Dissipative quantum dynamics simulations

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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

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

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

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

Egger & Mak, PRB 1994
Blocking always reduces sign problem

- New MC weight for sampling blocks:
  \[ W'[B] = \sum_{X \in B} W[X] \Phi[X] \]

- New phase factor \( \Phi'[B] \) numerically stable!
- This will never make the sign problem worse:
  \[ \langle \Phi' \rangle \geq \langle \Phi \rangle \]
Proof

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

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

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

- 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

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

\[ L(t) = \int_0^\infty \frac{d\omega}{\pi} J(\omega) \cosh[\omega(\hbar \beta / 2 - it)] / \sinh(\hbar \beta / 2) \]
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
  \[ C(t) = \text{Re}\left\langle\sigma_z(t)\sigma_z(0)\right\rangle \]

- Occupation probability with nonequilibrium preparation: \( \sigma_z(t=0)=+1 \) : \( P(t) = \left\langle\sigma_z(t)\right\rangle \)

- Forward rate (ET) for \( t_{\text{transient}} < t_{\text{plateau}} < t_{\text{relax}} \)
  \[
  k_f(t) = \frac{2}{\hbar \beta Z_A} \text{Im} \; \text{tr} \left[ e^{-\beta H} h_A(0) h_A(t) \right] 
  \]
  \[
  h_A = (1 + \sigma_z) / 2 
  \]
  \[
  Z_A = \text{tr} \left[ e^{-\beta H} h_A \right] 
  \]
Analytical results

- Noninteracting blip approximation (NIBA)
  \[ P(t) = E_{2(1-\alpha)} \left( -\left( \Delta_{\text{eff}} t \right)^{2(1-\alpha)} \right) \]
  \[ \Delta_{\text{eff}} \propto \Delta (\Delta / \omega_c)^{\alpha/(1-\alpha)} \]
  \[ \text{Leggett et al., RMP 1997} \]

- NIBA exact at \( \alpha=1/2 \) ! Essentially exact expansion exists for \( \alpha=1/2-\varepsilon \)
  \[ \text{Egger, Grabert & Weiss, PRE 1997} \]

- Advanced quantum field theory techniques:
  Exact results for arbitrary \( \alpha \) in scaling limit
  \[ \text{Lesage & Saleur, PRL 1998} \]
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 $\alpha=1/2$, NIBA inaccurate for $\alpha=0.7$
Coherent-incoherent transition

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

*Egger, Grabert & Weiss, PRE 1997*
Weak-to-intermediate coupling

- 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

Egger, Mühlbacher & Mak, PRE 2000
Spin-boson simulations:

**PRO**
- Numerically exact for arbitrary parameters (e.g. spectral density)
- Very powerful for intermediate-to-strong dissipation, e.g. ET-dissipation helps!
- 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.
  
  \[ \text{Postma, Teepen, Yao, Grifoni \& Dekker, Science 2001} \]

- Strong transmission: Fabry-Perot resonances observed in nanotubes
  
  \[ \text{Liang et al., Nature 2001} \]
Single-wall carbon nanotubes

- Prediction: SWNT is a Luttinger liquid with $g \approx 0.2$
  - 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

\[ G_{\text{peak}}^{\text{exp}} \propto T^{3+2/g} \]

but

\[ G_{\text{peak}}^{\text{seq}} \propto T^{2+1/g} \]
Luttinger liquid with double barrier

Hamiltonian (single-channel case, symmetric barriers)

\[ H = \frac{v_F}{2} \int dx \{ \Pi^2 + g^{-2} (\nabla \vartheta)^2 \} + V_0 \sum_{\pm} \cos \{ \sqrt{4\pi} \vartheta (\pm d / 2) + e V t \pm \pi N_0 \} \]

Current-voltage characteristics

\[ I = G_0 V + \frac{e}{\sqrt{\pi}} \left\langle \partial_t \vartheta \right\rangle \quad \text{with} \quad G_0 = \frac{e^2}{h} \]

Goal: compute linear conductance using QMC

\[ G(T, N_0, V_0, g, d) \]

Hügge & 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

\[ \frac{G}{G_0} = 1 - \lim_{t \to \infty} \partial_t I_B(t) \]

stable up to sufficiently long timescales, no need to use multilevel blocking
Noninteracting limit \((g=1)\)

Refermionization: exact conductance

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

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

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

\[ \alpha_{0.6} = 0.72 \]
\[ \alpha_{0.3} = 0.84 \]
Coherent resonant tunneling

Low T, arbitrary transmission:
Universal scaling

\[ G(N_0, T, V_0, d, g)/G_0 = f_g(X) \]

\[ X = cT^{g-1} |N_0 - 1/2| \]

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

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

Kane & Fisher, PRB 1992
Weak transmission: Peak height

\[
\frac{G_p}{G_0} \propto T^{3+2/g}
\]

Sequential tunneling

Coherent resonant tunneling

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