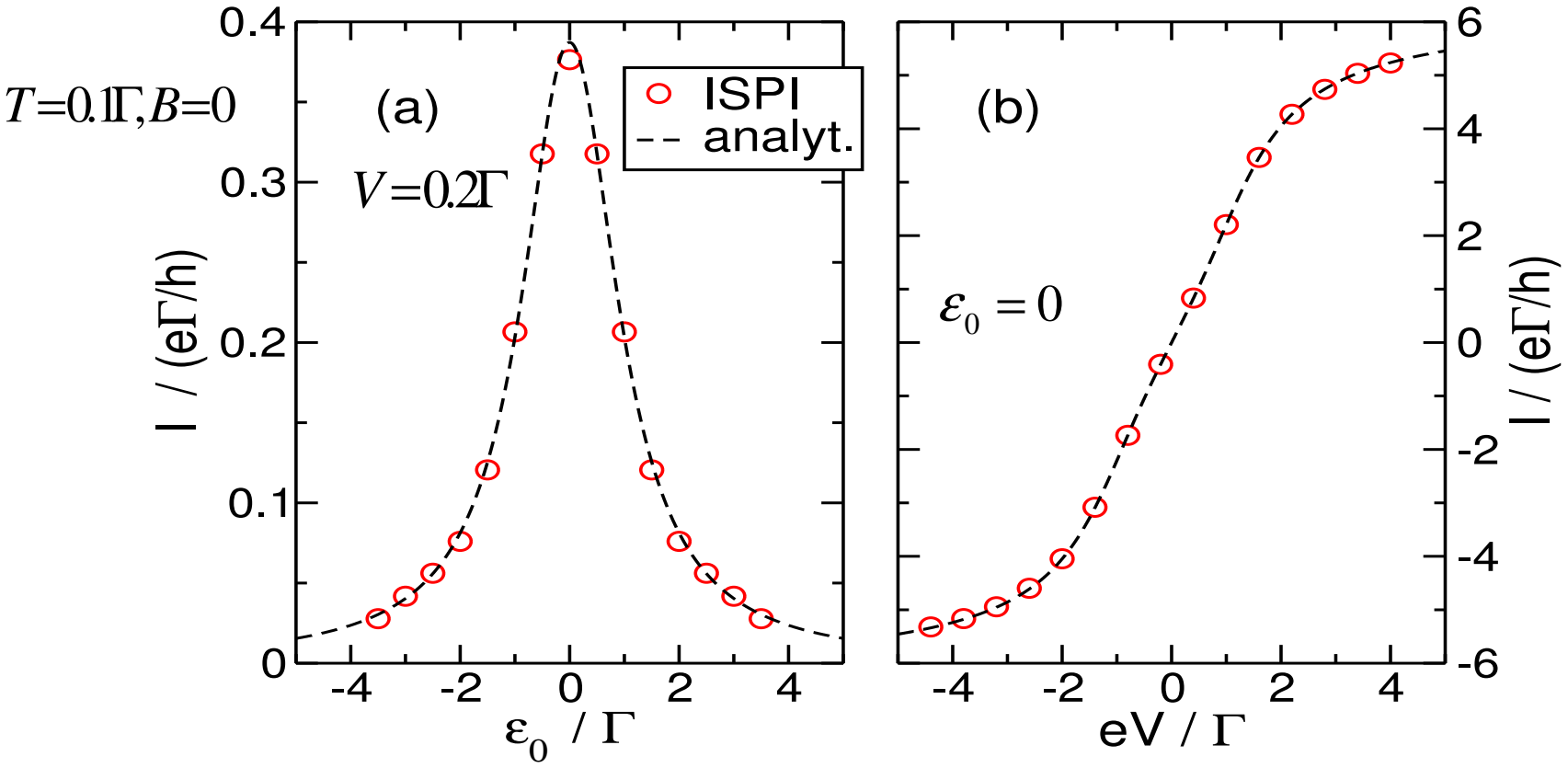



# Results: time dependence of current




Current saturates after initial transient: steady state value.
Upper curve: value agrees with nonequilibrium Kondo theory value *(Rosch et al., PRL 2003)* for $eV >> T_K (= 0.29\,\Gamma)$

# Warm up check: Noninteracting case

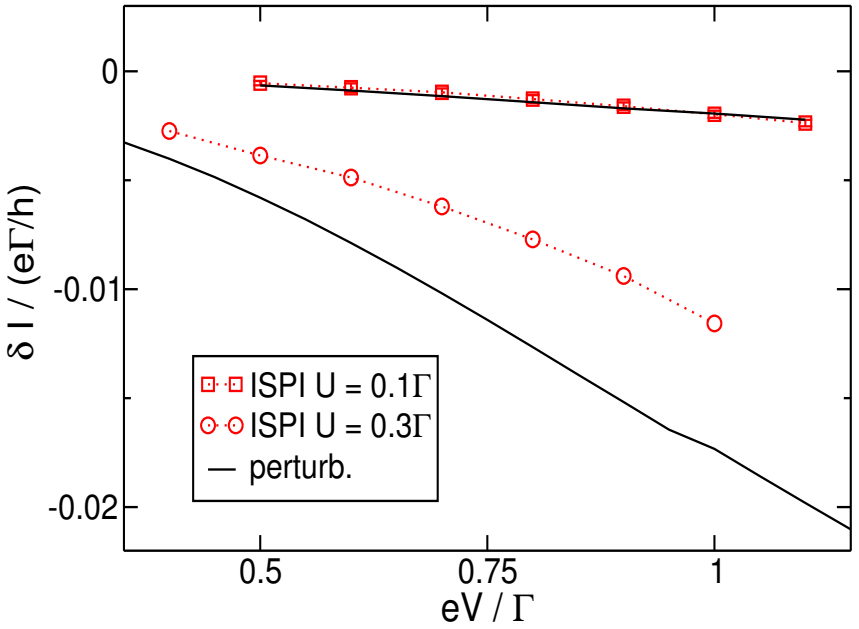


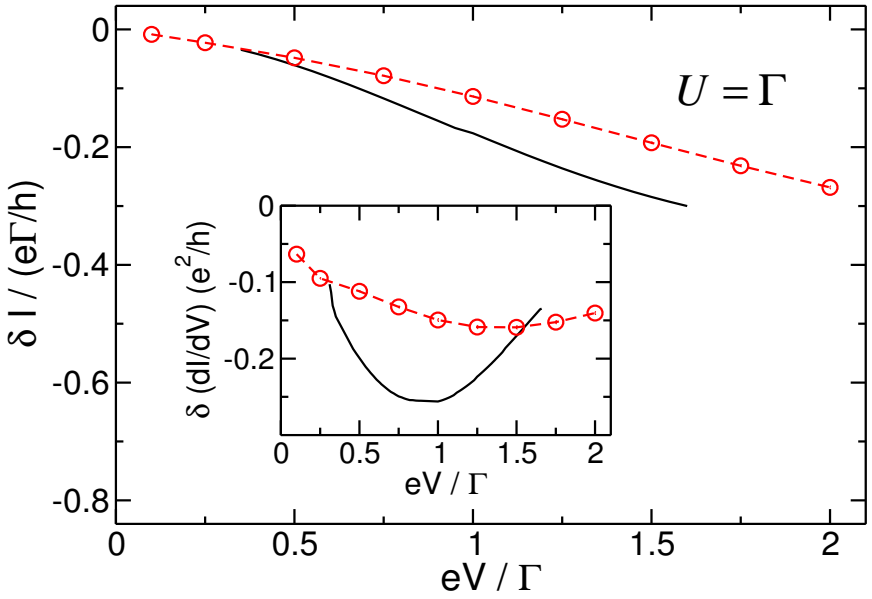

**Now: checks for interacting case…**

# Perturbation theory in U

$$\delta I = I(U) - I(U=0)$$

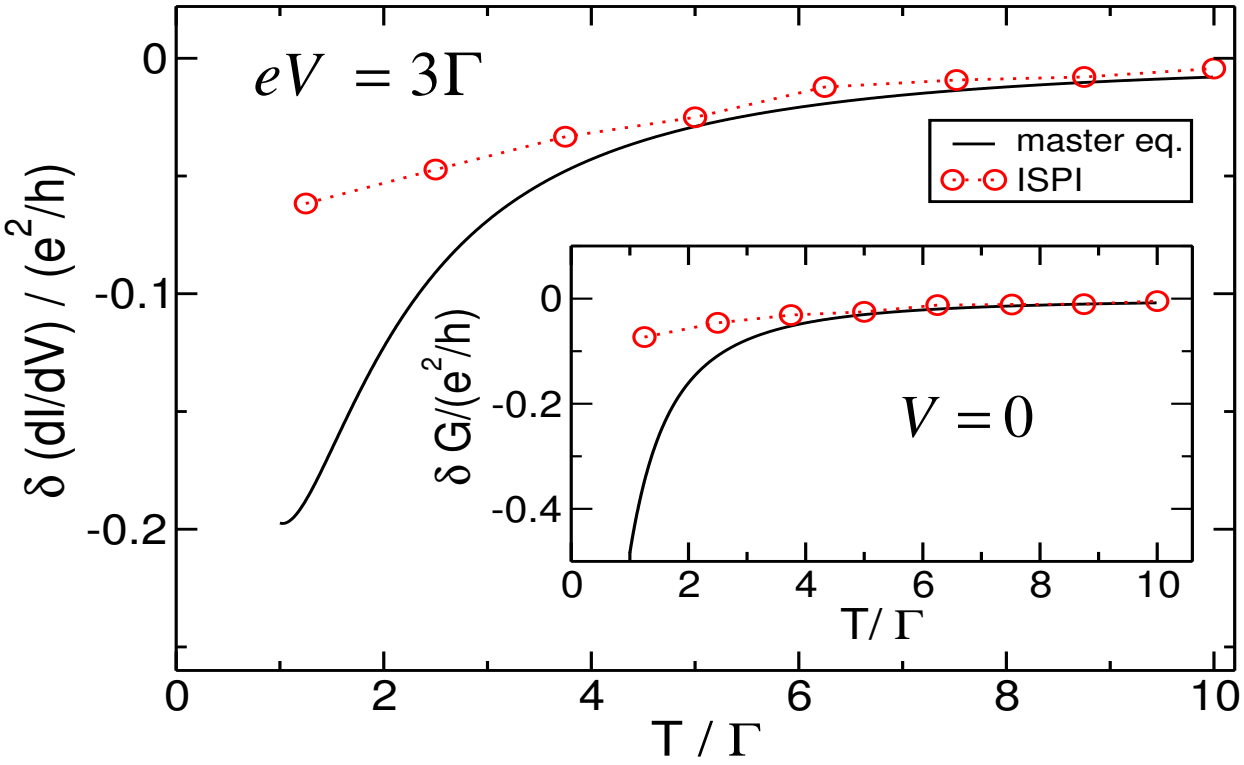
$$\varepsilon_0 = B = 0, T = 0.1\Gamma$$




Interaction corrections to the current compared to second-order perturbation theory in U

# Master equation results vs ISPI

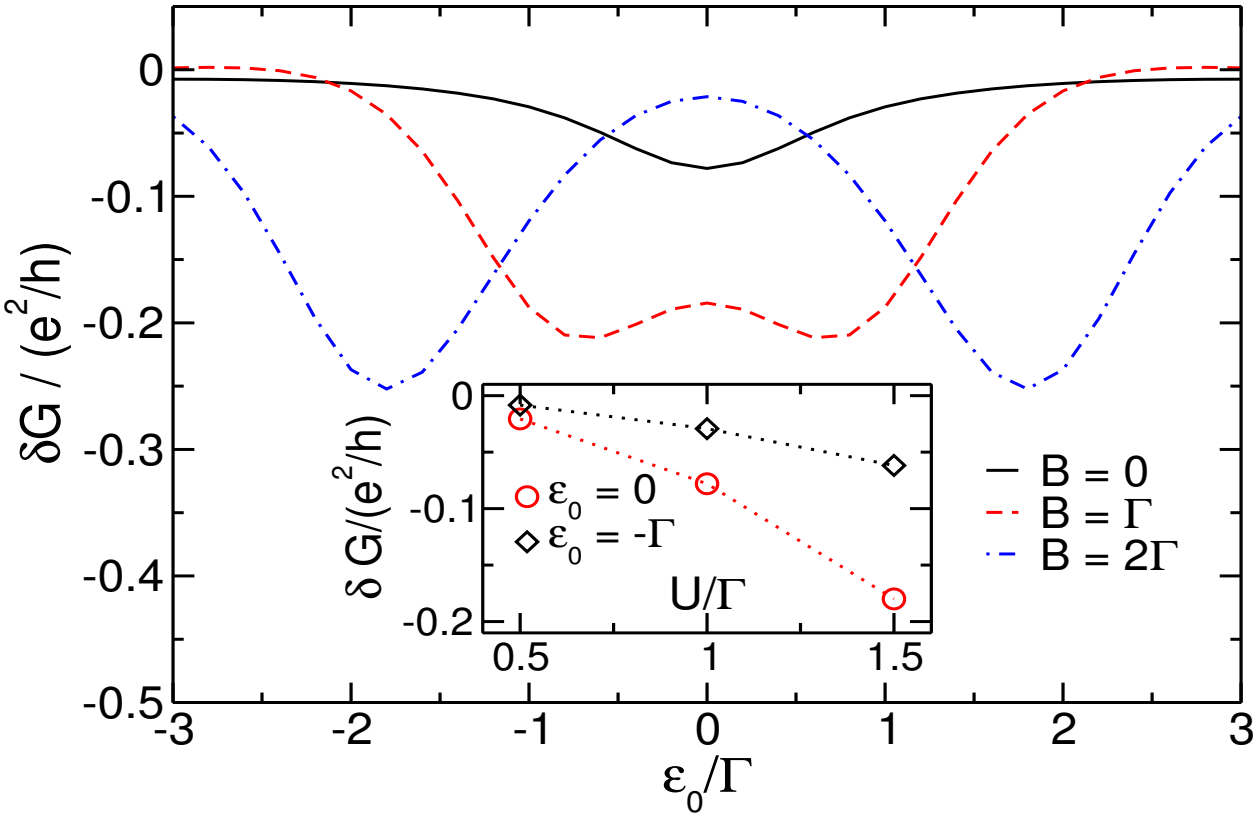



$\varepsilon_0 = B = 0$

$U = \Gamma$

Master equation in sequential tunneling approximation leads to quantitative agreement for T>4Γ, otherwise quantum coherence important!

# Linear conductance: Zeeman effects



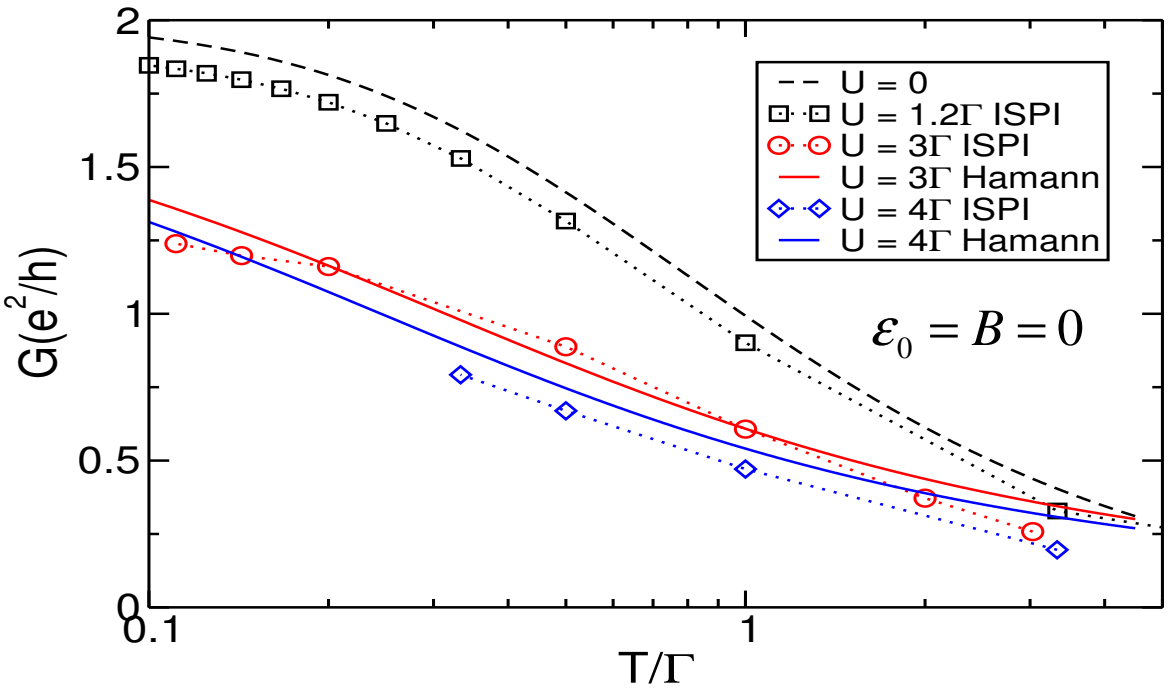

$U = \Gamma$

$T = 0.1\Gamma$

*Inset: B=0*

Zeeman field splitting of peaks, interaction corrections are largest near peaks

# Towards the deep Kondo regime




$T_K$=0.38Γ

$T_K$=0.29Γ

Linear conductance for $T>T_K$ compared to Hamann's result (PR 1967), which agrees with NRG (Costi, 1994) in this regime…

**Temperatures below $T_K$ : difficult to reach convergence !**

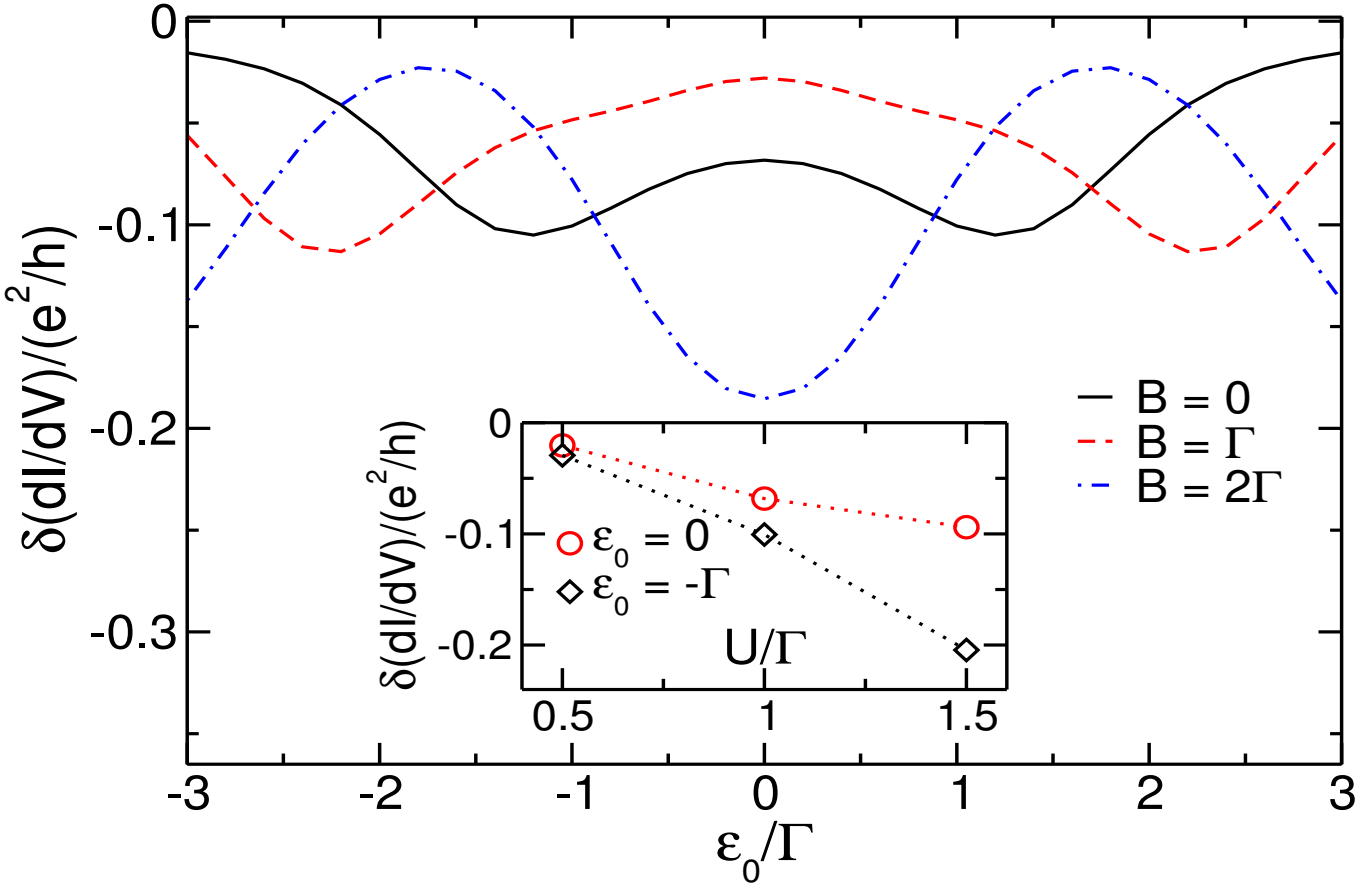
# Nonlinear conductance

$eV = 3\Gamma$

$T = 0.1\Gamma$

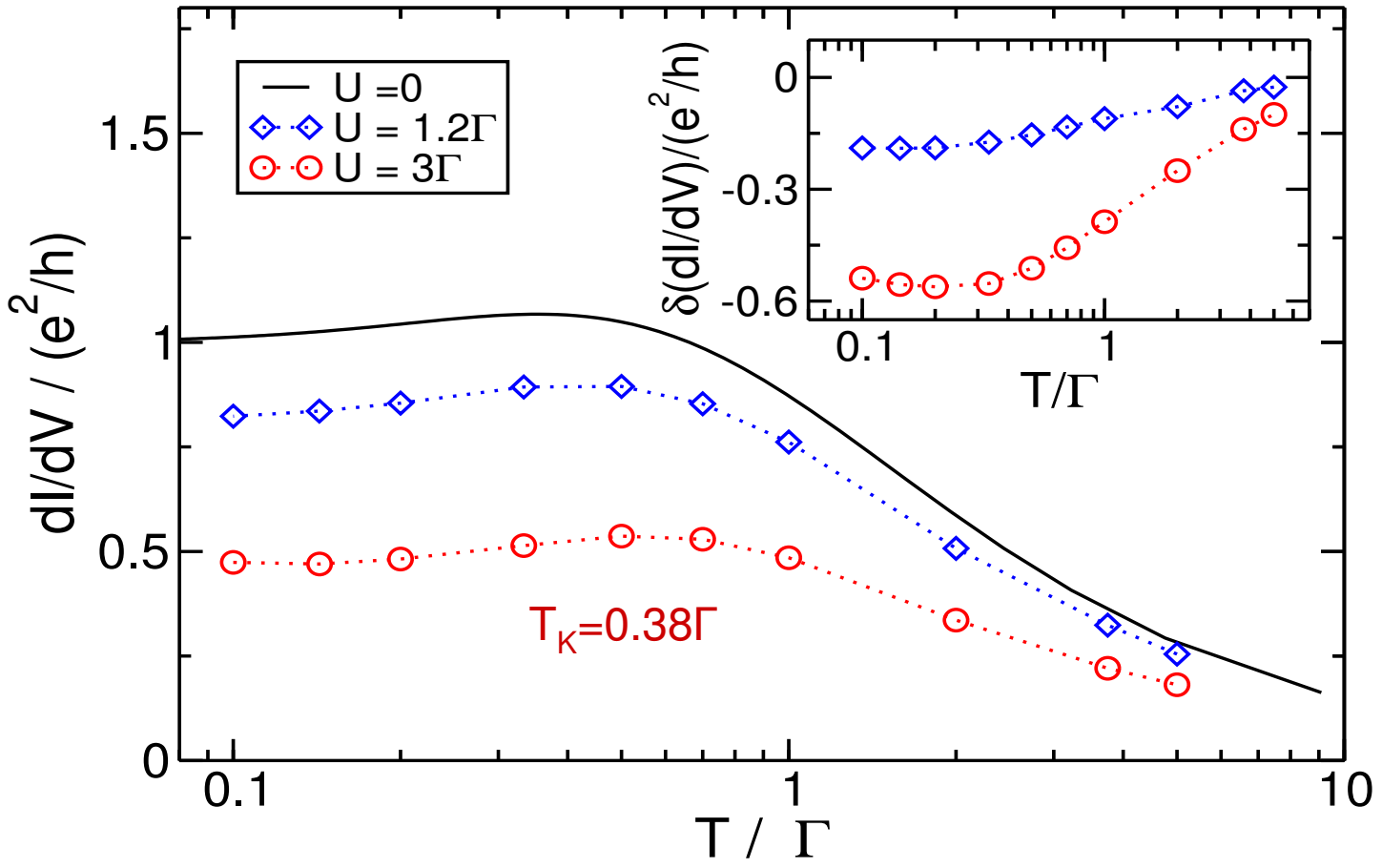
$U = \Gamma$

*Inset: B=0*




Fourfold peak splitting with bias and Zeeman field

# Nonlinear differential conductance




$eV = 2\Gamma$

$\varepsilon_0 = B = 0$

# Conclusions & outlook

- ISPI = Iterative Simulation of Path Integrals
- Useful numerical scheme for nonequilibrium quantum transport through correlated dots/molecules (except near T=V=0)
- Future applications
  - Systematic study of nonequilibrium Kondo regime
  - Other models (spin-fermion models, interacting resonant level, dot coupled to vibration mode…)
  - Other quantities (e.g. shot noise: two source fields)

Ref.: **PRB 77, 195316 (2008)**