

How To Win Friends and Influence Functionals

The Influence Functional approach to quantum and classical systems

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October 4, 2019

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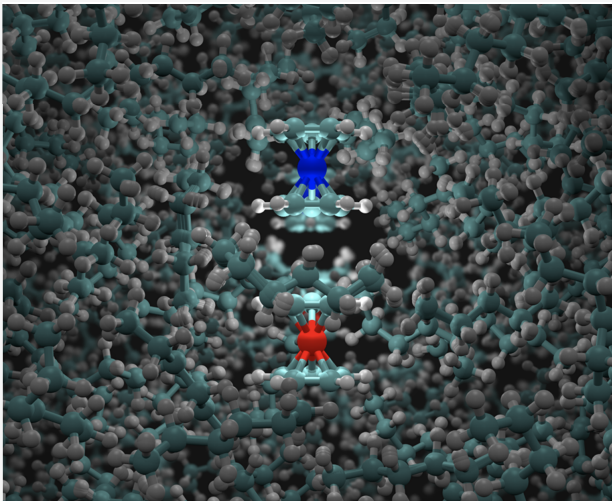
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This Talk

This talk is about a powerful technique for describing the dynamics of an open system known as the **influence functional**. Here we will discuss:

- The applications of influence functionals
- How influence functionals are defined and used
- The exact stochastic equations that can be derived from them.
- Their utility in establishing rigorous classical limits.

What are Influence functionals?



- Influence functionals are a path integral technique, where the environmental part of an open system is expressed as single functional.
- They have numerous applications, both analytical and numerical.

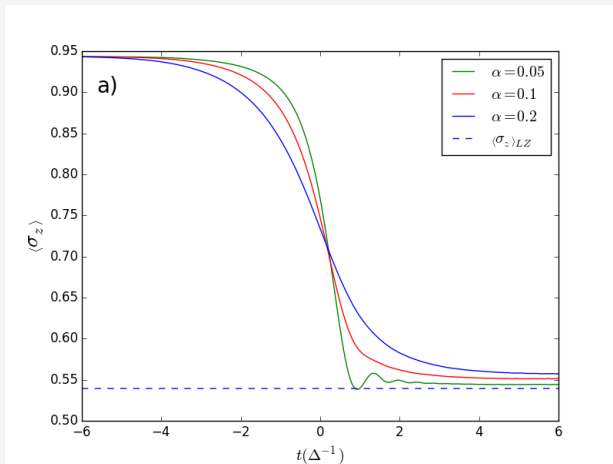
Spin Boson Model

Mappings

- Qubit in environment
- Kondo model
- Bio-molecular friction transfer

Applications

- Quantum computing
- Josephson junctions
- Exotic matter



Equations Derived With Influence Functionals

- One particularly useful application of influence functionals is their use in deriving **exact** equations.
- One example is the **Stochastic Liouville Equation**

Stochastic Liouville Equation

$$i\hbar\partial_t\tilde{\rho}(t) = \left[\hat{H}_Q(t), \tilde{\rho}(t)\right] - \eta(t) [\hat{q}(t), \tilde{\rho}(t)] - \frac{\hbar}{2}\nu(t) \{\hat{q}(t), \tilde{\rho}(t)\}$$

Generalised Langevin Equation

$$m\ddot{q}(t) = -V'(q, t) - 2 \int_0^t dt' \dot{q}(t') \gamma(t - t') + \eta_{\text{cl}}(t)$$

Equations Derived With Influence Functionals

- One particularly useful application of influence functionals is their use in deriving **exact** equations.
- One example is the **Stochastic Liouville Equation**

Classical Limit?

- The **SLE** and **GLE** are clearly closely related to each other.
- If we take the classical limit in a heuristic manner, we find that $\lim_{\hbar \rightarrow 0}$ **SLE** leads to:

$$m\ddot{q}(t) = -V'(q, t) + \eta_{\text{cl}}(t)$$

Generalised Langevin Equation

$$m\ddot{q}(t) = -V'(q, t) - 2 \int_0^t dt' \dot{q}(t') \gamma(t - t') + \eta_{\text{cl}}(t)$$

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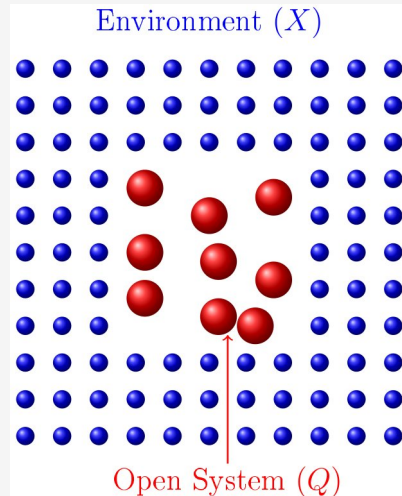
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Evolving The Density Matrix

- For a global system described with canonical coordinates q, p and x, k , the total Hamiltonian may be characterised as

$$H_{\text{tot}} = H_Q + H_X + V_{QX}$$

- To find $\hat{\rho}_Q(t)$, we evolve $\hat{\rho}_0^{\text{tot}}$ before tracing over the environment.



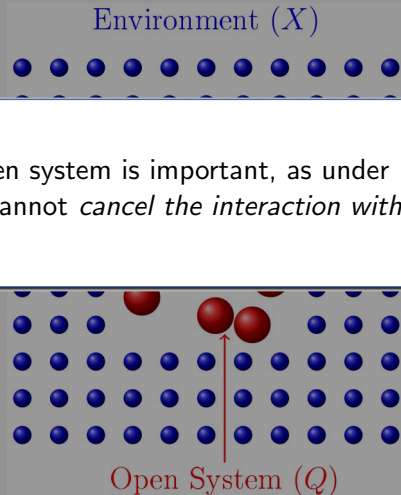
Evolving The Density Matrix

- For a global system described

The Influence of the Environment

Understanding the effect of an environment on an open system is important, as under ordinary circumstances a system's internal dynamics cannot *cancel the interaction with its surroundings...*

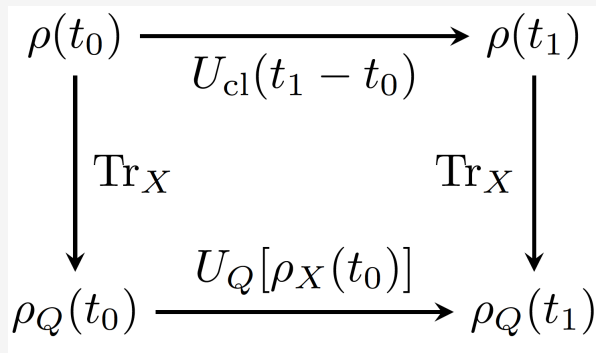
- To find $\hat{\rho}_Q(t)$, we evolve $\hat{\rho}_0^{\text{tot}}$ before tracing over the environment.



Brexit Means Brexit



The Goal of Influence Functionals



- We would like to describe the evolution of the open system without referring to its environment.
- To do so, we require an effective propagator U_Q .
- This is achieved with the **influence functional**.

The Goal of Influence Functionals

- We would like to describe the evolution

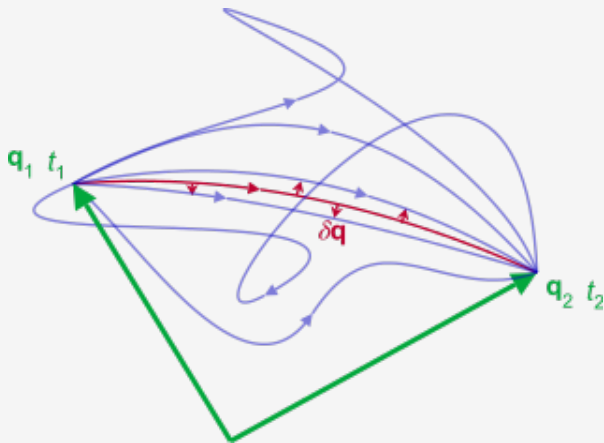
Reduced Density matrix

$$\begin{aligned} \rho_Q(q, q') = & \int d\bar{x} d\bar{x}' dx d\bar{q} d\bar{q}' U(q, x, t; \bar{q}, \bar{x}, 0) \\ & \times \rho_0^{\text{tot}}(\bar{q}, \bar{x}; \bar{q}', \bar{x}') U(\bar{q}', \bar{x}', 0; q', x, t) \end{aligned}$$

$$\rho_Q(t_0) \xrightarrow{U_Q[\rho_X(t_0)]} \rho_Q(t_1)$$

- This is achieved with the **influence functional**.

Path Integrals



- Influence functionals are a **path integral technique**
- Expressed as a path integral, the propagator of a state is

$$U(q_2, t_2; q_1, t_1) = \int_{q_1}^{q_2} \mathcal{D}q(t) e^{\frac{iS}{\hbar}}$$

Influence Functionals

- We have an expression for the reduced density matrix, but can we evaluate it?
- Feynman & Vernon (1963) developed a powerful formalism for dealing with systems of this type, using path integrals to describe the system of interest **without reference to the environment**.

$$\rho_{t_f}(q; q') = \frac{1}{Z} \int d\bar{q} d\bar{q}' \mathcal{D}q(t) \mathcal{D}q'(t) \left\{ \mathcal{F}[q(t), q'(t)] \right. \\ \left. \times \rho_0(\bar{q}; \bar{q}') \exp \left[\frac{i}{\hbar} S_q[q(t)] - \frac{i}{\hbar} S_q[q'(t)] \right] \right\}$$

Influence Functionals

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System Action

$S_q [q(t)]$ is the action of the isolated system evolving under the Hamiltonian $H_{\text{tot}} = H_Q$

$$\times \rho_0 (\bar{q}; \bar{q}') \exp \left[\frac{i}{\hbar} S_q [q(t)] - \frac{i}{\hbar} S_q [q'(t)] \right] \}$$

Influence Functionals

Influence Functional

$\mathcal{F}[q(t), q'(t)]$ is the *Influence Functional*. It characterises the environment's effect on the system.

$$\mathcal{F}[q(t), q'(t)] = \int \mathcal{D}\bar{X}(t) \rho_X(x_0; x'_0) \exp(iS_{\mathcal{F}}/\hbar)$$

$$\mathcal{D}\bar{X}(t) = dx_0 dx'_0 dx \mathcal{D}x(t) \mathcal{D}x'(t)$$

$$S_{\mathcal{F}} = S_X[x(t)] - S_X[x'(t)] + S_{QX}[q(t), x(t)] - S_{QX}[q'(t), x'(t)]$$

Using the Influence Functional

- Influence functionals can be evaluated numerically, but in some circumstances it is possible to derive **analytic** expressions.

- In this case they may be used to derive **effective** equations of motion for the reduced system.

- if $\mathcal{F}[q(t), q'(t')]$ can be decomposed into a product of the form

$$F[q(t), q'(t')] = \exp\left(\frac{i}{\hbar}\Phi_1[q(t)]\right) \exp\left(\frac{i}{\hbar}\Phi_2[q'(t')]\right)$$

- Then the effective propagator U_Q into a product of the form

$$U_Q[q(t), q'(t')] = \tilde{U}_Q[q(t)] \tilde{U}_Q^\dagger[q'(t')]$$

- from which an **effective** equation of motion may be found.

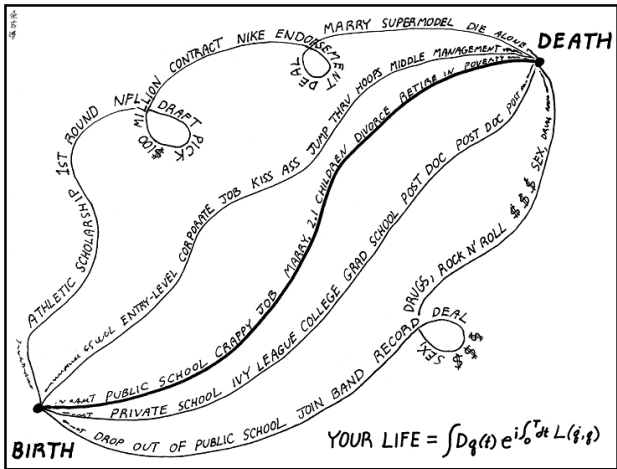
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The Path Integral Formulation of Your Life

- Influence functionals do not have to be restricted to quantum mechanics!
- A connection can be made to the classical limit of quantum results using the **Classical Influence Functional**
- Doing so requires a Hilbert space formulation of classical mechanics, in order to construct a **classical path integral**

What is Koopman von-Neumann mechanics?

- **Koopman von-Neumann (KvN)** mechanics was proposed in 1932 as a Hilbert space formulation of classical mechanics, providing an operational framework to assess classical problems.
- In both KvN and quantum mechanics, the **propagator** is a unitary transformation of the form:

$$\hat{U}(t) = e^{-i\hat{A}t}$$

Classical

- $[\hat{q}, \hat{p}] = 0$
- $\dot{\phi} = \{H, \phi\}$
- $\hat{A} = \hat{K} = \frac{\hat{p}}{m} \hat{\lambda} - \hat{V}'(x) \hat{\theta}$

Quantum

- $[\hat{q}, \hat{p}] = i$
- $\dot{\phi} = -i\hat{H}\phi$
- $\hat{A} = \hat{H}$

What is Koopman von-Neumann mechanics?

- Koopman von-Neumann (KvN) mechanics was proposed in 1932 as a Hilbert space formulation of classical mechanics, providing an operational framework to assess classical problems

Bopp Operators

$\hat{\lambda}$ and $\hat{\theta}$ are *Bopp operators*, defined by their commutation relations:

$$[\hat{x}, \hat{\lambda}] = [\hat{p}, \hat{\theta}] = i$$

$$[\hat{\lambda}, \hat{\theta}] = [\hat{\lambda}, \hat{p}] = [\hat{\theta}, \hat{x}] = 0$$

- $\phi = \{H, \phi\}$

- $\hat{A} = \hat{K} = \frac{\hat{p}}{m} \hat{\lambda} - \hat{V}'(x) \hat{\theta}$

- $\phi = -iH\phi$

- $\hat{A} = \hat{H}$

Constructing a Classical Path Integral

- In order to derive the Classical influence functional, we require a [Classical Path Integral](#).
- Given the KvN propagator

$$\hat{U}_{\text{cl}} = e^{-it\hat{K}}$$

- We can find a representation for it in phase space

$$U_{\text{cl}}(q_f, p_f, t_f; q_i, p_i) = \left\langle q_f, p_f \left| e^{-it_f \hat{K}} \right| q_i, p_i \right\rangle.$$

- Just like in the quantum case, this propagator can be expressed as a [path integral](#):

$$U_{\text{cl}}(q_f, p_f, t_f; q_i, p_i) = \int_{x_i, p_i}^{x_f, p_f} \underbrace{\mathcal{D}q \mathcal{D}p \mathcal{D}\lambda \mathcal{D}\theta}_{\mathcal{D}Q} e^{iR}$$

- Since the classical wavefunction and probability density are evolved by the same equation, this propagator can be used to evolve *both*.

Constructing a Classical Path Integral

- In order to derive the Classical influence functional, we require a **Classical Path Integral**.
- Given the KvN propagator

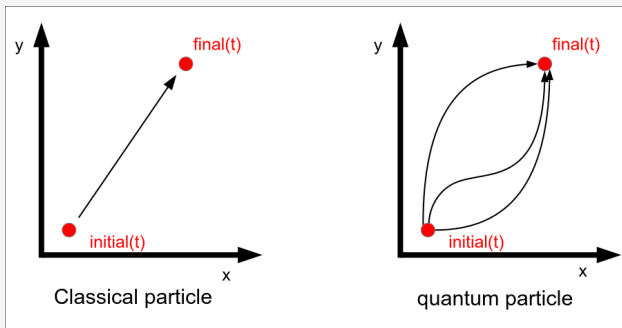
$$\hat{U}_{\text{cl}} = e^{-it\hat{K}}$$

The Classical "Quantum Action"

$$R = \int_0^{t_f} dt \left[\lambda(t) \left(\dot{x}(t) - \frac{p(t)}{m} \right) + \theta(t) (\dot{p}(t) + V'(x, t)) \right]$$

$$U_{\text{cl}}(q_f, p_f, t_f; q_i, p_i) = \int_{x_i, p_i}^{x_f, p_f} \underbrace{\mathcal{D}q \mathcal{D}p \mathcal{D}\lambda \mathcal{D}\theta}_{\mathcal{D}Q} e^{iR}$$

- Since the classical wavefunction and probability density are evolved by the same equation, this propagator can be used to evolve *both*.



- Classical path integral for total system is as expected (a delta functional).
- The path integral describing a *reduced* system is much more interesting.
- The process of tracing out the environment results in a non-trivial sum of trajectories.

Classical Influence Functional

- Evolving the composite system with the path integral propagator, and tracing out the environment gives:

$$\rho_Q(q_f, p_f, t_f) = \int dx_f dk_f \left(\int \mathcal{D}Q \mathcal{D}X dq_0 dp_0 dx_0 dk_0 e^{iR} \rho_0 \right)$$

- Using the influence functional it is possible to describe an *effective* propagator for the reduced system $U_Q [\rho_X(t_0)]$.

$$U_Q(q_f, p_f, t_f) = \int \mathcal{D}q(t) \mathcal{D}\theta_Q(t) \mathcal{F}[q(t), p(t), \theta_Q(t)] \exp \left(i \int_0^{t_f} dt \left[\theta_Q(t) \left(m\ddot{q} + \frac{\partial V_Q}{\partial q} \right) \right] \right)$$

Classical Influence Functional

- Evolving the composite system with the path integral propagator, and tracing out the

The form of this propagator depends on the influence functional, which is in turn a functional of the **initial environment state**.

$$\mathcal{F}[q(t), p(t), \theta_Q(t)] = \int dx_0 dk_0 dx_f dk_f \mathcal{D}x(t) \mathcal{D}\theta_X(t) \rho_X(x_0, k_0, q_0, p_0) \\ \times \exp \left(i \int_0^{t_f} dt \left[\theta_X(t) \left(m_k \ddot{x} + \frac{\partial V_{QX}}{\partial x} + \frac{\partial V_X}{\partial x} \right) + \theta_Q(t) \frac{\partial V_{QX}}{\partial q} \right] \right)$$

$$U_Q(q_f, p_f, t_f) = \int \mathcal{D}q(t) \mathcal{D}\theta_Q(t) \mathcal{F}[q(t), p(t), \theta_Q(t)] \exp \left(i \int_0^{t_f} dt \left[\theta_Q(t) \left(m \ddot{q} + \frac{\partial V_Q}{\partial q} \right) \right] \right)$$

Under certain circumstances an effective equation of motion may be defined from the influence functional. This is the case when it is possible to express $\mathcal{F}$ as

$$\mathcal{F}[q(t), p(t), \theta_Q(t)] = \exp \left(i \int_0^{t_f} dt \theta_Q(t) \chi[q(t), p(t)] \right) \quad (1)$$

where $\chi[q(t), p(t)]$ is an arbitrary functional of the phase space coordinates only. In the case, the effective equation of motion will be:

$$m\ddot{q} = -\frac{\partial V_Q}{\partial q} - \chi[q, \dot{q}] \quad (2)$$

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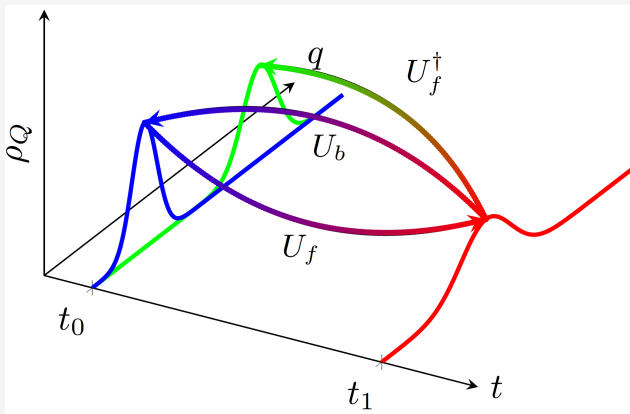
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The Effective Propagator

In both the classical and quantum cases, the effective propagator U_Q is now a functional of the **environment state** at the initial time. The “true” effective propagator for a system depends on the point in time it is being evolved from.

- $U_f = U_Q [\rho_X(t_0)]$
- $U_b = U_Q^\dagger [\rho_X(t_1)]$



Effective Propagators

Applying Influence functionals

- Using influence functionals, it is possible to derive both the [Stochastic Liouville equation](#) and [Generalised Langevin Equation](#).
- To do so, we must specify an environment and interaction Hamiltonian.
- We will use the [Caldeira-Leggett \(CL\)](#) model

$$H_{\text{tot}} = H_Q + \frac{1}{2} \sum_n (m_n \dot{x}_n^2 + m_n \omega_n^2 x_n^2) - q \sum_n c_n x_n + \frac{q^2}{2} \sum_n \frac{c_n^2}{m_n \omega_n^2}.$$

- Furthermore, we will specify that the environment is initially in thermal equilibrium.
In both cases, the influence functional can be expressed as

$$\mathcal{F} = e^{\Phi}$$

Quantum Influence Functional

Quantum

$$\begin{aligned}\Phi [q(t), q'(t)] &= \frac{i}{2\hbar} \int_0^{t_f} dt \int_0^{t_f} dt' K^R (t - t') \epsilon (t) \epsilon (t') \\ &\quad - \frac{1}{\hbar} \int_0^{t_f} dt \int_0^{t_f} dt' [\theta (t - t') K^I (t - t')] \epsilon (t) y (t')\end{aligned}$$

$$\epsilon (t) = q (t) - q' (t) \quad y (t) = \frac{1}{2} (q (t) + q' (t))$$

$$K^R (t - t') = \int_0^\infty d\omega I (\omega) \coth \left(\frac{1}{2} \hbar \beta \omega \right) \cos (\omega t)$$

$$K^I (t) = - \int_0^\infty d\omega I (\omega) \sin (\omega t)$$

Classical Influence Functional

Classical

$$\begin{aligned}\Phi[q(t), p(t), \theta_Q(t)] = & 2i \int_0^{t_f} dt \theta_Q(t) \int_0^t dt' q(t') \frac{d\gamma(t-t')}{dt'} \\ & - \int_0^{t_f} dt \int_0^t dt' \theta_Q(t) k_B T \gamma(t-t') \theta_Q(t')\end{aligned}$$

$$\gamma(t-t') = \int_0^\infty \frac{d\omega}{\omega\pi} I(\omega) \cos(t-t')$$

- In order to use the influence functional as part of an effective equation of motion, it must conform to the following functional form:

Classical

$$\mathcal{F}[q(t), p(t), \theta_Q(t)] = \exp \left(i \int_0^{t_f} dt \theta_Q(t) \chi[q(t), p(t)] \right)$$

Quantum

$$\mathcal{F}[q(t), q'(t')] = \exp \left(\frac{i}{\hbar} \Phi_1[q(t)] \right) \exp \left(\frac{i}{\hbar} \Phi_2[q'(t')] \right)$$

- In order to use the influence functional as part of an effective equation of motion, it must conform to the following functional form:

Classical

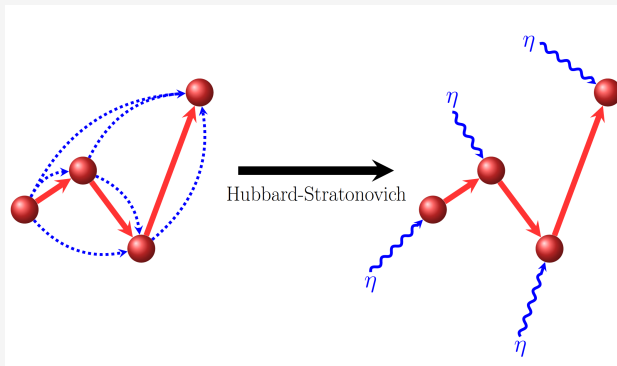
Problem

There is a **problem** here. Neither the quantum or classical influence functional is of a form from which an equation of motion can be derived. Is there a solution?

$$\mathcal{F}[q(t), q'(t')] = \exp\left(\frac{-i}{\hbar}\Phi_1[q(t)]\right) \exp\left(\frac{-i}{\hbar}\Phi_2[q'(t')]\right)$$

The Hubbard-Stratonovich Transformation

Use the [Hubbard-Stratonovich Transformation](#)!



- The HS transformation can be considered as converting a system of two body potentials into a set of independent particles in a fluctuating field.

The Hubbard-Stratonovich Transformation

Fourier-Transforming a Gaussian

$$\begin{array}{ccc}
 & & \langle e^{ikx} \rangle_r \\
 & & \updownarrow \\
 e^{-\frac{1}{2\sigma}x^2} & \xrightarrow{\text{Fourier}} & \int dx \, e^{-\frac{1}{2\sigma}x^2} e^{ikx} \\
 & & \updownarrow \\
 & & e^{-\frac{1}{2}\sigma k^2}
 \end{array}$$

into a set of independent particles in a fluctuating field.

Trajectories vs Distribution

Transformed Influence Functionals

Classical Propagator

$$\tilde{U}_{\text{cl}} = \int_{q_0, \dot{q}_0}^{q_f, \dot{q}_f} \mathcal{D}q(t) \delta \left[m\ddot{q}(t) + V'(q, t) + 2 \int_0^t dt' \dot{q}(t') \gamma(t - t') - \eta_{\text{cl}}(t) \right]$$

Quantum Propagator

$$\hat{U}^{\pm}(t_f) = \hat{T} \exp \left(-\frac{i}{\hbar} \int_0^{t_f} \hat{L}_Q(t) - \left[\eta(t) \pm \frac{\hbar}{2} \nu(t) \right] \hat{q}(t) dt \right)$$

Transformed Influence Functionals

Classical Propagator

Making Some Noise

$$\langle \eta(t) \eta(t') \rangle_r = \hbar \int_0^\infty \frac{d\omega}{\pi} I(\omega) \coth\left(\frac{1}{2}\omega\hbar\beta\right) \cos(\omega(t-t'))$$

$$\langle \eta(t) \nu(t') \rangle_r = -2i\Theta(t-t') \int_0^\infty \frac{d\omega}{\pi} I(\omega) \sin(\omega(t-t'))$$

$$\langle \eta_{\text{cl}}(t) \eta_{\text{cl}}(t') \rangle = \lim_{\hbar \rightarrow 0} \langle \eta(t) \eta(t') \rangle = \gamma(t-t')$$

Equations of Motions

Stochastic Liouville Equation

$$i\hbar\partial_t\tilde{\rho}(t) = \left[\hat{H}_Q(t), \tilde{\rho}(t)\right] - \eta(t) [\hat{q}(t), \tilde{\rho}(t)] - \frac{\hbar}{2}\nu(t) \{\hat{q}(t), \tilde{\rho}(t)\}$$

Generalised Langevin Equation

$$m\ddot{q}(t) = -V'(q, t) - 2 \int_0^t dt' \dot{q}(t') \gamma(t - t') + \eta_{\text{cl}}(t)$$

Classical Limit

- To show the SLE is equivalent in the classical limit to the GLE, we take the *effective* propagator of the reduced quantum system

$$\tilde{\rho}_{t_f}(q; q') = \int d\bar{q} d\bar{q}' \tilde{U}_{\text{eff}}(q, q', t_f; \bar{q}, \bar{q}', 0) \tilde{\rho}_0(\bar{q}; \bar{q}')$$

- Here $\tilde{U}_{\text{eff}}(q, q', t_f; \bar{q}, \bar{q}', 0)$ is $\hat{U}^+(t_f) \hat{U}^-(t_f)$ in path integral form.
- It is then possible to show:

$$\lim_{\hbar \rightarrow 0} \tilde{U}_{\text{eff}}(q, q', t_f; \bar{q}, \bar{q}', 0) = \tilde{U}_{\text{cl}}$$

Classical Limit

- To show the SLE is equivalent in the classical limit to the GLE, we take the *effective propagator of the reduced quantum system*

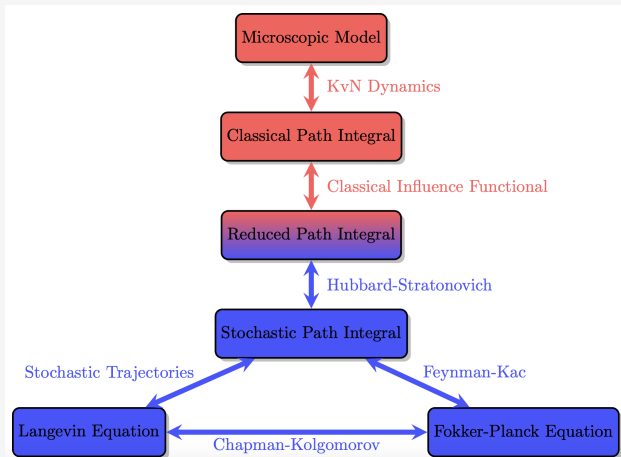
Propagator classical limit

$$\lim_{\hbar \rightarrow 0} \tilde{U}_{\text{eff}} = \int_{q_0, \dot{q}_0}^{q_f, \dot{q}_f} \mathcal{D}q(t) \delta [m\ddot{q}(t) + V'(q, t) - \eta_{\text{cl}}(t)] \exp \left(i \int_0^{t_f} dt q(t) \nu_{\text{cl}}(t) \right)$$

$$\langle \eta_{\text{cl}}(t) \nu_{\text{cl}}(t') \rangle_r = -2i\Theta(t - t') \frac{d\gamma(t - t')}{dt}$$

$\hbar \rightarrow 0$

Summing up



- Influence functionals are a useful technique in the analysis of physical systems.
- One application is in the derivation of exact classical and quantum stochastic equations.
- The formalism also helps to link classical results as the limit of their quantum equivalents.

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