Dissipative quantum dynamics simulations

Reinhold Egger
Institut für Theoretische Physik
Heinrich-Heine-Universität Düsseldorf
C.H. Mak, L. Mühlbacher, S. Hügle

Overview

- Real-time Path Integral Monte Carlo (PIMC) simulations for dissipative quantum systems
- Application 1: Spin-boson dynamics
- Application 2: Coherence for double-barrier tunneling in 1d quantum wires
- Conclusions

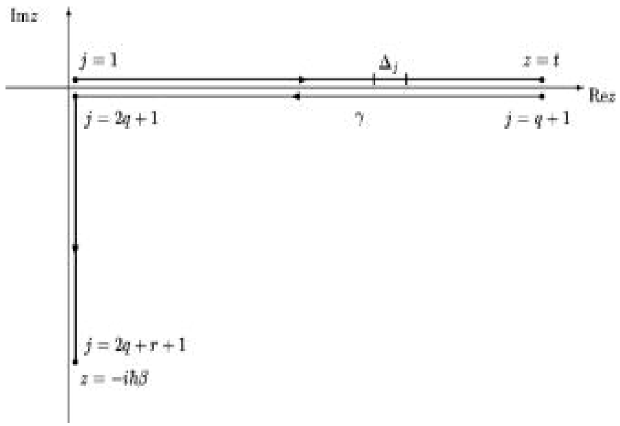
Real-time QMC: Sign problem

- Aim: Compute time-dependent quantities
  - Correlation functions (in or out of equilibrium)
  - Dynamical occupation probabilities
- QMC = stochastic evaluation of path integral
- Straightforward for positive definite weight, otherwise cancellations of different Feynman paths, signal-to-noise ratio $\propto \exp(-t/\tau_0)$
- Sign problem due to quantum interference of real-time trajectories, big problem!

Blocking strategy

Egger & Mak, PRB 1994

Start from discretized path integral expression, suitable for (brute-force) QMC



$$\langle A(t) \rangle = \frac{\langle A[X(t)]\Phi[X] \rangle_{W[X]}}{\langle \Phi[X] \rangle_{W[X]}}$$

Basic observation: Sign problem does not occur for small systems (small *t*)

➡ subdivide configuration space *{X}* into sufficiently small blocks *{B}*, first sum up interference within blocks

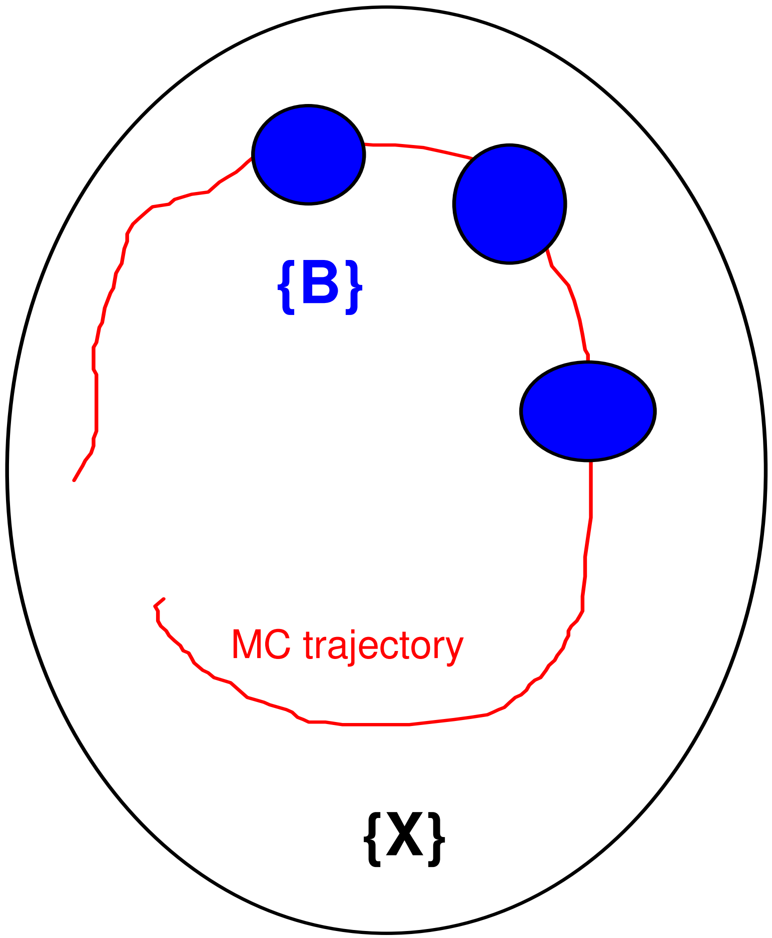
Blocking always reduces sign problem

- New MC weight for sampling blocks:

$$W'[B] = \left| \sum_{X \in B} W[X]\Phi[X] \right|$$

- New phase factor $\Phi'[B]$ numerically stable!
- This will never make the sign problem worse:

$$\left|\langle \Phi' \rangle\right| \geq \left|\langle \Phi \rangle\right|$$



Proof

$$\langle \Phi \rangle = \frac{\sum_X W[X]\Phi[X]}{\sum_X W[X]}$$

$$\langle \Phi' \rangle = \frac{\sum_B W'[B]\Phi'[B]}{\sum_B W'[B]} = \frac{\sum_X W[X]\Phi[X]}{\sum_B W'[B]}$$

$$\Rightarrow \quad \frac{|\langle \Phi' \rangle|}{|\langle \Phi \rangle|} = \frac{\sum_X W[X]}{\sum_B W'[B]} \geq 1$$

because

$$\sum_B W'[B] = \sum_B \left| \sum_{X \in B} W[X]\Phi[X] \right| \leq \sum_B \sum_{X \in B} W[X] = \sum_X W[X]$$

Multilevel blocking algorithm

Mak, Egger & Weber-Gottschick, PRL 1998
Mak Egger, JCP 1999

- For large system (long real time), too many blocks, again exponential sign problem
- Systematic implementation of blocking strategy using recursive algorithm, solve sign problem on different levels
- Implementation for dissipative quantum dynamics of spin-boson system has been demonstrated! *Egger, Mühlbacher & Mak, PRE 2000*

Application 1: Spin boson dynamics

Dissipative TLS (spin-boson model)

$$H = -\frac{\hbar\Delta}{2}\sigma_x + \frac{\hbar\varepsilon}{2}\sigma_z + \sum_i C_i x_i \sigma_z + H_B$$

- Two state system described by spin operators
- Harmonic oscillator bath, spectral density

$$J(\omega) = \frac{2\pi}{\hbar}\sum_i \frac{C_i^2}{m_i\omega_i}\delta(\omega-\omega_i) \approx 2\pi\alpha\omega e^{-\omega/\omega_c}$$

- Correlations $$L(t) = \int_0^\infty \frac{d\omega}{\pi} J(\omega)\frac{\cosh[\omega(\hbar\beta/2 - it)]}{\sinh(\hbar\beta/2)}$$

Spin boson model

- Simple but (sometimes) microscopic model for decoherence in qubits
- Close connection to Kondo problem
- Macroscopic quantum coherence in SQUIDs
- Electron transfer (ET) reactions in solids or chemical/biological systems
- For weak system-bath coupling: equivalent to Bloch-Redfield approach

Dynamics observables

- Equilibrium correlation function

$$C(t) = \mathrm{Re}\left\langle \sigma_z(t)\sigma_z(0)\right\rangle$$

- Occupation probability with nonequilibrium preparation $\sigma_z(t=0)=+1$: $P(t)=\left\langle \sigma_z(t)\right\rangle$
- Forward rate (ET) for $t_{transient} < t_{plateau} < t_{relax}$

$$k_f(t) = \frac{2}{\hbar\beta Z_A}\mathrm{Im}\ tr\left[e^{-\beta H} h_A(0) h_A(t)\right]$$

$$h_A = (1+\sigma_z)/2$$

$$Z_A = tr\left[e^{-\beta H} h_A\right]$$

Analytical results

- Noninteracting blip approximation (NIBA)

$$P(t) = E_{2(1-\alpha)}\left(-\left(\Delta_{eff}\, t\right)^{2(1-\alpha)}\right)$$

Leggett et al., RMP 1997

$$\Delta_{eff} \propto \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}$$

- NIBA exact at $\alpha=1/2$! Essentially exact expansion exists for $\alpha=1/2-\varepsilon$

Egger, Grabert & Weiss, PRE 1997

- Advanced quantum field theory techniques: Exact results for arbitrary α in scaling limit

Lesage & Saleur, PRL 1998

Spin-boson dynamics via PIMC

- Discretize Kadanoff-Baym contour
- Integrate out bath: Influence functional

$$\Phi[\sigma] = \sum_{j>k} L(t_j - t_k)\sigma_j \sigma_k$$

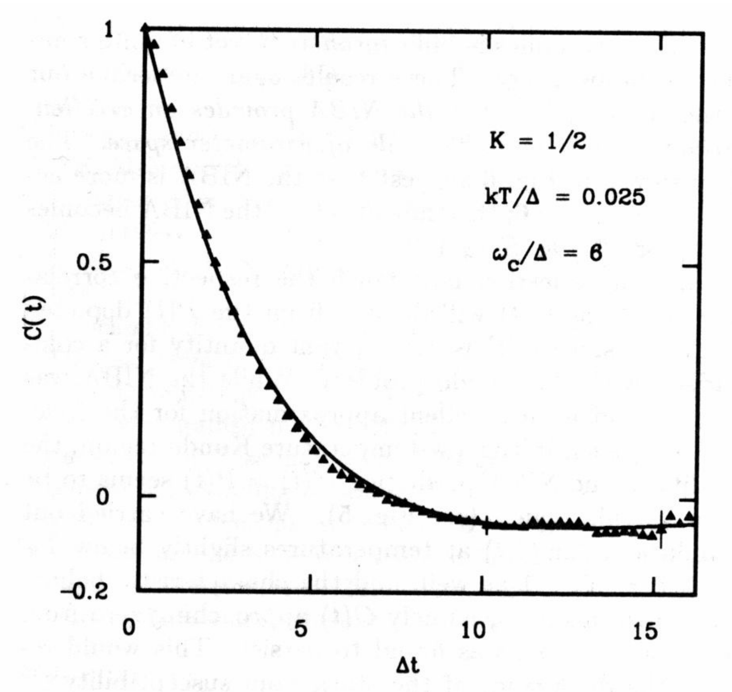
- Cyclic 1D Ising spin chain with unconventional long-range interactions

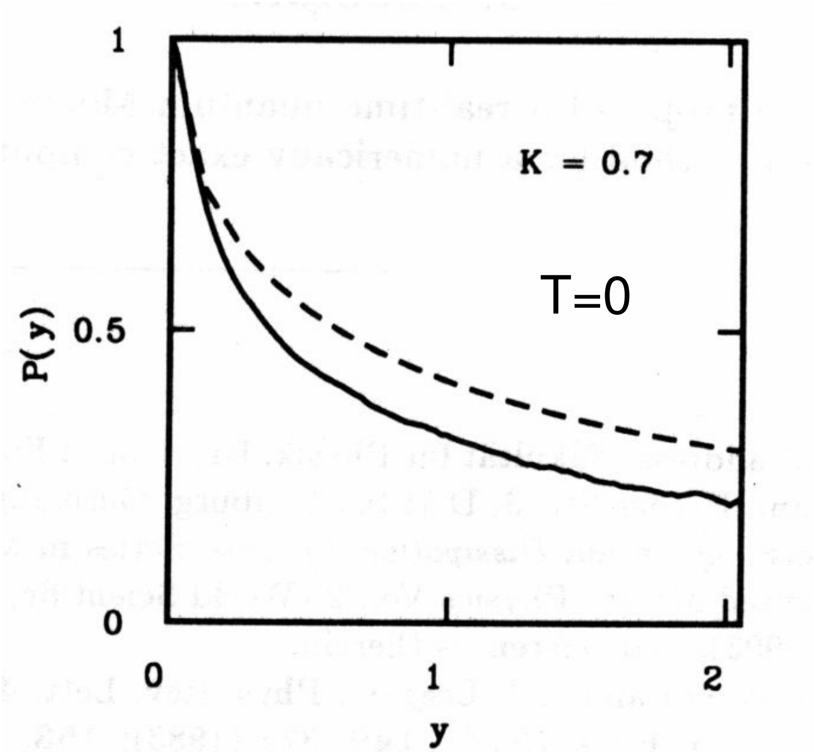
$$P(t) = Z^{-1} \sum_{\{\sigma\}} \sigma_t e^{iS_0[\sigma]} e^{-\Phi[\sigma]}$$

- Analytically trace out $\sigma_f + \sigma_b$
- Only sampling of quantum fluctuations $\sigma_f - \sigma_b$

Spin-boson dynamics

Egger & Mak, PRB 1994



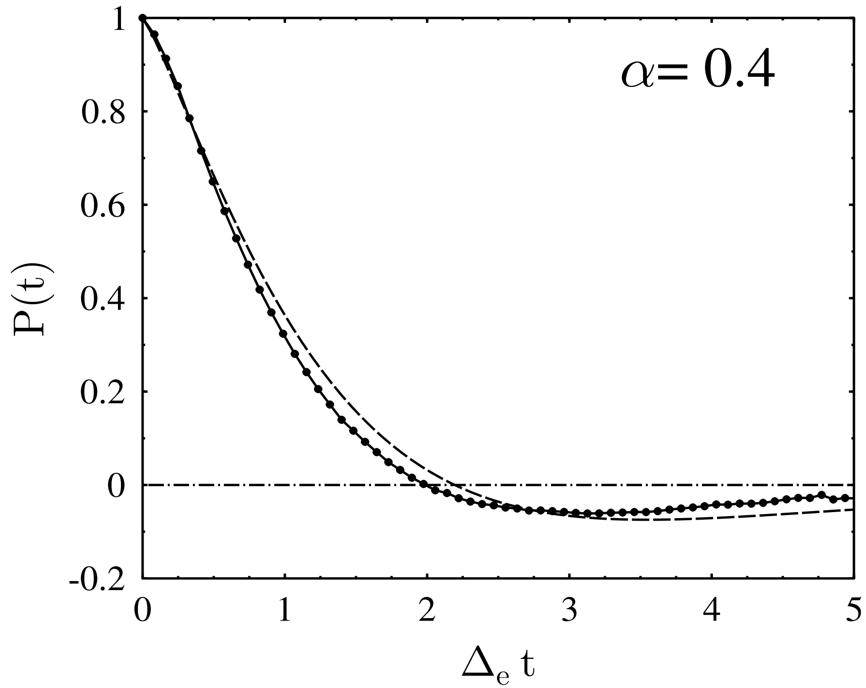


QMC accurate at α=1/2, NIBA inaccurate for α=0.7

Coherent-incoherent transition

Egger, Grabert & Weiss, PRE 1997

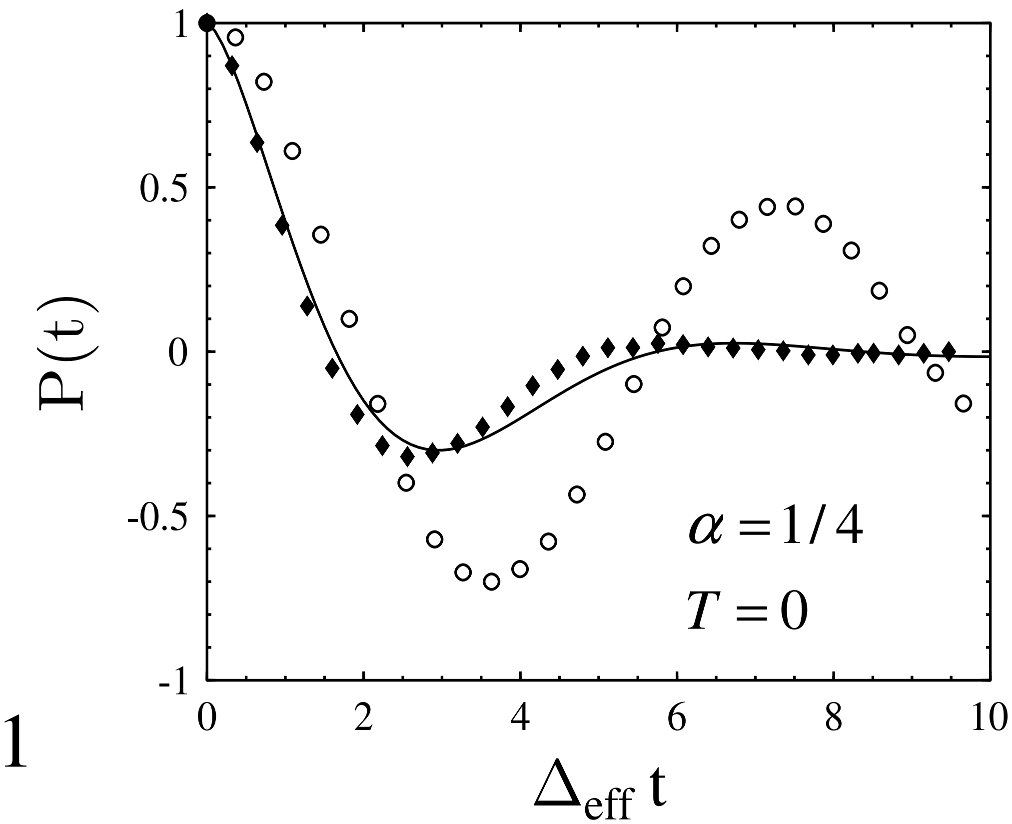
- Oscillatory dynamics in *P(t)* only for *α<1/2*
- Different criterion when analyzing *C(t):* Spectral function has only one quasielastic peak for *α>1/3*
- QMC covers all interesting timescales



Weak-to-intermediate coupling

Egger, Mühlbacher & Mak, PRE 2000

- More difficult, sign problem now more severe
- Multilevel blocking necessary
- Closed diamonds:
  $\omega_c / \Delta = 6$
  NIBA accurate
- Open circles: $\omega_c / \Delta = 1$
  NIBA breaks down



Spin-boson simulations:
PRO and CONTRA

PRO

- Numerically exact for arbitrary parameters (e.g. spectral density)
- Very powerful for intermediate-to-strong dissipation, e.g. ET - dissipation helps!
  Mühlbacher & Egger, JCP 2003, Chem. Phys. 2004
- Arbitrary quantities, in or out of equilibrium

CONTRA

- Numerically expensive
- Sign problem can be severe for low *T*, weak coupling and long times
- In practice useful even at low *T* for $\alpha \geq 0.1$

Application 2: Coherent and incoherent double-barrier tunneling in 1d wires

- Tunneling mechanism for transport through double-barrier structure in interacting 1D quantum wire, e.g. carbon nanotube?
- Recent nanotube experiments challenge established sequential tunneling theories

Postma, Teepen, Yao, Grifoni & Dekker, Science 2001

- Strong transmission: Fabry-Perot resonances observed in nanotubes *Liang et al., Nature 2001*

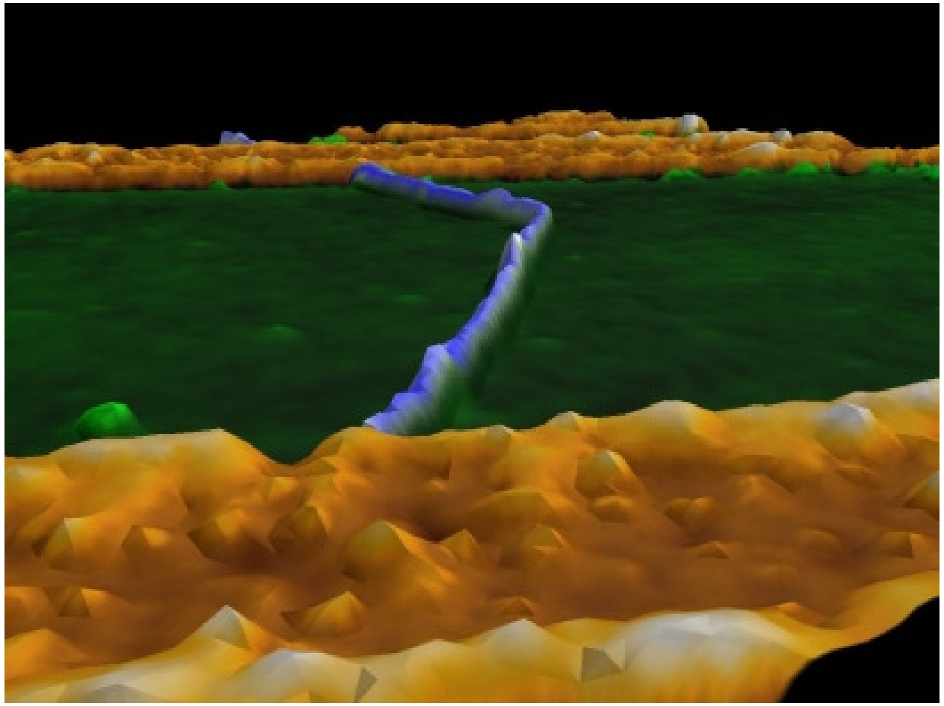
Single-wall carbon nanotubes

- Prediction: SWNT is a Luttinger liquid with
  g~0.2

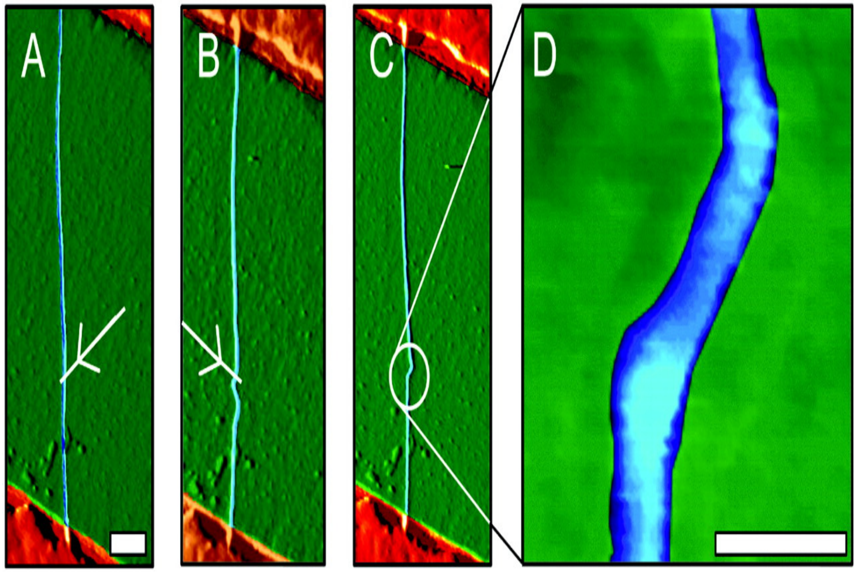
  Egger & Gogolin, PRL 1997
  Kane, Balents & Fisher, PRL 1997

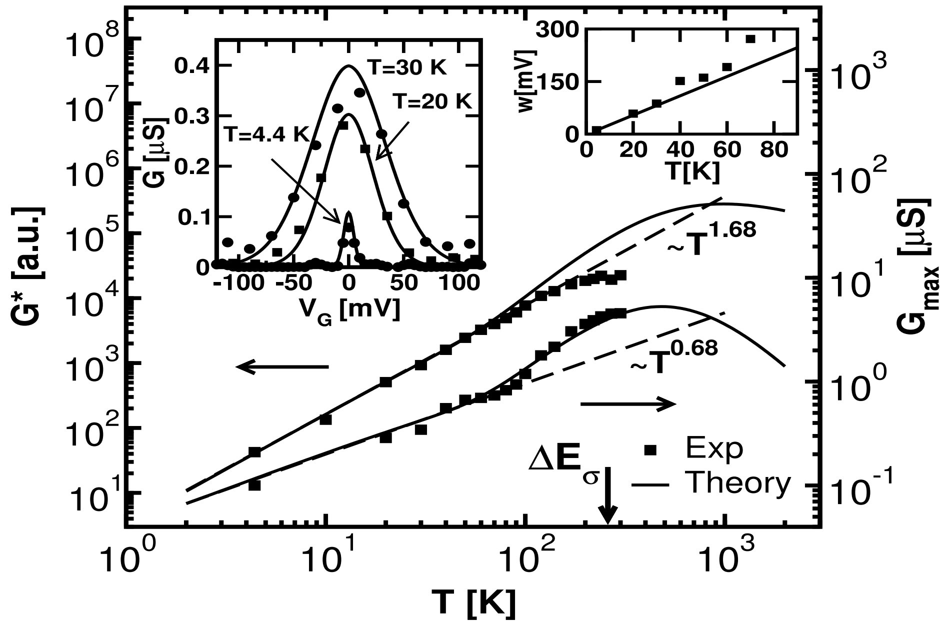
- Experiment: Luttinger power-law conductance through weak link, gives *g=0.22*

  Yao et al., Nature 1999
  Bockrath et al., Nature 1999



Weak transmission: Experiment





Postma et al., Science 2001

$$G_{peak}^{\exp} \propto T^{-3+2/g}$$

but $$G_{peak}^{seq} \propto T^{-2+1/g}$$

Luttinger liquid with double barrier

Hamiltonian (single-channel case, symmetric barriers)

$$H = \frac{v_F}{2}\int dx\left\{\Pi^2 + g^{-2}(\nabla\vartheta)^2\right\} + V_0\sum_{\pm}\cos\left\{\sqrt{4\pi}\vartheta(\pm d/2) + eVt \pm \pi N_0\right\}$$

Current-voltage characteristics

$$I = G_0 V + \frac{e}{\sqrt{\pi}}\left\langle \partial_t \vartheta \right\rangle \qquad \text{with } G_0 = e^2/h$$

Goal: compute linear conductance using QMC

$$G(T, N_0, V_0, g, d)$$

Hügle & Egger, EPL 2004

Map to dissipative tight binding model

Implement blocking strategy:

- Integration over all fields away from barriers
- Effective action describes two coupled Brownian particles in periodic potentials
- Spectral densities

$$J_{\pm}(\omega) = \pi g \omega \left[1 \pm \cos(\pi g^2 \omega / E_s)\right]$$

$$E_s = \pi v_F / d$$

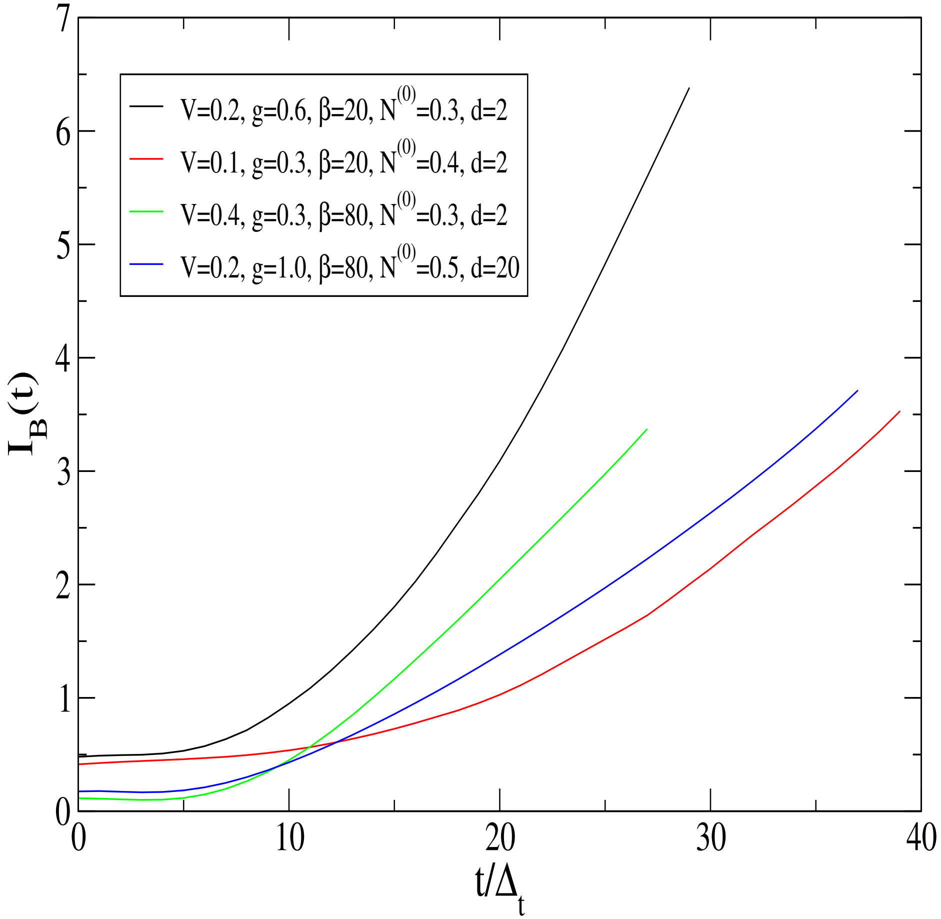
- Then map to Coulomb gas, trace over quasiclassical charges
- QMC for quantum fluctuations

Computing the conductance…

Conductance

$$G/G_0 = 1 - \lim_{t\to\infty} \partial_t I_B(t)$$

stable up to sufficiently long timescales, no need to use multilevel blocking



Noninteracting limit *(g=1)*

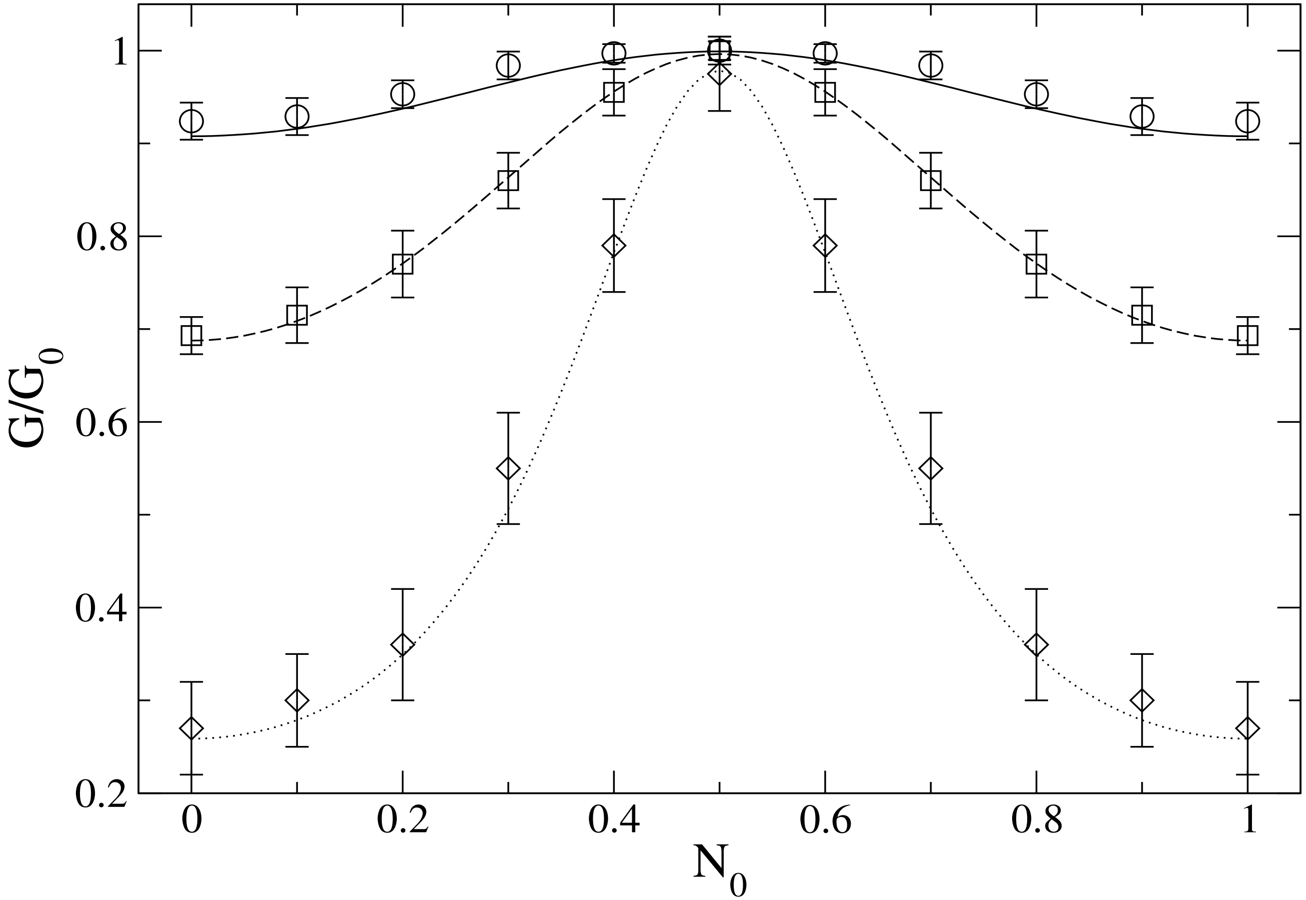
Refermionization: exact conductance

$$G/G_0 = \int_{-\infty}^{\infty} dE \, \frac{1}{4k_BT \cosh^2\left(E/2k_BT\right)} \frac{w^2}{w^2 + \cos^2\left[\pi N_0 + \pi E/E_s\right]}$$

$$w = \frac{(4-\lambda^2)^2}{8\lambda(4+\lambda^2)}, \lambda = \pi V_0/\omega_c \leq 2$$

allows for precise checks

Check QMC against *g=1* result



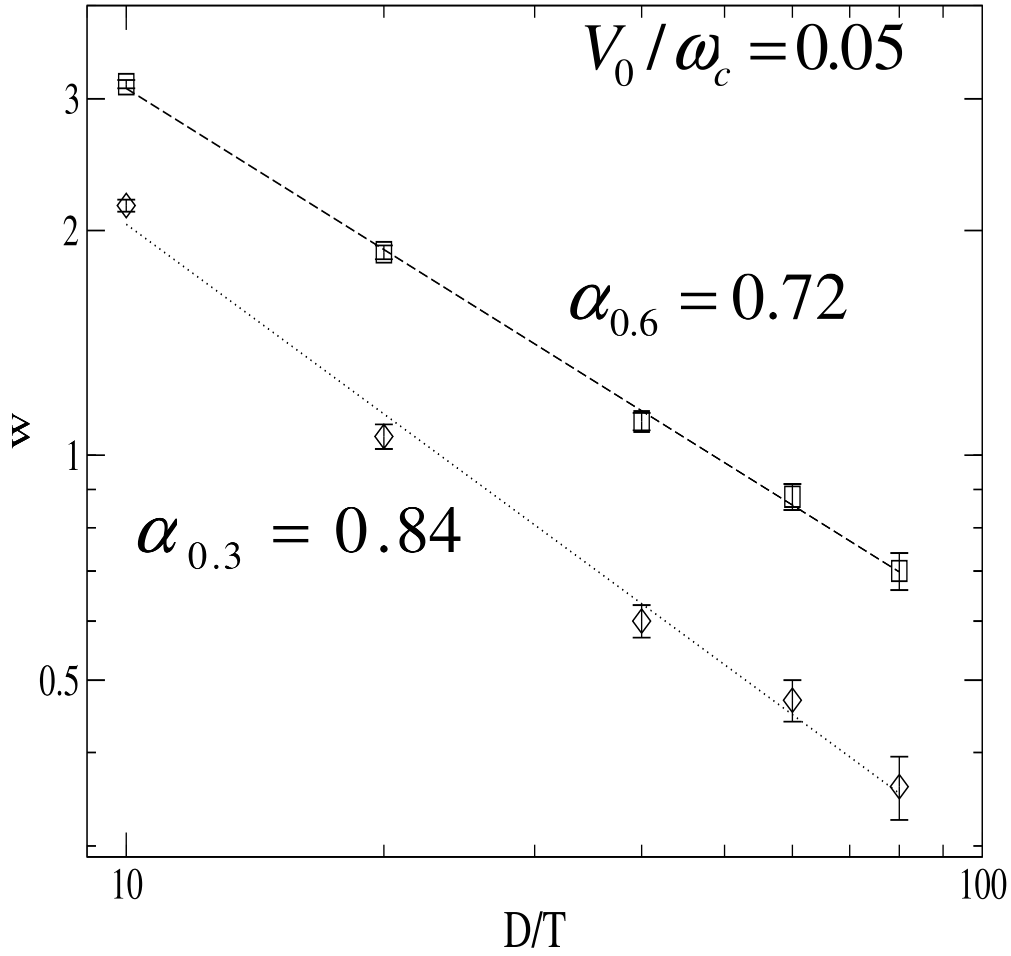
QMC reliable and accurate

Strong transmission behavior

- For $k_B T / \hbar\omega_c > 0.01$: *g=1* lineshape but with

$$w = w_g(T) \propto T^{\alpha_g}$$

- Fabry-Perot regime, broad resonance
- At lower *T*: Coherent resonant tunneling



Coherent resonant tunneling

Low T, arbitrary transmission:
Universal scaling

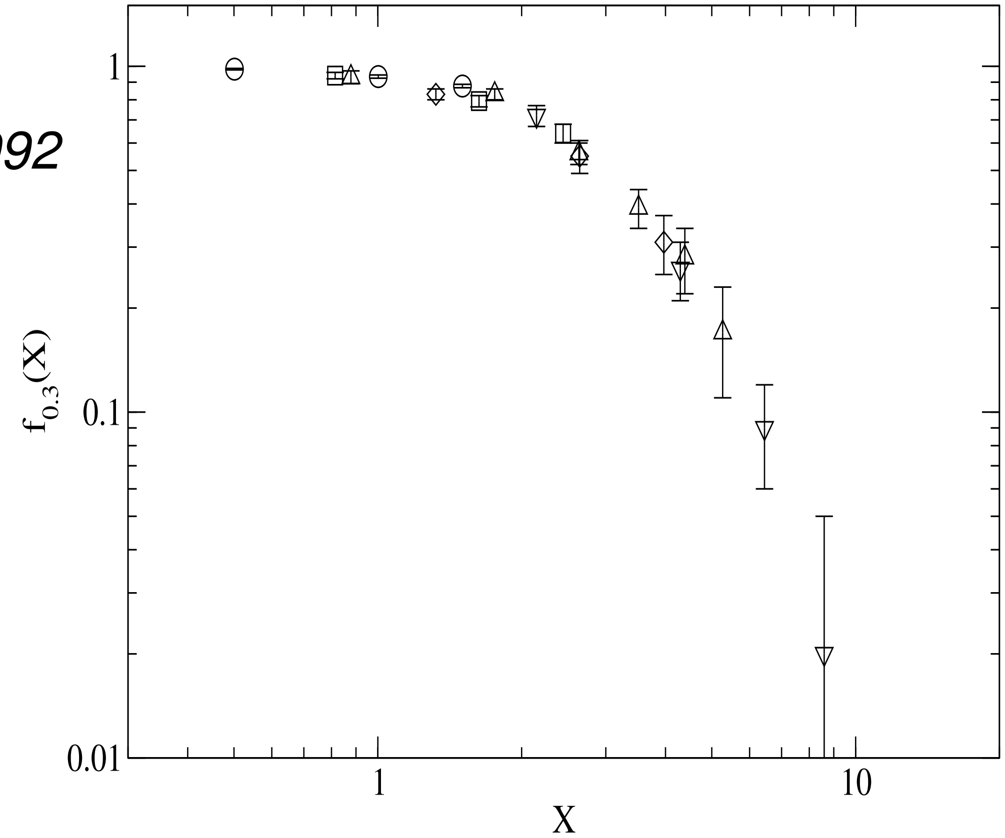
Kane & Fisher, PRB 1992

$$G(N_0, T, V_0, d, g)/G_0 = f_g(X)$$

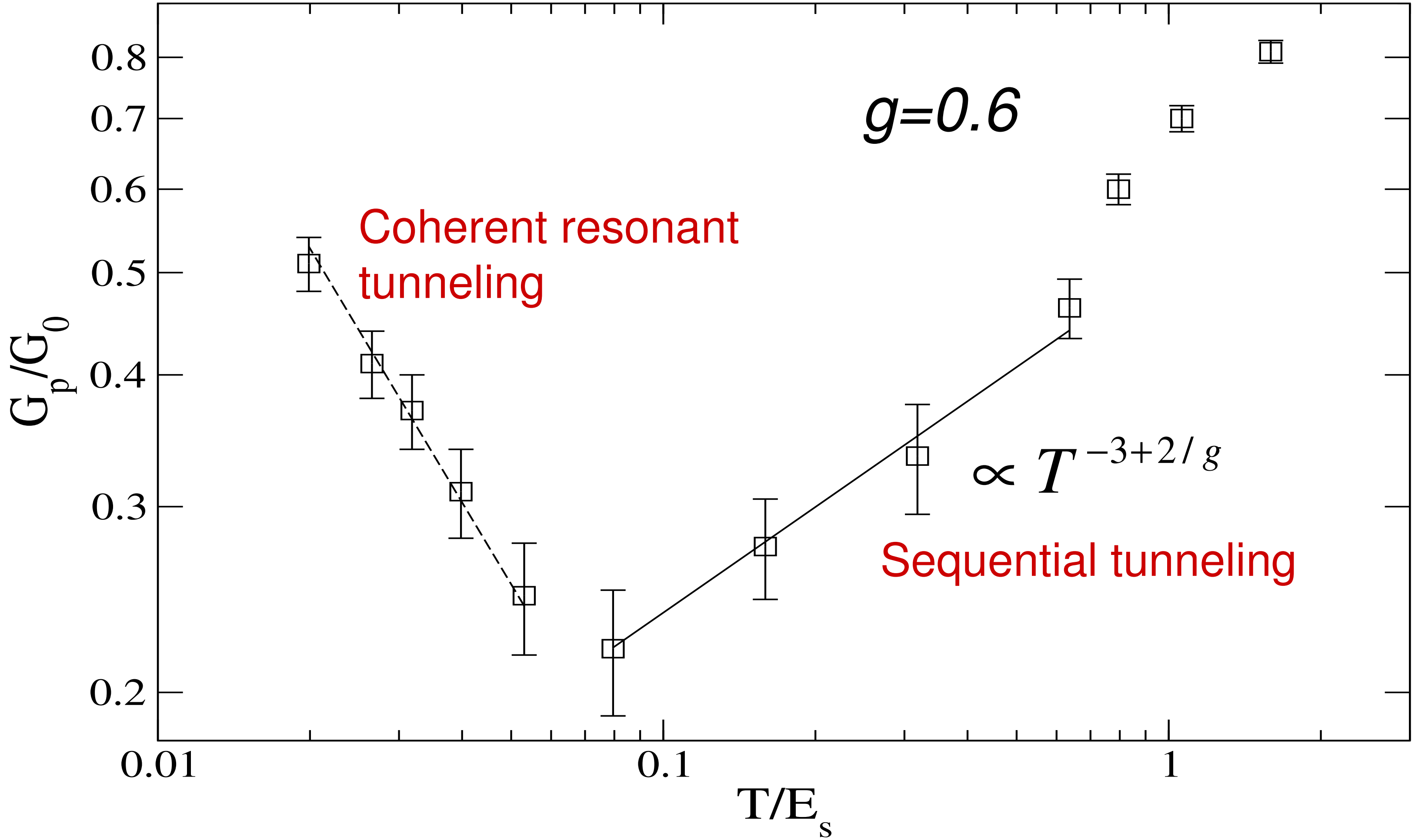
$$X = cT^{g-1}\left|N_0 - 1/2\right|$$

$$f(X \to 0) = 1 - X^2$$

$$f(X \to \infty) \propto X^{-2/g}$$



Weak transmission: Peak height



Hügle & Egger, EPL 2004

Correlated sequential tunneling

- QMC data appear to invalidate standard sequential tunneling picture
- Good agreement with experiment
- Theory proposal: correlated sequential tunneling processes *Thorwart, Grifoni et al., PRL 2002*

Conclusions

- Numerically exact route to dissipative quantum dynamics via real-time QMC
- Application 1: Spin-boson dynamics. Coherent-incoherent transition, comparison to NIBA.
- Application 2: Resonant tunneling in a Luttinger liquid. Strong-transmission lineshape, correlated tunneling