Time-dependent semiclassical simulation of (dissipative) quantum dynamics

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Overview

1. Semiclassical initial value representations (SC-IVR)
   - Thawed Gaussian Wavepacket Dynamics: TGWD
   - Frozen Gaussians: multiple trajectories for N DOF
2. Semiclassical hybrid dynamics (SCHD)
   - Combination of FGWD and TGWD
   - Interference Quenching in the Caldeira-Leggett (CL) model
3. Noise based approach to quantum Brownian motion
   - Hubbard-Stratonovich Uncompleting of the Square
   - Feynman-Vernon influence functional for CL model
   - Realization of stochastic semiclassical propagation
   - Anharmonic Brownian Motion
   - Dissipative tunneling

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Semiclassical Initial Value Representations (SC-IVR)

Heller's Thawed Gaussian Wavepacket Dynamics (TGWD)

$$\boxed{\Psi(x,t) = \left(\frac{\gamma_0}{\pi}\right)^{1/4} \exp\left\{-\frac{\gamma_t}{2}(x-q_t)^2 + \frac{i}{\hbar}p_t(x-q_t) + \frac{i}{\hbar}\delta_t\right\}}$$

$$\gamma_0, p_t, q_t \in \mathbf{R}, \qquad \gamma_\mathbf{t}, \delta_\mathbf{t} \in \mathbf{C}$$

Ansatz for the solution of the time-dependent Schrödinger equation

$$i\hbar\dot{\Psi}(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t)$$

E. J. Heller, J. Chem. Phys. ***62****, 1544 (1975)* second order Taylor expansion of potential around q_t leads to

$$\boxed{\dot{q}_t = \frac{p_t}{m} \qquad \dot{p}_t = -V'(q_t, t)}$$

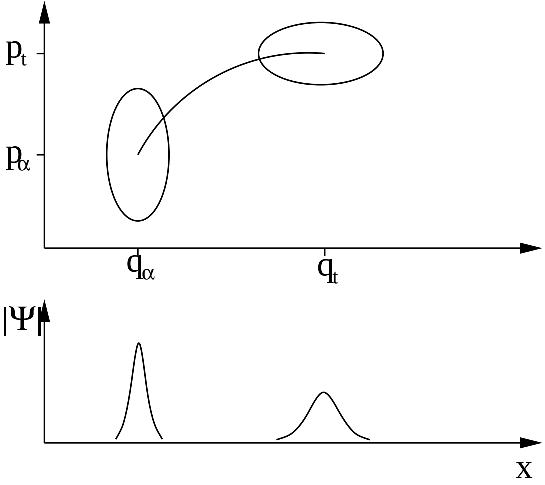
Hamilton's equations with initial conditions $(q_t, p_t) {=} (q_\alpha, p_\alpha)$

$$-i\hbar\dot{\gamma}_t = -\frac{\hbar^2}{m}{\gamma_t}^2 + V''(q_t, t)$$

time dependent width parameter γ_t with IC $\gamma_{t=0} = \gamma_0$

$$\dot{\delta}_t = \frac{p_t^2}{2m} - V(q_t, t) - \frac{\hbar^2}{2m}\gamma_t$$

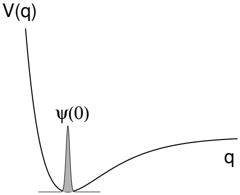
Thawed GWD: Phase- and position space

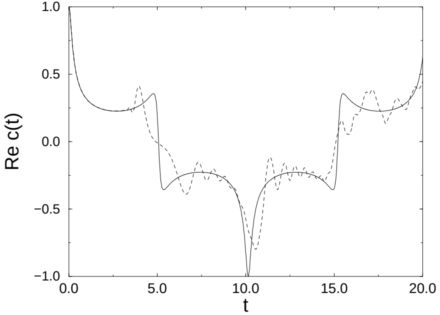


single trajectory initial value method

E. J. Heller, J. Chem. Phys. **62***, 1544 (1975)*

A simple example: Morse oscillator





$$c(t) = \langle \Psi(0) | \Psi(t) \rangle = \langle \Psi(0) | e^{-i\hat{H}t/\hbar} | \Psi(0) \rangle$$

Multiple trajectory method: Frozen Gaussians for N DOF

$$\Psi(\mathbf{x},t) = \int \mathrm{d}^N x' K(\mathbf{x},t;\mathbf{x}',0)\Psi(\mathbf{x}',0)$$

Initial value Herman-Kluk propagator

$$K(\mathbf{x},t;\mathbf{x}',0) \approx \int \frac{\mathrm{d}^N p' \mathrm{d}^N q'}{(2\pi\hbar)^N} \langle \mathbf{x}|g_\gamma(\mathbf{p}_t,\mathbf{q}_t)\rangle R e^{iS(\mathbf{p}',\mathbf{q}',t)/\hbar} \langle g_\gamma(\mathbf{p}',\mathbf{q}')|\mathbf{x}'\rangle$$

$$R(\mathbf{p}',\mathbf{q}',t) = \sqrt{\det \tfrac{1}{2}\left(\mathbf{m}_{pp} + \mathbf{m}_{qq} - \gamma i\hbar \mathbf{m}_{qp} - \frac{\gamma^{-1}}{i\hbar}\mathbf{m}_{pq}\right)} = \sqrt{|\mathbf{h}|}$$

- $|g_\gamma\rangle$ are Gaussians with fixed ("frozen") width parameter matrix
- Hamilton's principal function $S(\mathbf{p}',\mathbf{q}',t) = \int_0^t L dt'$
- initial value solutions of Hamilton's equations $\mathbf{p}_t(\mathbf{p}',\mathbf{q}'), \mathbf{q}_t(\mathbf{p}',\mathbf{q}')$

Heller ('81), Herman and Kluk ('84), Kay ('94), F.G. and Xavier ('98)

- $\mathbf{m}_{pp}, \mathbf{m}_{qq}, \ldots$ are elements of the stability (monodromy) matrix $\mathbf{M}$

$$\mathbf{M} = \begin{pmatrix} \mathbf{m}_{pp} & \mathbf{m}_{pq} \\ \mathbf{m}_{qp} & \mathbf{m}_{qq} \end{pmatrix} = \begin{pmatrix} \partial \mathbf{p}_t / \partial \mathbf{p}' & \partial \mathbf{p}_t / \partial \mathbf{q}' \\ \partial \mathbf{q}_t / \partial \mathbf{p}' & \partial \mathbf{q}_t / \partial \mathbf{q}' \end{pmatrix}$$

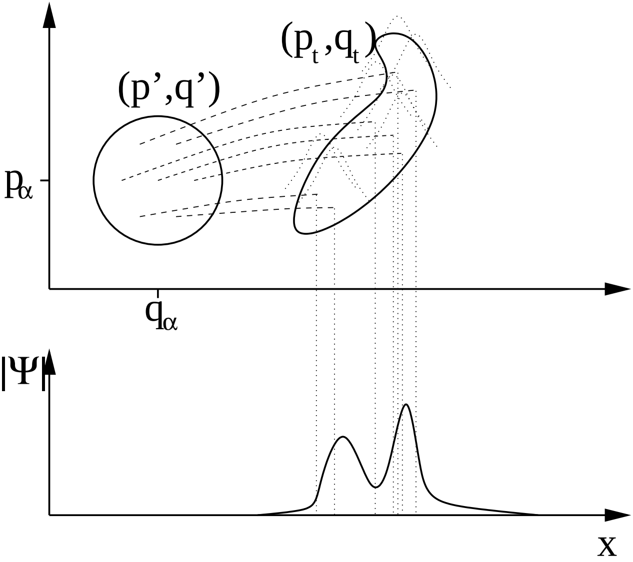
- $\mathbf{M}$ fulfills linear differential equation

$$\frac{d}{dt}\mathbf{M} = \begin{pmatrix} 0 & -H_{qq} \\ H_{pp} & 0 \end{pmatrix} \mathbf{M}$$

- H_{qq}, H_{pp}: Hessian

- purely classical input!
- symplectic integration routines (leap frog) $\Rightarrow$parallelization

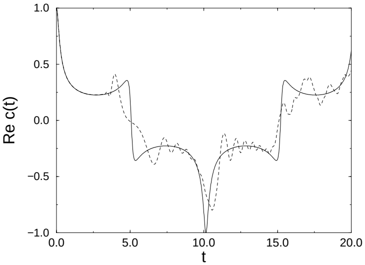
Frozen GWD: Phase- and position space



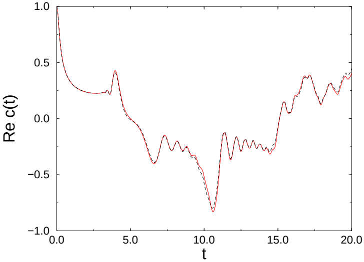
*multi*trajectory initial value method

Simple example revisited

TGWD/QM



FGWD/QM



HK-FGA

- Time-dependent initial value method for *arbitrary* dynamics
- no storage problems due to locality of classical mechanics
- Initial Gaussian $\Rightarrow |\langle g_\gamma|\Psi(0)\rangle|$ Monte Carlo weight
- SPA $\Rightarrow$Van Vleck-Gutzwiller propagator (boundary value problem)

$$K(\mathbf{x}, t; \mathbf{x}', 0) \sim \sum_j \left|\frac{1}{\det \mathbf{m}_{qp}}\right|^{1/2} \exp\{iS_j(\mathbf{x}, \mathbf{x}', t)/\hbar - i\pi\nu_j/2\}$$

- good long-time accuracy $\Rightarrow$ *Harabati et al JCP (2004)*
- no problems at caustics, HK-FGA is uniform $\Rightarrow$ *Kay ARPC (2005)*
- HK-FGA is unitary (in SPA) $\Rightarrow$ *Herman JCP (1986)*
- Approximation to CCS $\Rightarrow$ *Miller JPCB (2002), Shalashilin and Child CP (2004)*
- iterative improvement is possible $\Rightarrow$ *Zhang & Pollak PRL (2003), Hochman & Kay JPA (2008)*
- "on the fly" determination of forces is possible $\Rightarrow$ *Ceotto et al. PCCP (2009)*
- LSCIVR: classical Wigner dynamics (or CTMC) $\Rightarrow$ *Sun, Wang, Miller JCP (1998)*

Some applications

- "understanding" of quantum effects ⇒*van de Sand & Rost, PRL (1999)*
- (laser) driven systems ⇒*Zagoya et al, PRA Rapid (2012),...*
- non-adiabatic dynamics ⇒*Meyer & Miller, JCP (1981), Stock & Thoss, PRL (1997) (MMST)*
- hybrid method ⇒*Sun & Miller, JCP (1997), Ovchinnikov & Apkarian, JCP (1998), FG, JCP (2006)*
- environment-induced qc transition ⇒*Wang et al., JCP ('01), Goletz & FG, JCP ('09),....*
- dissipative relaxation dynamics ⇒*W. Koch et al., PRL (2008)*
- scattering dynamics ⇒*Miller, JCP (1970), FG, CPL (1996), Garashchuk, FG & Tannor, JCS (1997),...*
- electrons with/w/o magnetic fields ⇒*Harabati & Kay, JCP (2007), FG & Kramer, JPB (2011)*
- discrete breathers (FPUT) ⇒*Igumenshchev et al., Mol. Phys (2012), Zagoya et al., JPA (2014)*
- IR spectroscopy ⇒*Noid et al JCP (2003), Buchholz et al (2016)*
- interacting Bose particles ⇒*Simon and Strunz (2014), Ray et al (2016)*

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Semiclassical Hybrid Dynamics: SCHD

problem: exponential scaling of numerical effort in grid based qm $\sim 10^N$
possible solution: Frozen Gaussian Wavepacket Dynamics

$$\Psi_\alpha(\mathbf{x}, t) = \int \mathrm{d}^N x' K^{\mathrm{FGA}}(\mathbf{x}, t; \mathbf{x}', 0)\langle \mathbf{x}'|\Psi_\alpha(0)\rangle$$

$$\boxed{\Psi_\alpha(\mathbf{x}, t) = \int \frac{\mathrm{d}^N p' \mathrm{d}^N q'}{(2\pi\hbar)^N} \langle \mathbf{x}|g(\mathbf{p}_t, \mathbf{q}_t)\rangle R e^{\frac{i}{\hbar}S(\mathbf{p}', \mathbf{q}', t)} \langle g(\mathbf{p}', \mathbf{q}')|\Psi_\alpha(0)\rangle}$$

- ☺ Monte Carlo integration over initial conditions
- ☺ no storage problems due to locality of cm
- ☹ linear scaling not generic *M. L. Brewer, JCP* **111**, *6168 ('99)*
- ☹ expanding the exponent around $(\mathbf{p}_\alpha, \mathbf{q}_\alpha)$ ⇒TGWD: too crude!

Semiclassical Hybrid Dynamics: SCHD

"divide and conquer"

$$\mathbf{q}' = (\mathbf{q}'_1, \mathbf{q}'_2)$$

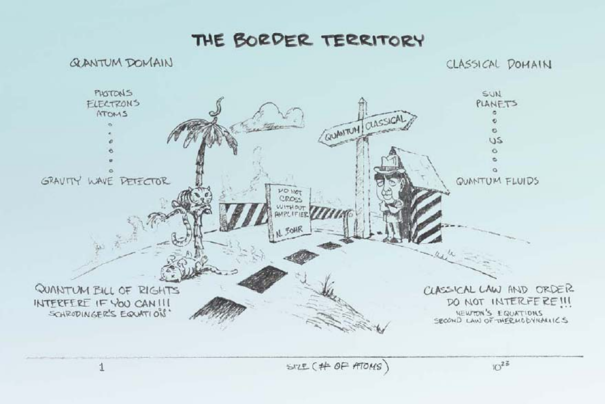
- $\mathbf{q}'_2$ are n "nearly harmonic" DOFs $\Rightarrow$TGWD
- $\mathbf{q}'_1$ are $N-n$ "strongly anharmonic" DOFs $\Rightarrow$FGWD

$$\boxed{\Psi_\alpha(\mathbf{x}, t) = \int \frac{\mathrm{d}^{N-n}p'_1 \mathrm{d}^{N-n}q'_1}{(2\hbar)^N \pi^{N-n}} \sqrt{\frac{\sqrt{\det \gamma}}{\pi^{N/2} \det \mathbf{A}_2}} R \exp\left\{\frac{1}{4}\mathbf{b}_2^{\mathrm{T}} \cdot \mathbf{A}_2^{-1} \cdot \mathbf{b}_2 + c_2\right\}}$$

$\mathbf{A}_2, \mathbf{b}_2, c_2$ contain fully coupled classical dynamics

FG, JCP **125**, *014111 (2006)*

Interference Quenching in the Caldeira-Leggett (CL) model



(quantum) system will behave classically if coupled to a (large) environment

W.H. Zurek, Physics Today 44, October, 36 - 44, (1991)

Caldeira-Leggett model for molecule in solution

$\mathbf{q}_1$ "system": 2 phase space variables (p, q)
$\mathbf{q}_2$ "bath": $2n$ phase space variables (p_j, x_j)

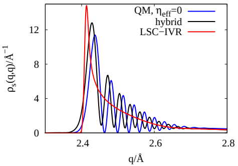
$$H = \frac{p^2}{2m} + V(q) + \sum_{j=1}^{n} \frac{p_j^2}{2m_j} + \frac{m_j\omega_j^2}{2}\left(x_j - \frac{c_j}{m_j\omega_j^2} q\right)^2$$

- counterterm $\sim q^2$ compensates for shift of minimum/frequency
- "system": Morse oscillator for I_2, $\omega_{\mathrm{S}} \approx 200\mathrm{cm}^{-1}$
- "bath": $T = 0$, discretized $(n = 20)$ Ohmic spectral density $J(\omega) = \eta\omega\Theta(\omega - \omega_c)$ with cutoff $\omega_c \approx 20\mathrm{cm}^{-1} \ll \omega_{\mathrm{S}}$ *H. Wang et al JCP '01*
- blue shift:

$$\lambda_0{}^2 = \frac{\omega_{\mathrm{S}}{}^2}{1 + \frac{2}{\pi}\frac{\eta}{m}\int_0^{\omega_c} d\omega(\omega^2 - \lambda_0{}^2)^{-1}}$$

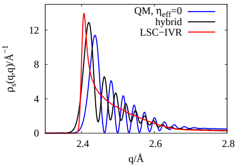
E. Pollak, PRA ***33****, 4244 (1986)*

Interference quenching, diagonal of $\hat{\rho}_\mathrm{S}(t) = \mathrm{Tr}_\mathrm{B}\hat{\rho}(t)$

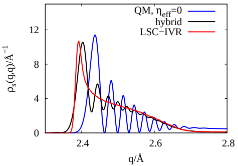


$\eta_\mathrm{eff} = 0.25$

t=192 fs



$\eta_\mathrm{eff} = 0.5$



$\eta_\mathrm{eff} = 1.0$

blue shift and transition to classicality

C.-M. Goletz and FG, JCP **130**, *244107 (2009)*

More recent SCHD developments

- mimicing an infinite bath *C.-M. Goletz, W. Koch and FG, CP* **375**, *227 (2010)*
- vibrational decoherence of molecules in clusters *Buchholz et al., J. Phys. Chem. A* **116**, *11199 (2012)*
- calculating IR response functions *F.G., Phys. Scr.* **91**, *044004 (2016)*
- combining SCHD with time averaging *M. Buchholz, FG, M. Ceotto, JCP* **144**, *094102 (2016)*

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Hubbard-Stratonovich Uncompleting of the Square

$$\sqrt{\pi/a}\exp\{-\overset{\downarrow}{b^2}/(4a)\} = \int dy\exp\{-ay^2 + i\overset{\downarrow}{b}y\}$$

M: Stochastic averaging, $\xi(t)$ Gaussian noise

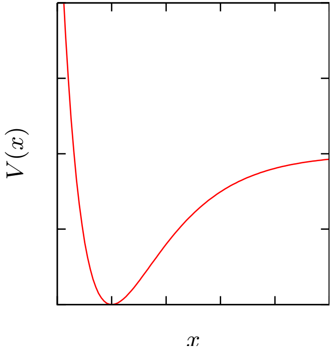
$$M[\exp\left(\frac{i}{\hbar}\int_{t_0}^{t} dt'\xi(t')q(t')\right)]$$

equivalent to

$$\exp\left(-\frac{1}{\hbar^2}\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt'' q(t')M[\xi(t')\xi(t'')]q(t'')\right)$$

J. Hubbard, PRL ***3****, 77 (1959)*

Diploar driving by noise



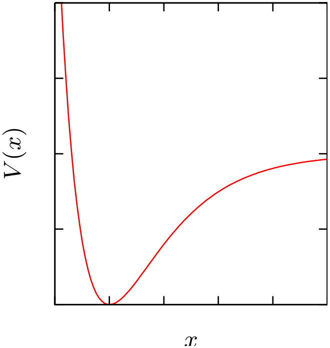
$$H(t) = H_S - \xi(t)\, q$$

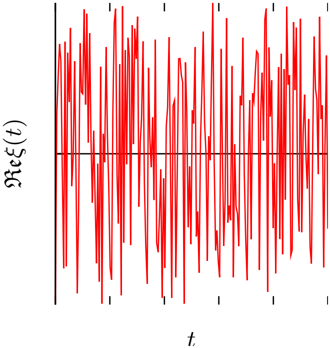
additional phase

$$\mathcal{F}_\xi[q_1, q_2] = M\left[\exp\left\{\frac{i}{\hbar}\int_{t_0}^{t} dt'\xi(t')\left[q_1(t') - q_2(t')\right]\right\}\right]$$

"forward path" q_1, "backward path" q_2

Diploar driving by noise





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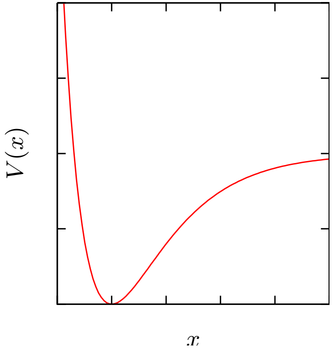
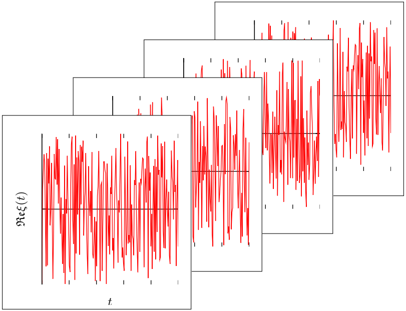




$$H\left(t\right) = H_S - \xi\left(t\right) q$$

additional phase

$$\mathcal{F}_{\xi}\left[q_1, q_2\right] = M\left[\exp\left\{\frac{i}{\hbar}\int_{t_0}^{t} dt' \xi\left(t'\right)\left[q_1\left(t'\right) - q_2\left(t'\right)\right]\right\}\right]$$

"forward path" q_1, "backward path" q_2

Reduced Density matrix evolution

$$\begin{aligned}\rho(q_f, q'_f, t) &= M[\rho_\xi(q_f, q'_f, t)] \\ &= \sum_{\text{paths}} e^{\frac{i}{\hbar}(S_{\rm S}[q_1]-S_{\rm S}[q_2])}\mathcal{F}[q_1, q_2]\rho(q_i, q'_i, t_0)\end{aligned}$$

- "completing the square" $\Rightarrow$non-Markovian dynamics

$$\mathcal{F}[q_1, q_2] = e^{-\frac{1}{\hbar^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''[q_1(t')-q_2(t')]M[\xi(t')\xi(t'')][q_1(t'')-q_2(t'')]}$$

- "uncompleting the square" $\Rightarrow$memory free dynamics + averaging

$$\mathcal{F}[q_1, q_2] = M e^{\frac{i}{\hbar}\int_{t_0}^{t} dt'\xi(t')[q_1(t')-q_2(t')]} = M\mathcal{F}_\xi[q_1]\mathcal{F}_{\xi^*}[q_2]$$

two summations: $\sum_{\text{paths}}$ and M

is this only a mathematical trick?

Feynman-Vernon influence functional for CL model

$$x \equiv q_1(t) - q_2(t), r \equiv [q_1(t) + q_2(t)]/2$$

$$\mathcal{F}[x,r] \;=\; e^{-\frac{1}{\hbar^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' x(t')[\mathrm{Re}L(t'-t'')x(t'')+2i\mathrm{Im}L(t'-t'')r(t'')]} \; e^{-\frac{i\mu}{\hbar^2}\int_{t_0}^{t} dt' x(t')r(t')}$$

$$\boxed{L(t) = \frac{\hbar}{\pi}\int d\omega J(\omega)\left(\coth\frac{\hbar\omega\beta}{2}\cos(\omega t) - i\sin(\omega t)\right)}$$

contains both fluctuation and dissipation

- $J(\omega) = \frac{\eta\omega}{(1+\omega^2/\omega_c^2)^2}$ Ohmic with algebraic cutoff
- $\beta = 1/kT$ inverse bath temperature
- $\mu = \frac{2}{\pi}\int_0^\infty d\omega \frac{J(\omega)}{\omega}$ due to "counter term" (preserving translational invariance in the free particle case)

R. P. Feynman and F. L. Vernon, Ann. Phys. (NY) **24**, *118 (1963)*

FV path integral ⇔ stochastic LvN differential equation

$$i\hbar\dot{\hat{\rho}} = [\hat{H}_{\mathrm{S}}, \hat{\rho}] - \xi(t)[\hat{q}, \hat{\rho}] + \frac{\mu}{2}[\hat{q}^2, \hat{\rho}] - \frac{\hbar}{2}\nu(t)[\hat{q}, \hat{\rho}]_+$$

with two (fluctuation and dissipation) *complex-valued* noise sources $z \equiv (\xi, \nu)$ with zero mean $M[\xi(t)] = M[\nu(t)] = 0$

$$\begin{aligned} M[\xi(t)\xi(t')] &= \mathrm{Re}L(t-t') \\ M[\xi(t)\nu(t')] &= (2i/\hbar)\Theta(t-t')\mathrm{Im}L(t-t') \\ M[\nu(t)\nu(t')] &= 0 \end{aligned}$$

- single realization *not* norm conserving (anticommutator!)
- stochastic averaging ⇒norm conserving dynamics
- incorporate counter term as delta-correlated noise term
- noise generation via FFT

Stochastic unraveling a la Stockburger/Grabert

$$\boxed{\hat{\rho} = |\Psi_1\rangle\langle\Psi_2|} \quad \Rightarrow \quad \dot{\hat{\rho}} = |\dot{\Psi}_1\rangle\langle\Psi_2| + |\Psi_1\rangle\langle\dot{\Psi}_2|$$

$$\begin{aligned} i\hbar|\dot{\Psi}_1\rangle &= [\hat{H}_\mathrm{S} - \xi(t)\hat{q} - \frac{\mu}{2}\hat{q}^2 - \frac{\hbar}{2}\nu(t)\hat{q}]|\Psi_1\rangle \\ i\hbar|\dot{\Psi}_2\rangle &= [\hat{H}_\mathrm{S} - \xi^*(t)\hat{q} - \frac{\mu}{2}\hat{q}^2 + \frac{\hbar}{2}\nu^*(t)\hat{q}]|\Psi_2\rangle \end{aligned}$$

$$\boxed{\hat{\rho}(t) = M|\Psi_1(t)\rangle\langle\Psi_2(t)|}$$

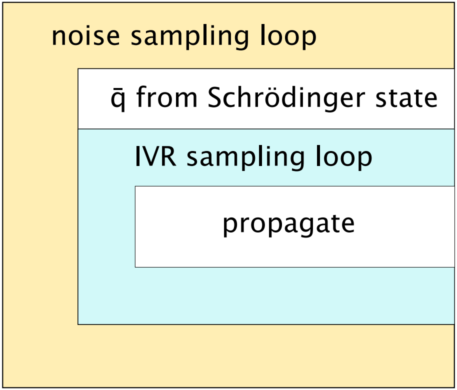
- Two independent complex noise “driven” Schrödinger eqns.
- Same initial conditions
- a) Herman-Kluk semiclassical propagation ⇒vibrational relaxation
  b) Bohmian Mechanics with complex action ⇒tunneling

J. Cao, Ungar and G. Voth JCP **104**, *4189 (96); W. T. Strunz et al PRL* **82**, *1801 ('99); J. T. Stockburger and H. Grabert, PRL* **88**, *170407 ('02), Y. Yan et al CPL* **395**, *216 ('04)*

Realization of stochastic semiclassical propagation

Elimination of diffusion of $\mathrm{Tr}(\rho)$ with guiding trajectory $\bar{q}$!
$\Rightarrow$norm conservation of single noise realization

nested sampling



W. Koch, FG, J. T. Stockburger, J. Ankerhold, CP **370**, *34 (2010)*

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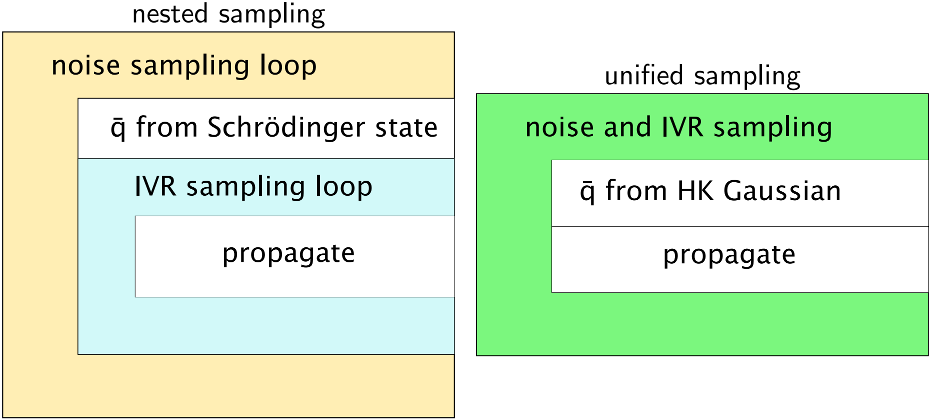

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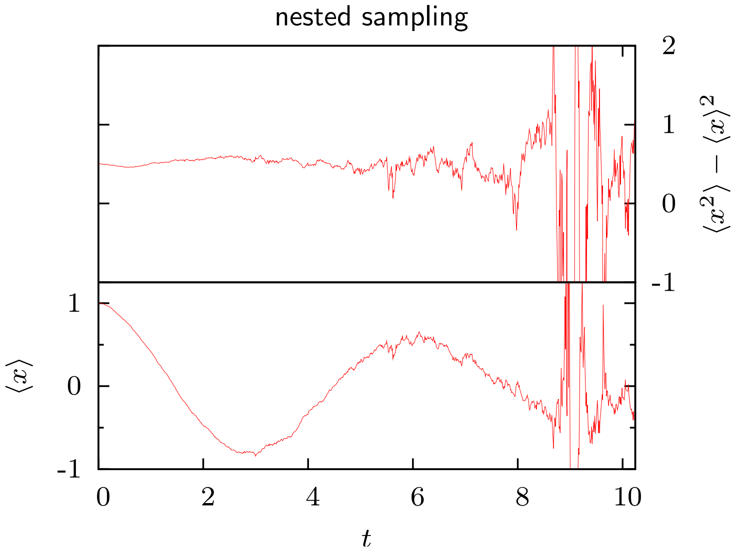
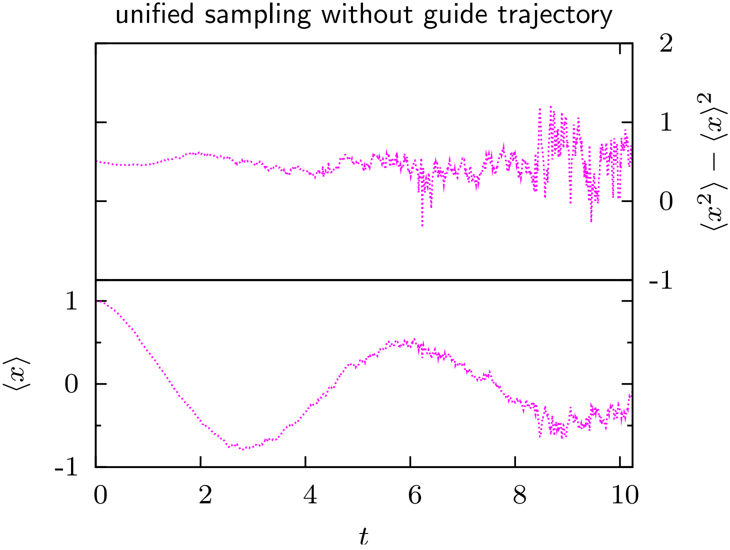
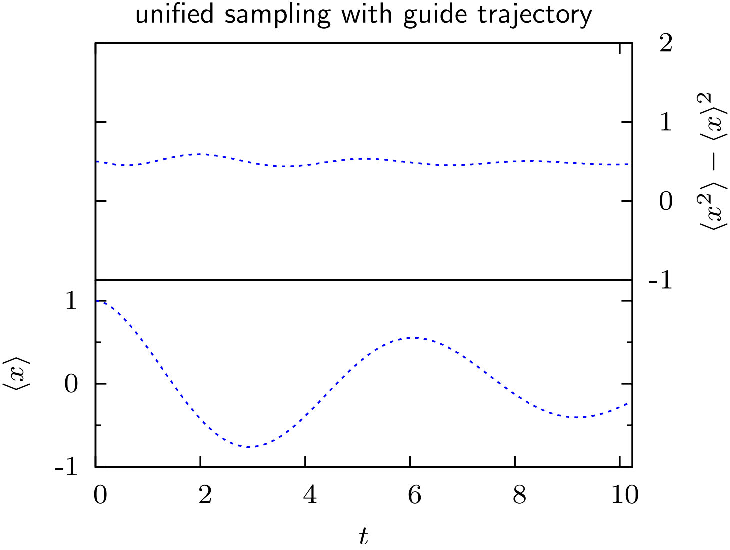
Improvement of Numerics: Brownian harmonic oscillator



Improvement of Numerics: Brownian harmonic oscillator



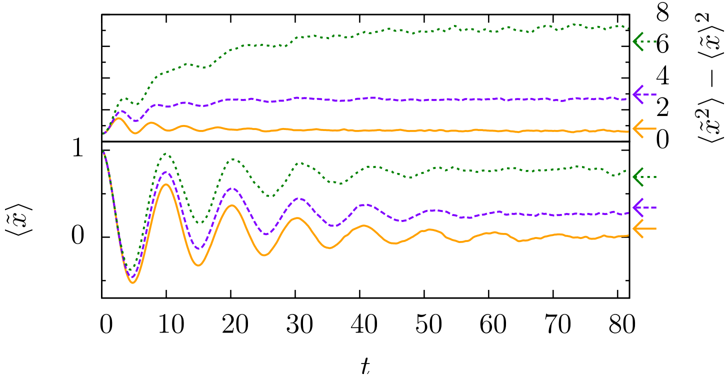
Improvement of Numerics: Brownian harmonic oscillator



Anharmonic Brownian Motion: Thermalization

$$\boxed{V = D(1 - \exp\{-\lambda\tilde{x}\})^2} \quad D = 30, \lambda = 0.08$$

$\eta = 0.1, \ T = 0.1, 1, 2$



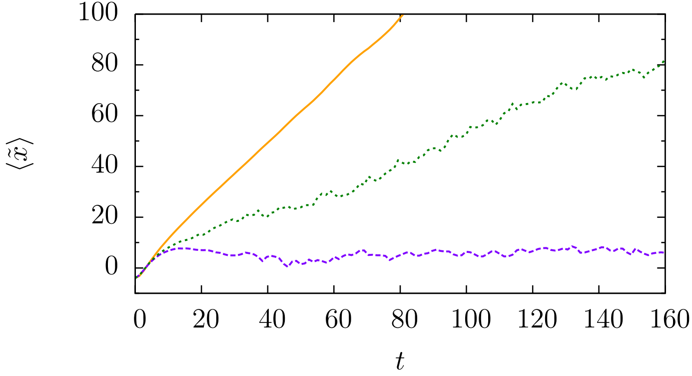
long time limit: "Boltzmann average"

W. Koch, FG, J. T. Stockburger, J. Ankerhold, PRL **100**, *230402 (2008)*

Trapping by Thermalization

$$\boxed{V = D(1 - \exp\{-\lambda\tilde{x}\})^2} \quad D = 1, \lambda = 0.2, \langle\tilde{x}\rangle(0) = -4$$

$$\eta = 0, 0.1, 0.1, \; T = 0.1, 2$$



W. Koch, FG, J. T. Stockburger, J. Ankerhold, CP **370***, 34 (2010)*

Dissipative tunneling through a parabolic potential in the Lindblad theory of open quantum systems

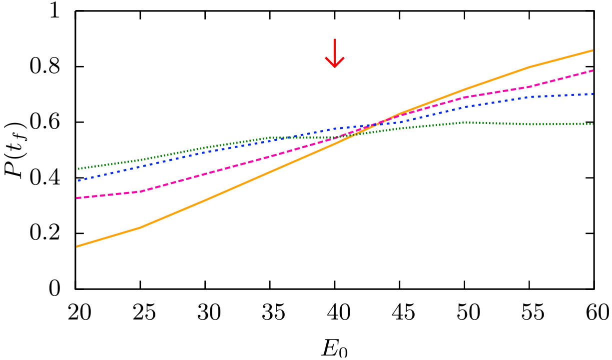
Isar, A., Sandulescu, A., and Scheid, W., The European Physical Journal D - Atomic, Molecular, Optical and Plasma Physics, 12:3-10 (2000)

. . . Caldeira and Leggett [1,2] concluded that dissipation tends to suppress quantum tunneling. Using a different method, Schmid obtained similar results in reference [13]. Widom and Clark [14] considered a parabolic potential barrier and found that dissipation enhances tunneling. Bruinsma and Bak [15] also considered tunneling through a barrier and found that at zero temperature the tunneling rate can be either increased or decreased by dissipation. Leggett [16] considered tunneling in the presence of an arbitrary dissipation mechanism and found that, normally, dissipation impedes tunneling, but he also found an anomalous case in which dissipation assists the tunneling process. Razavy [17] considered tunneling in a symmetric double-well potential and concluded that dissipation can inhibit or suppress tunneling. . . .

Dissipative tunneling through an Eckart barrier

$$\boxed{V = D/\cosh^2(\lambda x)} \; D = 40, \lambda = 4.32$$

$$\eta = 0.2 \;\; T = 400 \;\; \langle x_0 \rangle = -0.7, -1.7, -2.7, -3.7$$

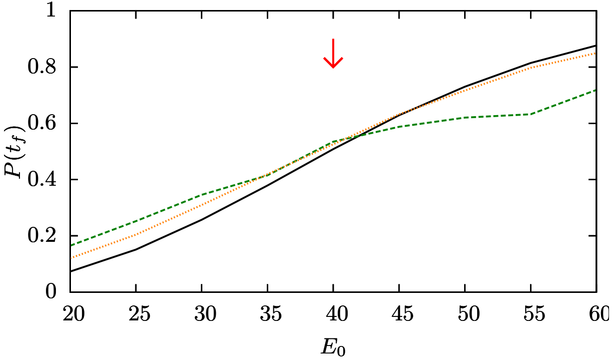


W. Koch, FG, D. J. Tannor, PRL **105**, *230 (2010)*

Dissipative tunneling through an Eckart barrier

$$\boxed{V = D/\cosh^2(\lambda x)} \quad D = 40, \lambda = 4.32$$

$$\eta = 0.2, 0.6 \quad T = 400 \quad \langle x_0 \rangle = -0.7$$



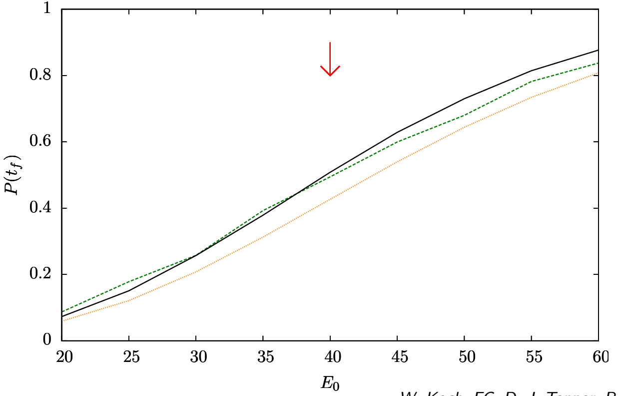
W. Koch, FG, D. J. Tannor, PRL **105**, *230 (2010)*

Non-Markovian dissipative tunneling

$$\boxed{V = D/\cosh^2(\lambda x)} \; D = 40, \lambda = 4.32$$

$$\eta = 0.4 \;\; T = 40 \;\; \langle x_0 \rangle = 0.7$$

BOMCA ($\omega_c = 10$) versus CLME



W. Koch, FG, D. J. Tannor, PRL **105**, *230 (2010)*

Conclusions and Outlook

- Semiclassical IVR: TGWD, Herman-Kluk FGWD
- Semiclassical hybrid dynamics combines TGWD and HK
- Transition to classicality in Caldeira-Leggett model
- Non-Markovian dissipative/decoherence dynamics via driving by complex noise: $\mathcal{F}[q_1, q_2] = M\mathcal{F}_\xi[q_1]\mathcal{F}_{\xi^*}[q_2]$
- (An)harmonic Brownian dynamics up to thermalization
- Dissipative tunneling
- *quantify non-Markovianity*
- *go beyond bilinear coupling*
- *better convergence: J. Stockburger, arXiv:1608.03438*
- *compare to HEOM*

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DFG: GR-1210/4-1,2

For your interest!