A path integral theory of heat flow through a system of qubits

Erik Aurell

QT60

Workshop on thermodynamics, thermoelectrics and transport in quantum devices

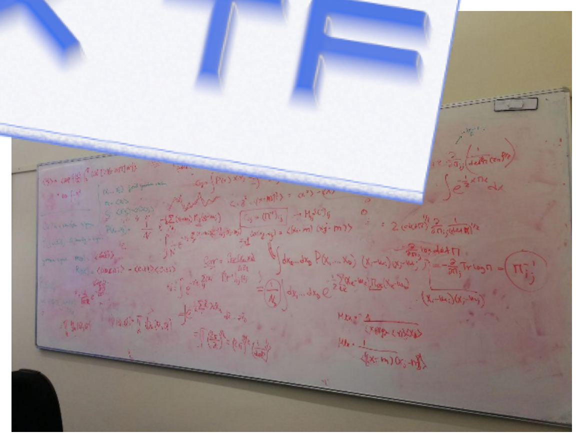
Work in progress

E.A., Bayan Karimi, Federica Montana, Jukka Pekola, Lamberto Rondoni (2018)

NORDITA qi2019

“New Directions in Quantum Information”

April 1-26 2019



Channel Capacity
Thermodynamics
Synchronization
Future

http://www.nordita.org/qi2019

Hyvää syntymäpäivää!

Happy Birthday!

С днем рождения!

Grattis på födelsedagen!

Why theory?

More precisely: why not a theory based on perturbation theory and Golden Rule?

Reason 1: Jukka and collaborators have already done it (Karimi & Pekola *Phys Rev B* 2017; Ronzani et al *Nature Commun* 2018)

Reason 2: eventually one would like to be able to treat heat in a quantum system interacting both weakly and strongly with a bath, or baths.

Why path integrals?

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The Lagrangian formulation of quantum mechanics (i.e. path integrals) is equivalent to the more standard Schrödinger and Heisenberg pictures, but often leads to more complicated ways to arrive at the same result. So why bother?

Path integrals are easier for global properties e.g. large deviations (e.g. escape rates from metastable states)

Famous results were first time or almost first time found this way (superfluidity in He^4, quantum Brownian motion, …)

Because one can…

KTH VETENSKAP OCH KONST
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Qubit path integrals

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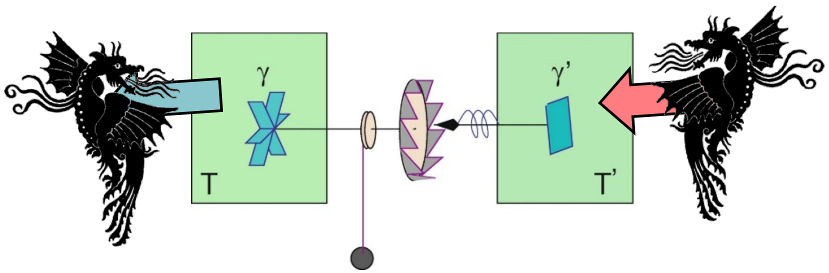


Discrete system state, harmonic oscillator (bosonic) bath(s), same or different bath temperatures,…

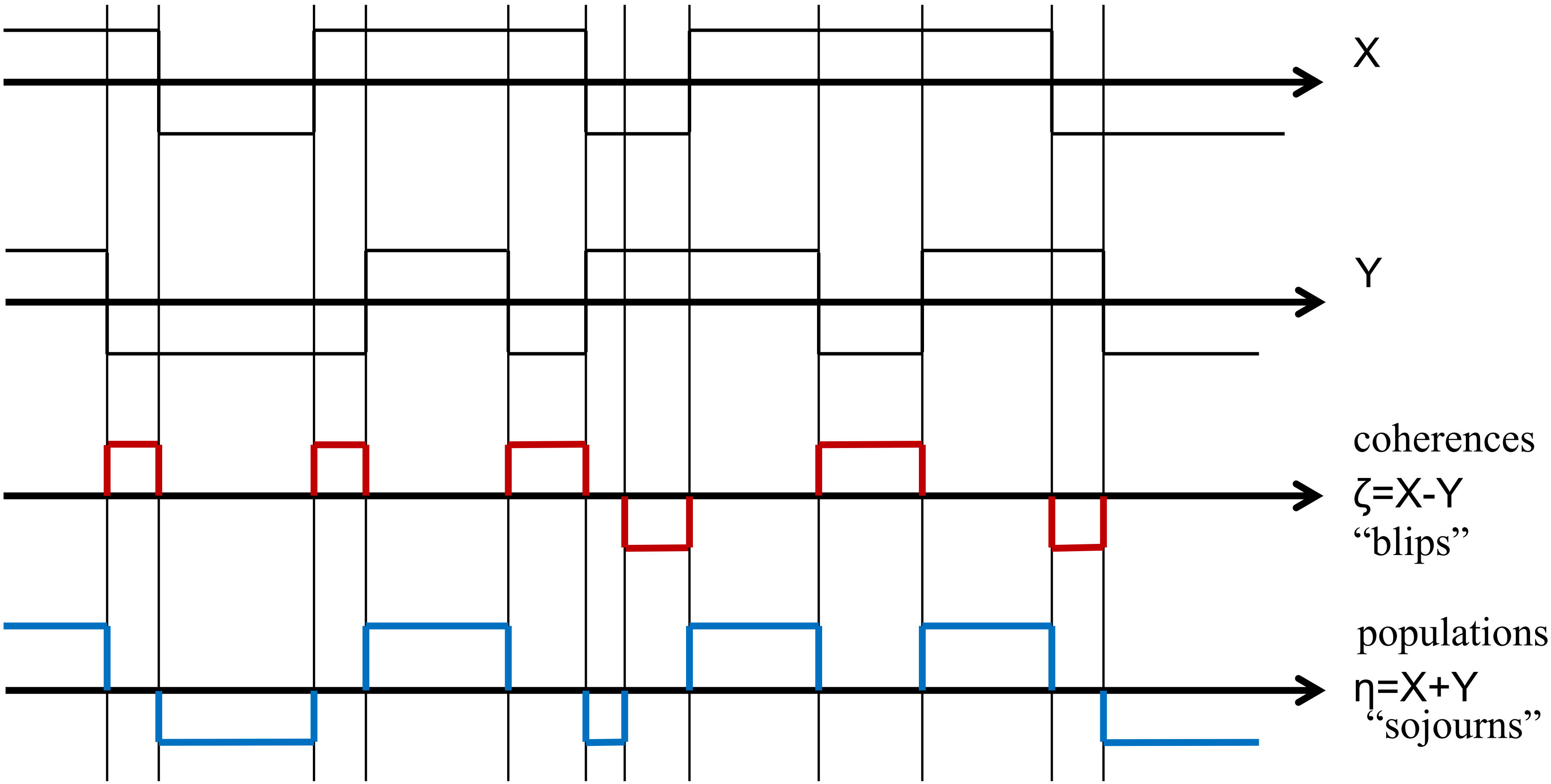
Path integrals were developed in the 80ies by Leggett and others for spin systems interacting with harmonic oscillator environments like

$$H = \frac{1}{2}\sum_a \mu_a \prod_{i\in\partial a} \hat{\sigma}_z^i - \frac{\hbar}{2}\sum_i \Delta_i \hat{\sigma}_x^i + \sum_{b,i} C_{b,i}\hat{\sigma}_z^i q_b + \frac{1}{2}\sum_b \frac{p_b^2}{m_b} + m_b\omega_b^2 q_b^2$$

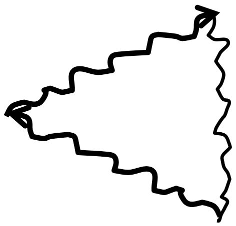
The oscillators are for brevity written classically. Inserting complete sets of states between time slices produces sequences of up and down states which can be interpreted as piece-wise constant "spin histories". The spin paths jump between ½ and -½ with rates Δ_i.

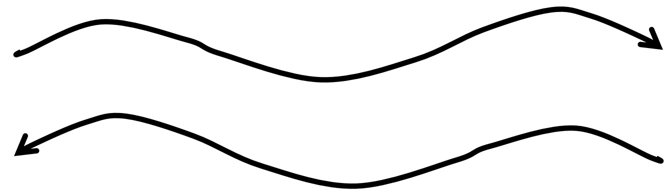
Leggett et al 1987: interactions between "blips" and "sojourns"

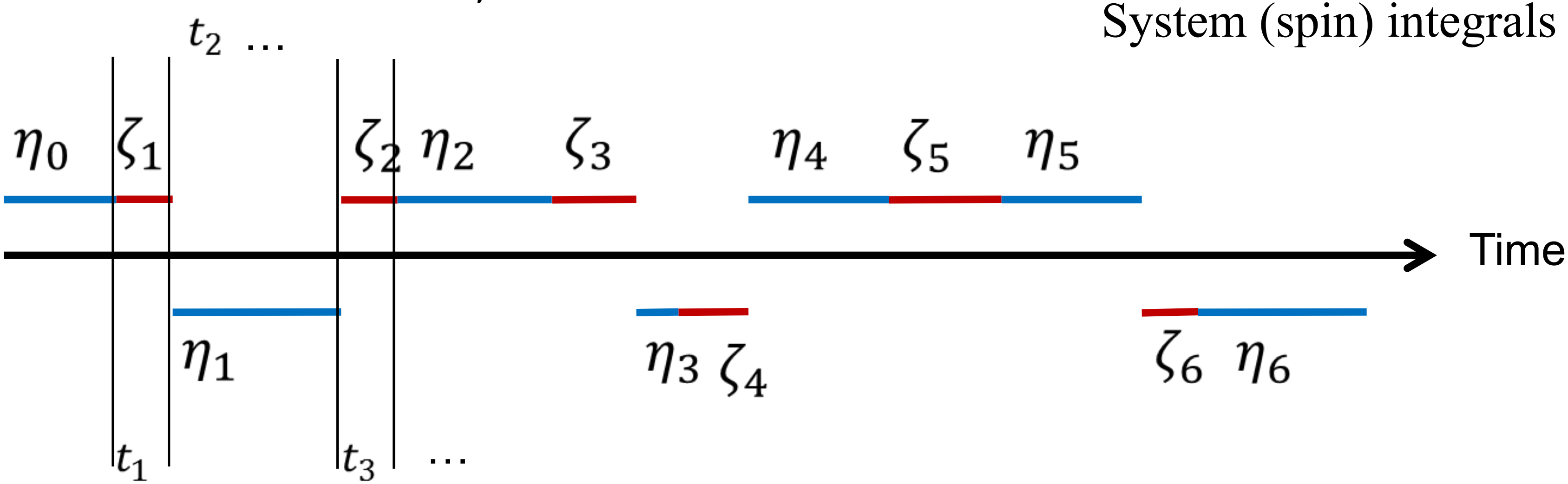
One needs two paths for each spin to represent the development of the density matrix, one for the path integral of U and one for the path integral of U^{-1}.



One integrates out the bosonic bath(s) (Feynman-Vernon theory)



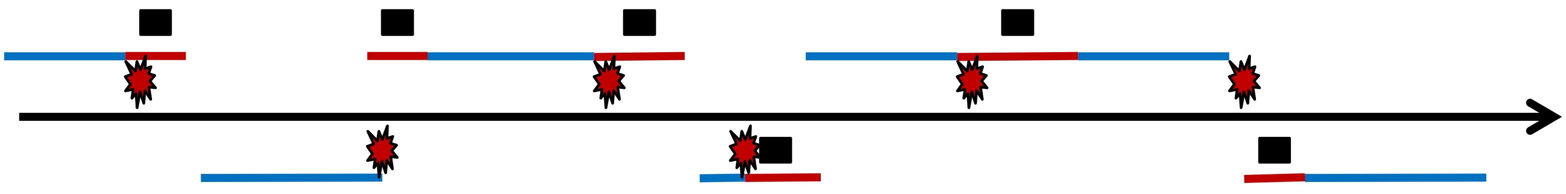




Result: pair-wise interactions between periods when the forward and backward spin histories are the same (“sojourns”), and when they are opposite (“blips”). Depend on second primitive functions (two integrations) of Feynman-Vernon kernels.

Propagators in “non-interacting blip approximation” (NIBA)

$$K_{FV} = \int \mathcal{D}X\mathcal{D}Y\, e^{\frac{i}{\hbar}S_S[X]}\, e^{-\frac{i}{\hbar}S_S[Y]}\, e^{\frac{i}{\hbar}S_i[X,Y]-\frac{1}{\hbar}S_r[X,Y]}$$



$$S_r[X,Y] = \sum_j S_j + \sum_{jk} \xi_j \xi_k \Lambda_{jk}$$

$$S_i[X,Y] = \sum_j \sum_{k<j} \xi_j \eta_k X_{jk}$$

NIBA means to neglect all terms except S_j (■) and $X_{j,j-1}$ (✱).

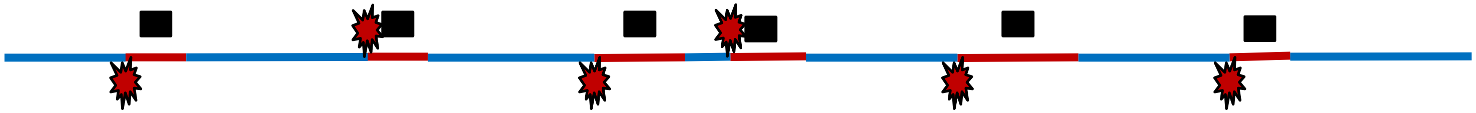
$$S_j = \int_{t_{2j-1}}^{t_{2j}} \int_{t_{2j-1}}^{s} k_r(s,u)\,du\,ds$$

$$\Lambda_{jk} = \int_{t_{2j-1}}^{t_{2j}} \int_{t_{2k-1}}^{t_{2k}} k_r(s,u)\,du\,ds$$

$$X_{jk} = \int_{t_{2j-1}}^{t_{2j}} \int_{t_{2k}}^{t_{2k+1}} k_i(s,u)\,du\,ds$$

These effective interactions summarize the influence of the bath on system development (Leggett et al, Weiss, a large literature….)

Depressing fact for path integral afficionados…



NIBA for the spin-boson problem also follows from relaxation theory after a polaron transform

$$H \to S^{-1} H S \qquad S = \exp i \sum_{b,i} \hat{\sigma}_z^i \frac{C_{b,i}}{\hbar \omega_b^2} \hat{p}_b$$

$$H = \frac{1}{2}\sum_a \mu_a \prod_{i \in \partial a} \hat{\sigma}_z^i - \frac{\hbar}{2}\sum_i \Delta_i \left(\hat{\sigma}_+^i e^{-i\Omega_i} + \hat{\sigma}_-^i e^{i\Omega_i} \right) + \frac{1}{2}\sum_b \frac{p_b^2}{m_b} + m_b \omega_b^2 q_b^2 \qquad \Omega_i = \sum_b 2 \frac{C_{b,i}}{\hbar \omega_b^2} \hat{p}_b$$

NIBA is thus a kind of perturbation in the jump rates Δ_i .

Aslangul, Pottier & Saint-James, *Journal de Physique* **46**:20131-2045 (1985); **47**:1657-1661 (1986)
Dekker, *Physical Review A* **35**:1436 (1987) [one page paper!]

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Heat is different

Let heat be change in bath energy (not interaction energy).

For strong-coupling thermodynamics (Seifert, Jarzynski, Hänggi,…), I refer to EA *Phys Rev E* **97**:042112 (2018).

The polaron transform now does not help because it would mix the bath energy and the interaction energy.

On the other hand, path integrals for these quantities have now been worked out by several groups Aurell & Eichhorn (2015), Weiss and collaborators (Carrega *et al* 2015:2016), and others.

Probability distribution of bath energy change

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$$P(\Delta E_B, f|i)$$

Joint probability of observing bath energy change ΔE_B and final system state $|f\rangle$, conditioned on initial system state $|i\rangle$ and the bath initially in an equilibrium state.

$$G_{if}(\nu) = \int e^{i\nu\Delta E_B} P(\Delta E_B, f|i) d\Delta E_B$$

a generating function

This generating function of the change in bath energy, aka full counting statistics (FCS), can be written as a modified Feynman-Vernon transition probability

$$G_{if}(\nu) = \mathrm{Tr}_B\left[\langle f|e^{i\nu H_B} U\left(|i\rangle\langle i|\otimes e^{-i\nu H_B}\rho_B^{eq}\right)U^\dagger|f\rangle\right]$$

After integrating out the bath FCS is a functional of the system history only, describing the distribution of bath energy changes if the bath would be measured before and after the process.

Full Counting Statistics

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Ignoring the final state of the system....

$$G_i(\nu) = \int e^{i\nu\Delta E_B} P(\Delta E_B|i) d\Delta E_B$$

$$G_i(\upsilon) = \mathrm{Tr}_{SB}\left[e^{i\upsilon H_B} U\left(|i\rangle\langle i| \otimes e^{-i\upsilon H_B}\rho_B^{eq}\right)U^\dagger\right]$$

Then in principle the answer must look like this...

$$G_i(\nu) = \int \mathcal{D}X\mathcal{D}Y e^{\frac{i}{\hbar}S[X]-\frac{i}{\hbar}S[Y]+\frac{i}{\hbar}S_i[X,Y]-\frac{1}{\hbar}S_r[X,Y]+\mathfrak{I}_\nu^{(2)}[X,Y]+\mathfrak{I}_\nu^{(3)}[X,Y]} 1_{X_f,Y_f}$$

The new functionals depend on the paths, the parameters, and the time difference

$$\mathfrak{I}_\nu^{(2)} = \iint (X_s Y_{s'} - X_{s'} Y_s) \sum_\omega f^{(2)}(\nu,\beta,\omega)\ \sin\omega(s-s')\, ds' ds$$

E.A.

Phys Rev E **97**:062117

$$\mathfrak{I}_\nu^{(3)} = \iint (X_s Y_{s'} + X_{s'} Y_s) \sum_\omega f^{(2)}(\nu,\beta,\omega)\ \cos\omega(s-s')\, ds' ds$$

(formulas for the coefficient functions later)

Path integral heat for spins

$$G_i(\nu) = \int \mathcal{D}X\mathcal{D}Y e^{\frac{i}{\hbar}S[X] - \frac{i}{\hbar}S[Y] + \frac{i}{\hbar}S_i[X,Y] - \frac{1}{\hbar}S_r[X,Y] + \Im_\nu^{(2)}[X,Y] + \Im_\nu^{(3)}[X,Y]} 1_{X_f, Y_f}$$

For heat there are both blip-blip and sojourn-sojourn interactions. In a sojourn-blip interactions, the sojourn can additionally be both before a blip and after a blip.

$$\Im_\nu^{(3)} = -\sum_j S_j + \sum_j \tilde{S}_j - \sum_{jk} \xi_j \xi_k \Lambda_{jk} + \sum_{jk} \eta_j \eta_k \tilde{\Lambda}_{jk}$$

$$\Im_\nu^{(2)} = \sum_{jk} \xi_j \eta_k X_{jk}^{(\nu)}$$

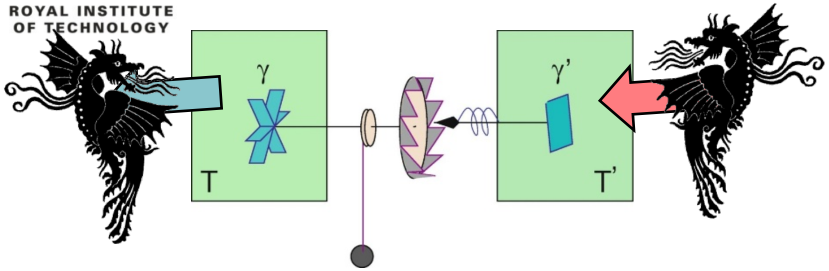
NIBA is OK for an Ohmic bath, and to first order in ν.

$$\Im_\nu^{(3)} \approx -\sum_j S_j + \sum_j \tilde{S}_j$$

$$\Im_\nu^{(2)} \approx \sum_j \xi_j \eta_j X_{jj}^{(\nu)} + \xi_j \eta_{j-1} X_{j,j-1}^{(\nu)}$$

I am still working on getting this into shape…

More spin dynamics



Discrete system state, bosonic bath, Ohmic or not Ohmic spectrum

Path integrals for general spin dynamics are nowadays supposed text book stuff *cf*. Atland & Simons ”Condensed Matter Field Theory” 2nd Edition 2010.

These path integrals for spin are built on Klauder’s coherent-state path integrals. I even recently published a paper using this approach myself*. How to use it for quantum heat is however less clear.

* “Global Estimates of Errors in Quantum Computation by the Feynman–Vernon Formalism” *Journal of Statistical Physics* **171**:745-767 (2018)

Large deviations

$$f^{(2)} = \frac{1}{2} - \frac{\sin(\omega\hbar\nu)\sin\left(\omega\hbar(\nu - i\beta)\right)}{4\sinh^2\left(\frac{\omega\hbar\beta}{2}\right)}$$

$$f^{(3)} = -\frac{i}{2}\cos(\omega\hbar\nu)\coth\left(\frac{\omega\hbar\beta}{2}\right) + \frac{1}{2}\sin(\omega\hbar\nu)$$

My version of these heat kernels

Phys Rev E **97**:062117

App A, Eqs A13-A20

NB, not clear if other authors (Weiss et al, Funo and Quan) get exactly these results. Not so easy to check. Partly comes back to the definition of heat as change in bath energy only or some other combination.

A main interest should be large υ (large but rare heat). There should be combination effects of υ, temperature and the spectral shape.

One can also look at correlations between heat in different baths connected to one and the same system.

Thanks

Federica Montana
Lamberto Rondoni

Jukka Pekola
Bayan Karimi