New developments in numerical studies of quantum time-evolution based on the real-time path integral

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Johannes Gutenberg-Universität Mainz, Germany

Ref.)
[1] JN, Katsuta Sakai, Atis Yosprakob,
JHEP 09 (2023) 110, e-Print: 2307.11199 [hep-th]
[2] Chien-Yu Chou, JN, e-Print: 2407.17724 [gr-qc]
[3] JN, Hiromasa Watanabe, e-Print: 2408.16627 [quant-ph]

Two approaches to quantum time-evolution

1) Schrödinger equation

equivalent

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

Hamiltonian

2) Feynman path integral

$$\Psi(x_{\mathsf{f}}, t_{\mathsf{f}}) = \int \mathcal{D}x(t)\,\Psi(x(t_{\mathsf{i}}), t_{\mathsf{i}})\, e^{iS[x(t)]}$$

$$S = \int L\, dt$$

action

Lagrangian

advantageous for:

- applications to large numbers of d.o.f. (including QFT)
- extensions to QG (diffeomorphism) and matrix model (nonperturbative strings)
- possible applications of powerful Monte Carlo simulation (important sampling)

Progress in real-time path integral

- quantum mechanics :
$$\Psi(x_{\mathrm{f}}, t_{\mathrm{f}}) = \int_{x(t_{\mathrm{f}})=x_{\mathrm{f}}} \mathcal{D}x(t)\, \Psi(x(t_{\mathrm{i}}), t_{\mathrm{i}})\, e^{iS[x(t)]/\hbar}$$

- quantum gravity (“time” is one of the dynamical variables)
$$\Psi[h] = \int \mathcal{D}g_{\mu\nu}\, e^{iS[g]/\hbar}$$

- IKKT matrix model nonperturbative formulation of string theory
(“time” is an emergent concept)
$$Z = \int dA_\mu\, e^{iS[A]}$$

the oscillating behavior

conceptual problem : How to define the oscillating integral

➡ Picard-Lefschetz theory

technical problem : How to overcome the sign problem in MC sim.

➡ the generalized (Lefschetz) thimble method

(including the “Worldvolume approach” of Fukuma-Matsumoto (’20))

Plan of the talk

0. Introduction
1. Generalized thimble method and the Picard-Lefschetz theory
2. A new picture of quantum tunneling
3. Quantum tunneling at the beginning of the universe
4. Quantum decoherence from saddle points
5. Summary and discussions

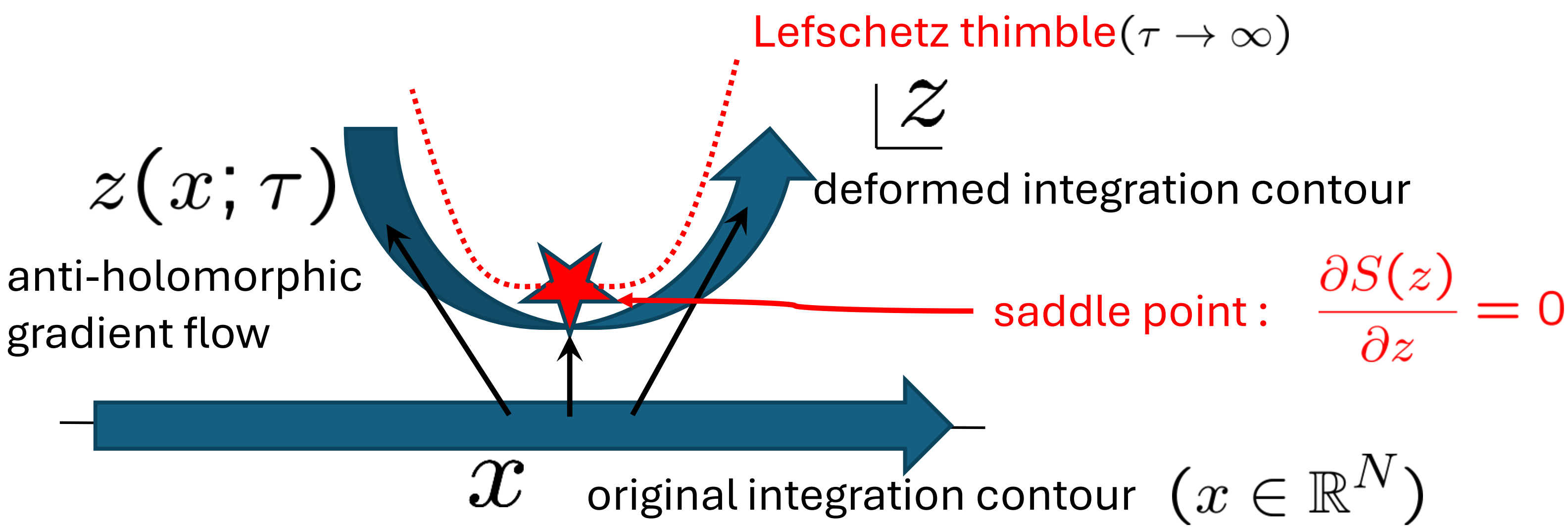
1. Generalized thimble method and the Picard-Lefschetz theory

The generalized thimble method

Fukuma's talk on Sept.??

Alexandru, Basar, Bedaque, Ridgway, Warrington, JHEP 1605 (2016) 053

$$Z = \int_{\mathbb{R}^N} dx\, e^{-S(x)} \qquad S(x) \in \mathbb{C}$$



Solve $\frac{\partial}{\partial \sigma} z_k(x;\sigma) = \overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$ from $\sigma = 0$ to $\sigma = \tau$

with the initial condition $z(x;0) = x \in \mathbb{R}^N$

➡ One obtains a one-to-one map from x to $z(x;\tau)$, which defines a contour deformation. (Cauchy's theorem)

An important property of the gradient flow

complex-valued!

$$\frac{d}{d\sigma}S(z(x;\sigma)) = \frac{\partial S(z(x;\sigma))}{\partial z_k}\frac{\partial z_k(x;\sigma)}{\partial \sigma}$$

$$= \frac{\partial S(z(x;\sigma))}{\partial z_k}\overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$$

$$= \left|\frac{\partial S(z(x;\sigma))}{\partial z_k}\right|^2$$

real positive !

anti-holomorphic gradient flow

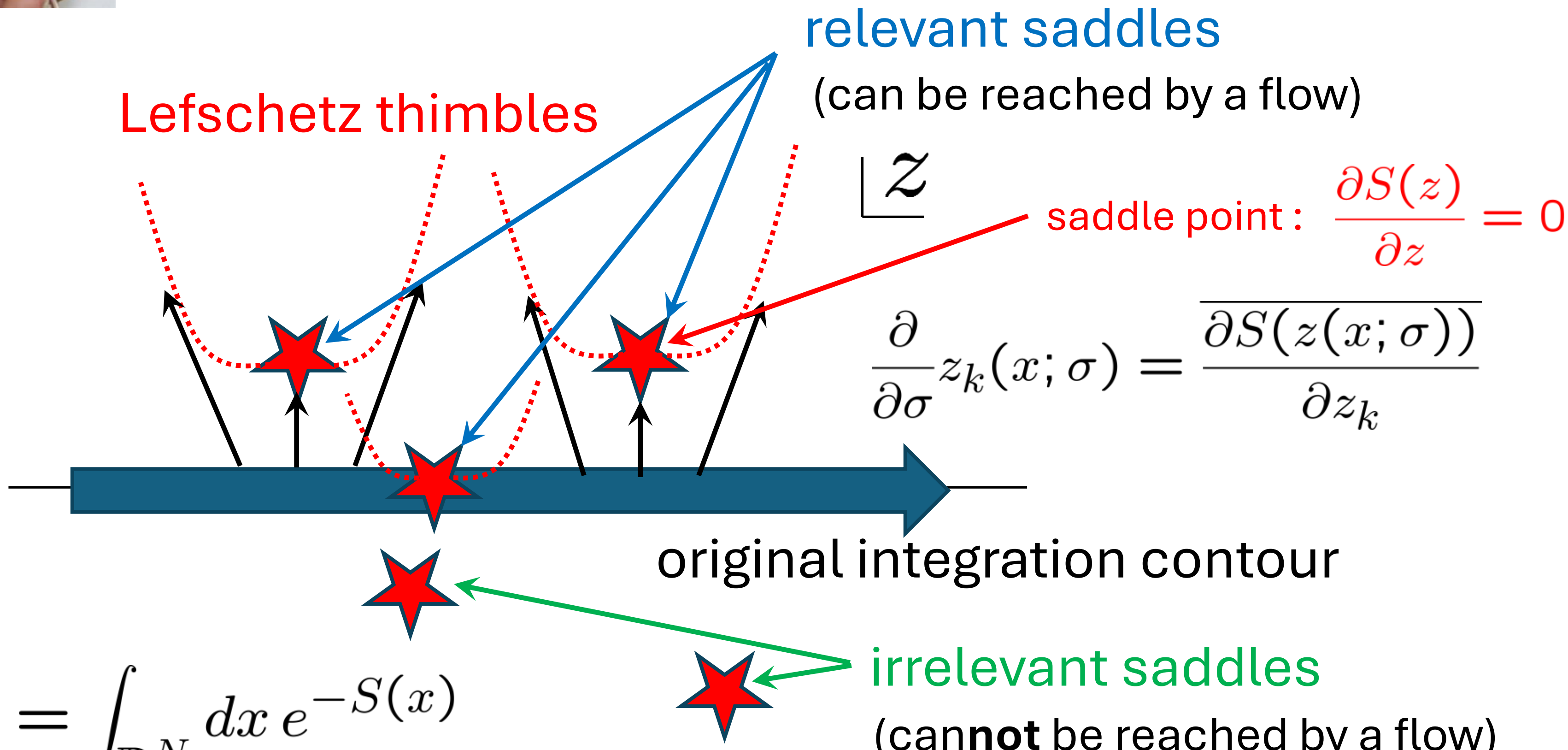
$$\frac{\partial}{\partial \sigma}z_k(x;\sigma) = \overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$$

Real part of the action increases along the flow,
while the imaginary part is kept constant.

The imaginary part tends to become constant
as the flow time increases. (Sign problem is solved !)

Picard-Lefschetz theory $(\tau \to \infty)$

multi-dimensional version of steepest descent method



$$Z = \int_{\mathbb{R}^N} dx\, e^{-S(x)}$$

An oscillating integral can be made well defined uniquely.
No ambiguity in the choice of integration contour.

2. A new picture of quantum tunneling

JN, Katsuta Sakai, Atis Yosprakob,
“A new picture of quantum tunneling in the real-time path integral
from Lefschetz thimble calculations”
JHEP 09 (2023) 110, e-Print: 2307.11199 [hep-th]

Time-evolution of the wave function

$$\Psi(x_\mathsf{f}, t_\mathsf{f}) = \int_{x(t_\mathsf{f}) = x_\mathsf{f}} \mathcal{D}x(t)\, \Psi(x(t_\mathsf{i}), t_\mathsf{i})\, e^{iS[x(t)]}$$

$$S[x(t)] = \int dt \left\{ \frac{1}{2} m \left(\frac{dx}{dt} \right)^2 - V(x) \right\}$$

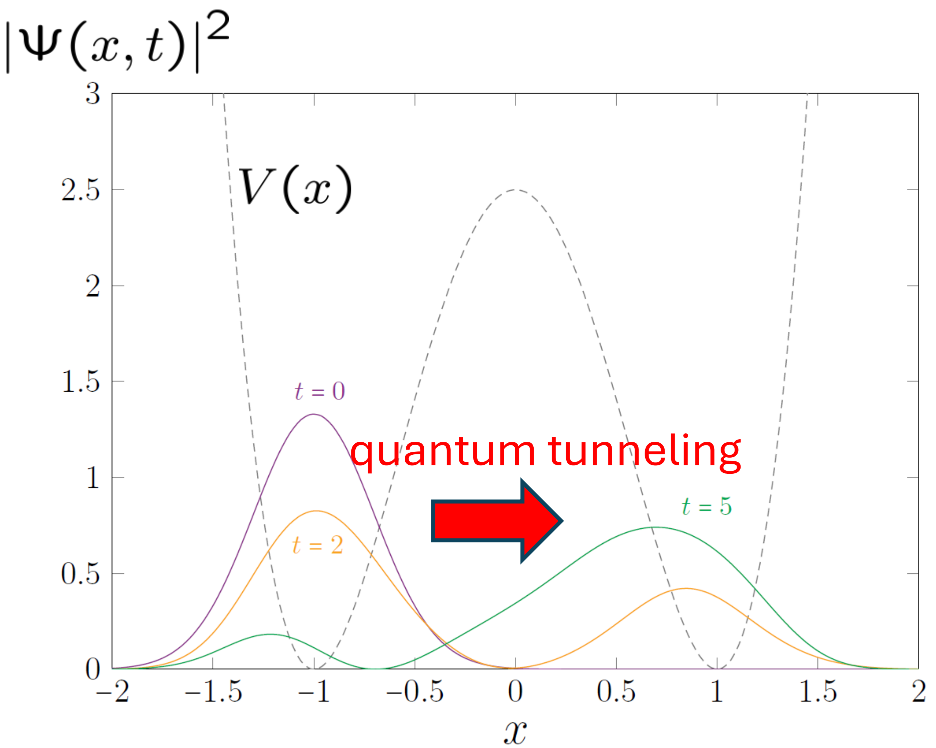
$$V(x) = \alpha(x^2 - 1)^2 \qquad \alpha = 2.5$$

$$\Psi(x, t_\mathsf{i}) = \exp\left\{ -\frac{1}{4\sigma^2} (x - b)^2 \right\}$$

$$\sigma = 0.3 \ , \quad b = -1$$

$$x_\mathsf{f} = 1$$

$$T \equiv t_\mathsf{f} - t_\mathsf{i} = 2$$

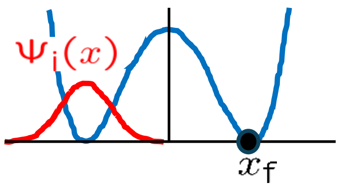


Discretize the time as:

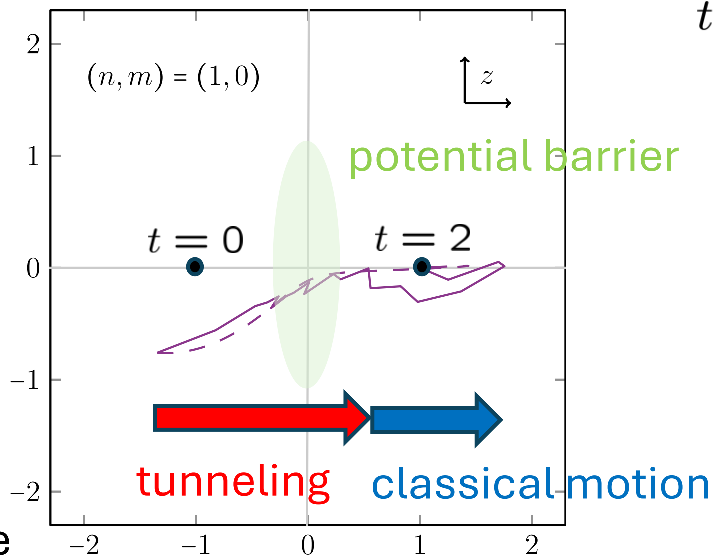
$$\begin{aligned} x_n &= x(t_n) \\ t_n &= \frac{n}{N} T \qquad (n = 0, \cdots, N) \end{aligned}$$

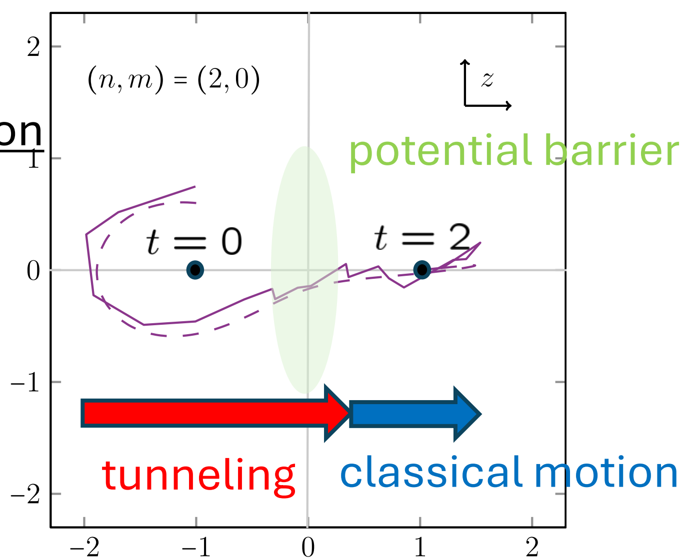
$$N = 20$$

Results of GTM (with flow time integration *a la* Fukuma-Matsumoto)



typical config $z(t)$ at large τ





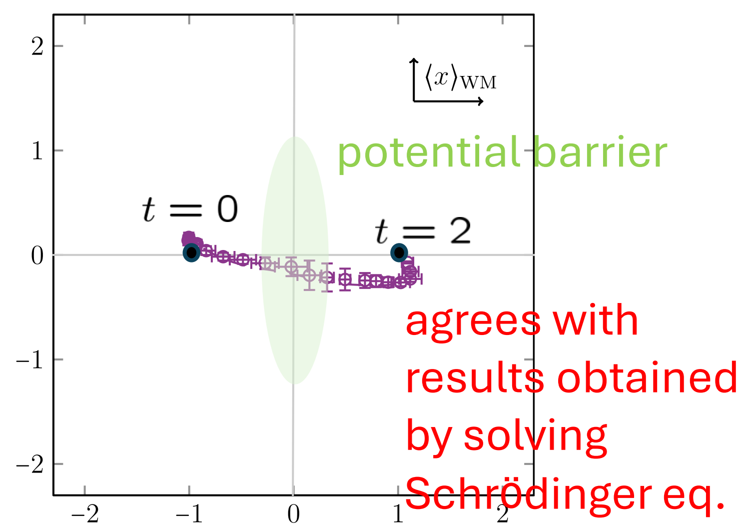
(Rem)
The dashed line represents the closest <u>complex solution</u> <u>of the EOM</u>.

Koike-Tanizaki ('14)

$N_\tau = 10$, $0.2 < \tau < 4$
$t_{\rm HMC} = 1.0$, $N_{\rm HMC} = 10$

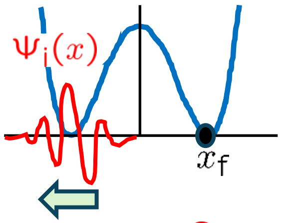
ensemble average
("weak value" of $x(t)$)

$$\frac{\langle x_{\rm f}|e^{-i\hat{H}(T-t)}\hat{x}e^{-i\hat{H}t}|\Psi_{\rm i}\rangle}{\langle x_{\rm f}|e^{-i\hat{H}(T-t)}e^{-i\hat{H}t}|\Psi_{\rm i}\rangle}$$



Quantum tunneling is represented by complex trajectories.

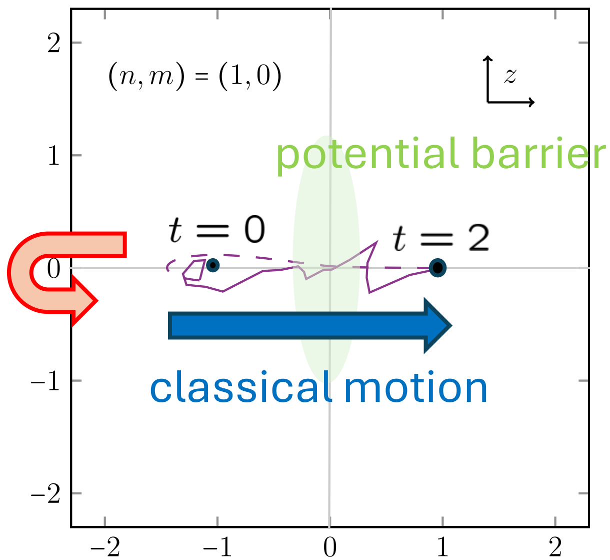
Introducing momentum in the initial state

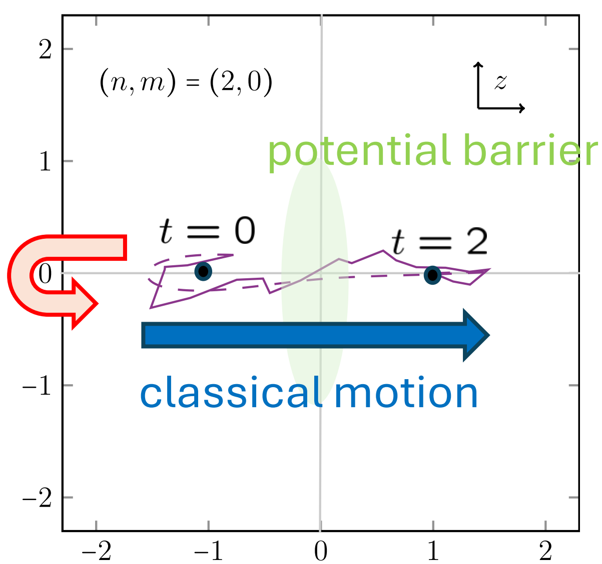


$p = -2$

initial momentum

typical config $z(t)$ at large τ





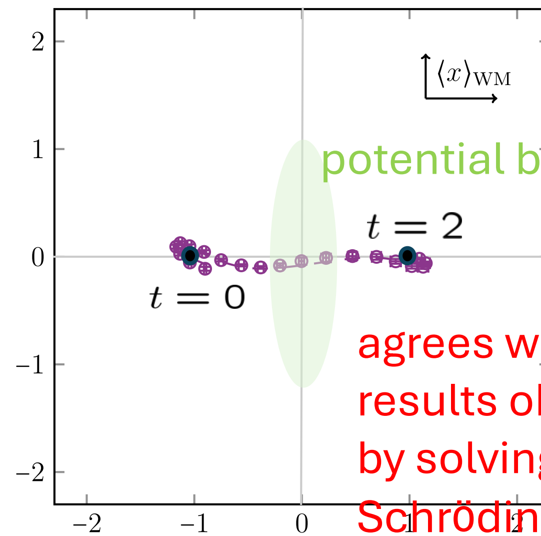
(Rem)
The dashed line represents the closest <u>complex solution of the EOM</u>.

Koike-Tanizaki ('14)

$$\Psi(x,t_{\rm i}) = \exp\left\{-\frac{1}{4\sigma^2}(x+1)^2 + i\,p\,x\right\}$$

$p = -2$

$$\left(\begin{array}{l}\text{ensemble average} \\ (\text{“weak value” of } x(t)) \\ \dfrac{\langle x_{\rm f}|e^{-i\hat{H}(T-t)}\hat{x}e^{-i\hat{H}t}|\Psi_{\rm i}\rangle}{\langle x_{\rm f}|e^{-i\hat{H}(T-t)}e^{-i\hat{H}t}|\Psi_{\rm i}\rangle}\end{array}\right)$$



agrees with results obtained by solving Schrödinger eq.

Classical motion over the barrier becomes dominant.
→ almost real trajectories

A new understanding of quantum tunneling

$$\Psi(x_\mathsf{f}, t_\mathsf{f}) = \int_{x(t_\mathsf{f})=x_\mathsf{f}} \mathcal{D}x(t)\, \Psi(x(t_\mathsf{i}), t_\mathsf{i})\, e^{iS[x(t)]/\hbar}$$

initial wave function $\Psi(x, t_\mathsf{i}) = \varphi(x)\, e^{ipx/\hbar}$

$\varphi(x)$ is assumed to have a finite support $\Delta \equiv [x_\mathsf{min}, x_\mathsf{max}]$

$\hbar \to 0$

Classical EOM

$$\frac{\delta S[x(t)]}{\delta x(t)} = 0$$

Boundary condition

$$x(t_\mathsf{i}) \in \Delta\,, \quad \dot{x}(t_\mathsf{i}) = \frac{p}{m}$$
$$x(t_\mathsf{f}) = x_\mathsf{f}$$

- If real $x(t)$ exists, it is a relevant & dominant saddle.

→ real trajectory
emergence of classical motion

- If real $x(t)$ does **not** exist, the relevant saddle with min. $\mathrm{Im}S(> 0)$ dominates.

$$|\text{prob. amplitude}| \sim e^{-\mathrm{Im}S[x^\star]/\hbar}$$

(instanton-like suppression)

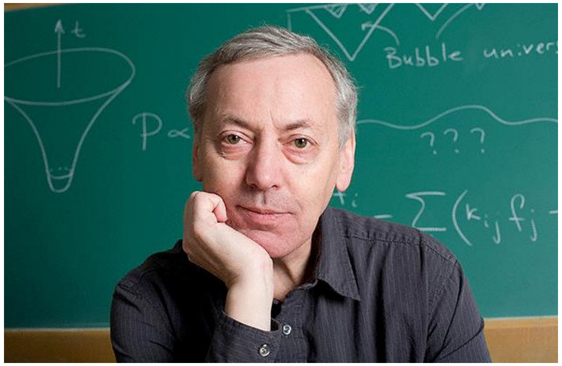
→ complex trajectory
semi-classical description of quantum tunneling

Can be observed by using the weak measurement

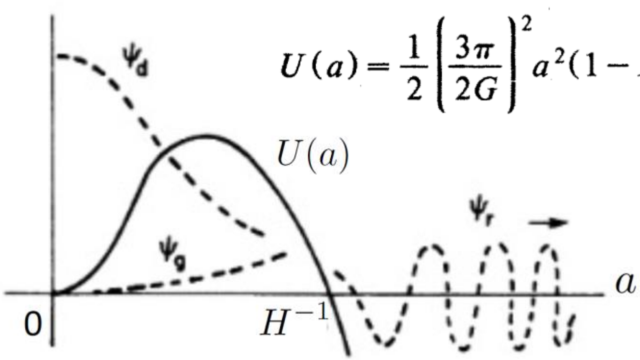
3. Quantum tunneling at the beginning of the universe

Chien-Yu Chou, JN,
"Monte Carlo studies of quantum cosmology by the generalized Lefschetz thimble method"
e-Print: 2407.17724 [gr-qc]

How did the Universe begin ?



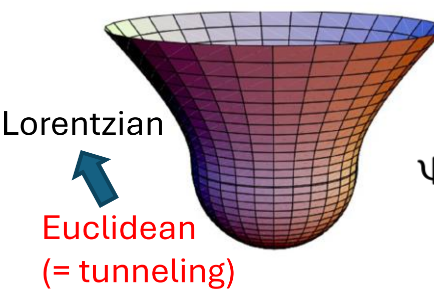
A. Vilenkin
“Creation of Universes from Nothing”
Phys.Lett.B 117 (1982) 25



$$U(a) = \frac{1}{2}\left(\frac{3\pi}{2G}\right)^2 a^2(1 - H^2a^2)$$

tunneling from nothing

J. B. Hartle and S. W. Hawking
“Wave function of the Universe”
Phys. Rev. D 28,(1983) 2960



$$\Psi[h] = \int \mathcal{D}g_{\mu\nu}\, e^{-S[g]/\hbar}$$

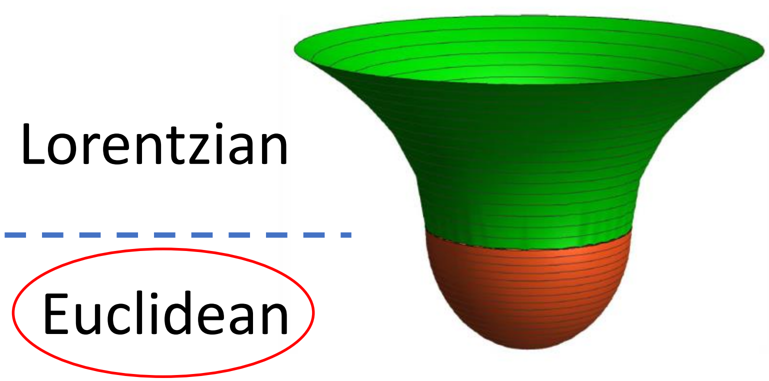
Path integral over
Euclidean geometry

no-boundary wavefunction

Quantum Cosmology

Issues in quantum cosmology

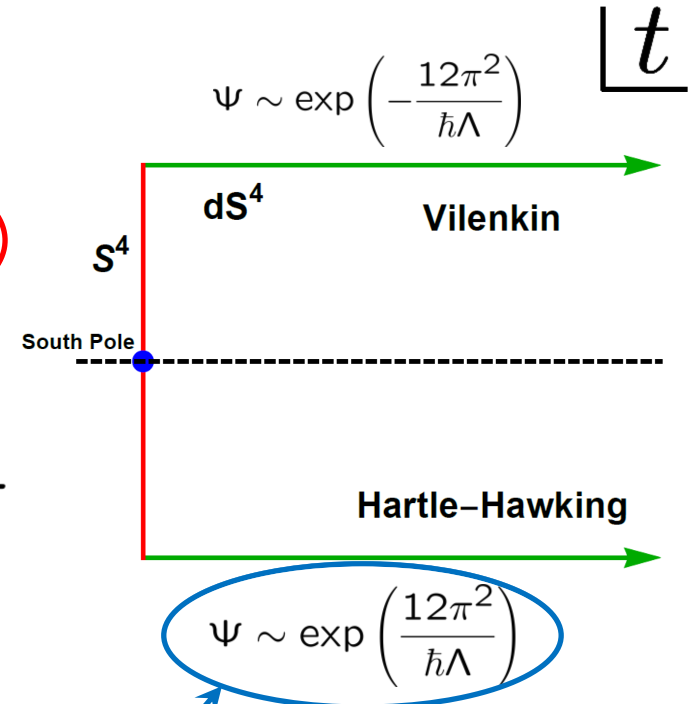
- Vilenkin's proposal seems to have **instability** in fluctuations due to the "wrong" Wick rotation.



tunneling at the beginning of the Universe

$$t = i\tau$$

$$t = -i\tau$$



- Hartle-Hawking's proposal seems to be **incompatible** with the inflation scenario since it favors $\Lambda = 0$.

- Which is the relevant saddle point ?

mini-superspace model

Halliwell-Louko, Phys.Rev.D 39 (1989) 2206

Assuming homogeneous, isotropic, closed space-time

$$ds^2 = a^2(\eta)(-N(\eta)^2 d\eta^2 + d\Omega_3{}^2)$$

η : conformal time

scale factor   lapse function

Einstein-Hilbert action

$$S_{\mathsf{EH}}[a, N] = 6\pi^2 \int d\eta \left\{ -\frac{1}{N} \left(\frac{da}{d\eta} \right)^2 + N V(a) \right\}$$

$$V(a) = a^2 - \frac{\Lambda}{3} a^4$$

change of variables: $\begin{cases} q = a^2 \\ d\eta = a^{-2}(t) dt \end{cases}$

$$ds^2 = -\frac{N^2}{q(t)} dt^2 + q(t)\, d\Omega_3{}^2$$

$N = \text{const.}$ (reparam. inv.)

$$S_{\mathsf{EH}}[q, N] = 6\pi^2 \int_0^1 dt \left\{ -\frac{1}{4N} \left(\frac{dq}{dt} \right)^2 + N \left(1 - \frac{\Lambda}{3} q \right) \right\}$$

$q(t)$ can be integrated out by the Gaussian integral

Integration over N has ambiguity in the choice of contour.

Picard-Lefschetz theory → Vilenkin's saddle becomes relevant.

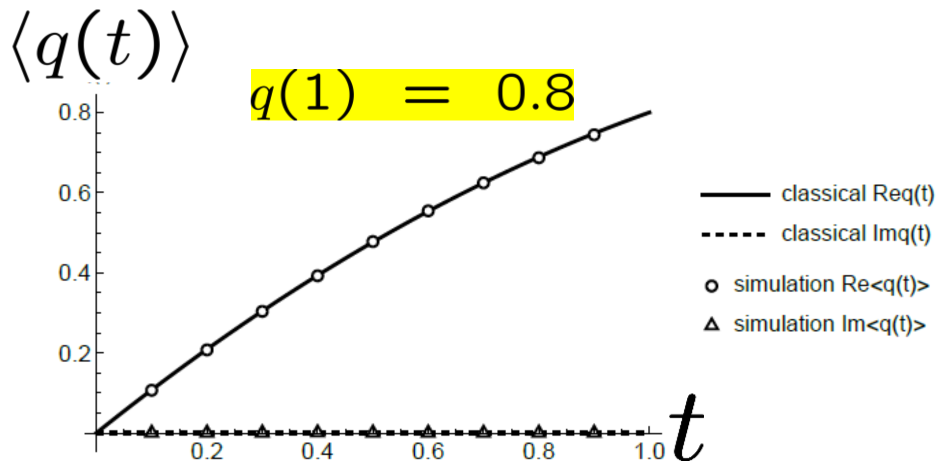
Feldbrugge-Lehners-Turok, Phys.Rev.D 95 (2017) 10, 103508, 1703.02076 [hep-th]

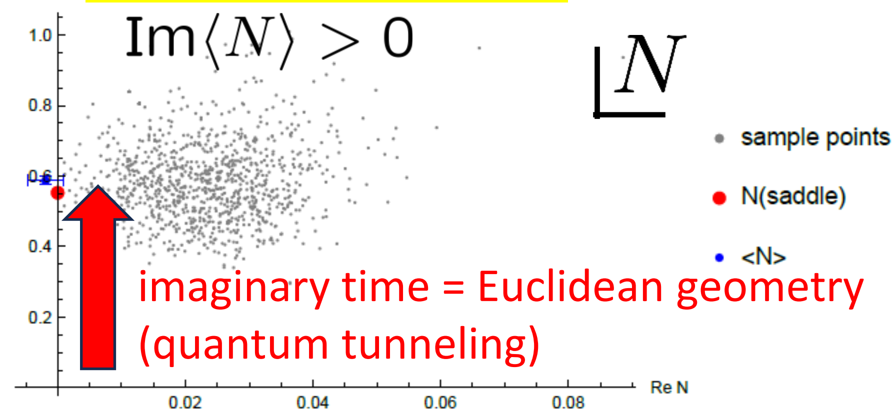
Simulating quantum cosmology

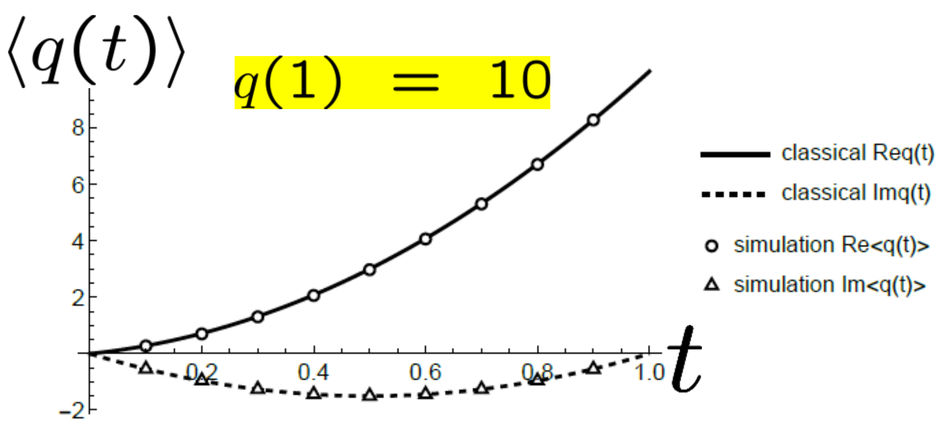
$q(0) = 0$ "no boundary" condition
$\Lambda = 3$

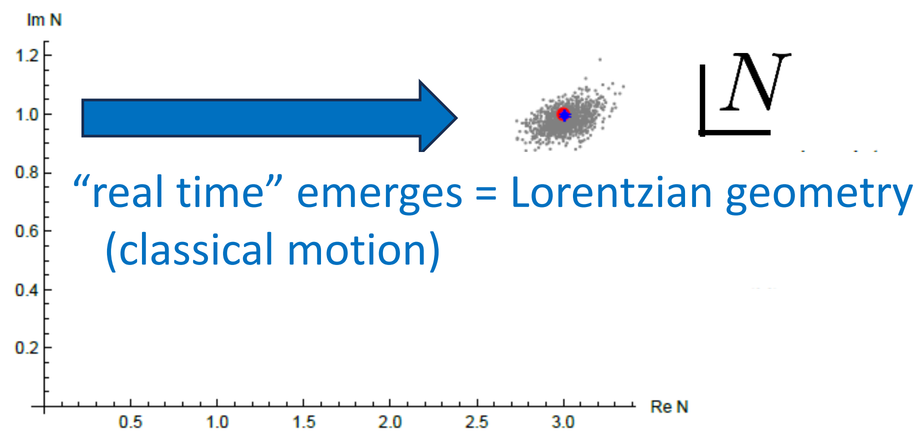
Chou-JN, 2407.17724 [gr-qc]

Vilenkin's saddle point becomes relevant.









Next step : Add tensor modes and investigate the instability issue.

4. Quantum decoherence from saddle points

JN, Hiromasa Watanabe, “Quantum decoherence from saddle points”
e-Print: 2408.16627 [quant-ph]

Couple the system to an environment

$$L \;=\; L_{\mathcal{S}} + L_{\mathcal{E}} + L_{\text{int}}$$

Caldeira-Leggett ('83)

$$L_{\mathcal{S}} = \frac{1}{2} M \dot{x}(t)^2 - \frac{1}{2} M \omega_{\mathrm{b}}^2 x(t)^2 \ ,$$

$$L_{\mathcal{E}} = \sum_{k=1}^{N_{\mathcal{E}}} \left\{ \frac{1}{2} m\, \dot{q}^k(t)^2 - \frac{1}{2} m\, \omega_k^2\, q^k(t)^2 \right\} \ ,$$

$$L_{\text{int}} = c\ x(t) \sum_{k=1}^{N_{\mathcal{E}}} q^k(t) \ ,$$

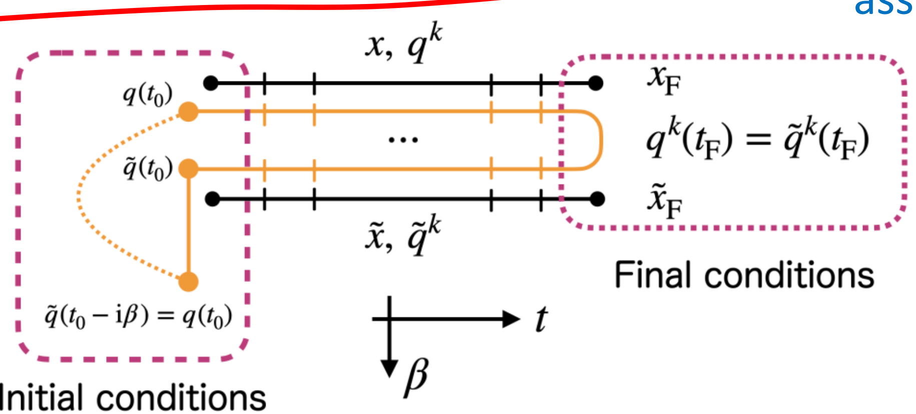
reduced density matrix after tracing out the environment

$$\rho_{\mathcal{S}}(x_{\mathsf{F}}, \tilde{x}_{\mathsf{F}}; t_{\mathsf{F}}) = \int \mathcal{D}x \mathcal{D}\tilde{x} \prod_{k=1}^{N_{\mathcal{E}}} \mathcal{D}q^k \mathcal{D}\tilde{q}^k \mathcal{D}\tilde{q}_0^k \, \mathrm{e}^{-S_{\text{eff}}(x, \tilde{x}, q, \tilde{q}, \tilde{q}_0)} \ ,$$

$$S_{\text{eff}}(x, \tilde{x}, q, \tilde{q}, \tilde{q}_0) = -\mathrm{i} \left\{ S(x, q) - S(\tilde{x}, \tilde{q}) \right\} + S_0(\tilde{q}_0) + \frac{1}{4\sigma^2}(x_0^2 + \tilde{x}_0^2)$$

Gaussian initial state assumed for the system

Environment initially in thermal equilibrium with temperature $1/\beta$



Tracing out environment $\mathcal{E}$

Exact results from saddle points

JN, Hiromasa Watanabe, e-Print: 2408.16627 [quant-ph]

Introducing $X_\mu = \{x_i, \tilde{x}_i, q_i^k, \tilde{q}_i^k, (\tilde{q}_0^k)_j\}$

$$S_{\text{eff}}(x, \tilde{x}, q, \tilde{q}, \tilde{q}_0) = \frac{1}{2} X_\mu \mathcal{M}_{\mu\nu} X_\nu - C_\mu X_\mu + B$$

saddle point: $\bar{X}_\mu = \left(\mathcal{M}^{-1}\right)_{\mu\nu} C_\nu$

$$X_\mu = \bar{X}_\mu + Y_\mu$$

Integrating Y_μ,

$$\rho_S(x_{\text{F}}, \tilde{x}_{\text{F}}; t_{\text{F}}) = \frac{1}{\sqrt{\det \mathcal{M}}} \text{e}^{-\mathcal{A}} ,$$

$$\mathcal{A} = B - \frac{1}{2} C_\mu \left(\mathcal{M}^{-1}\right)_{\mu\nu} C_\nu$$

Quantum decoherence is captured by complex saddle points.
(analogous to what we have found for quantum tunneling)

Disappearance of interference pattern

γ : coupling with environment
β : inverse temperature

JN, Hiromasa Watanabe, in preparation

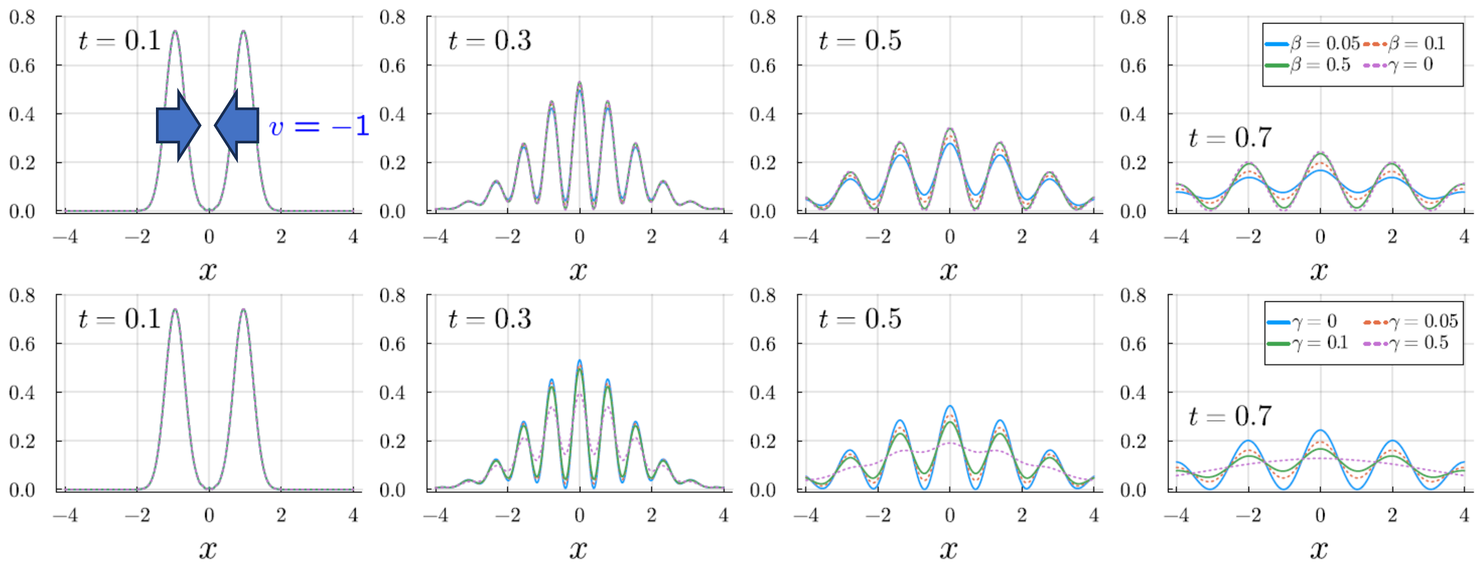
$(N_{\mathcal{E}} = 64,\ \omega_{\mathrm{cut}} = 2.0,\ \omega_{\mathrm{r}} = 0,\ \sigma = 0.1)$

$\rho_S(x, x; t)$

$t = 0$ $\quad t = 0.3$ $\quad t = 0.5$ $\quad t = 0.7$

$\beta = 0.5,\ 0.1,\ 0.05$
$(\gamma = 0.1)$

$\gamma = 0.05,\ 0.1,\ 0.5$
$(\beta = 0.05)$



Master eq. (with Born and Markov approximations)

$$\frac{d}{dt}\rho_S(x, \tilde{x}; t) = K(x, \tilde{x})\rho_S(x, \tilde{x}, t)\ , \qquad (\omega_{\mathrm{r}} \ll \omega_{\mathrm{cut}} \ll T = \beta^{-1})$$

$$K(x, \tilde{x}) = \frac{\mathrm{i}}{2M}\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial \tilde{x}^2}\right) - \frac{\mathrm{i}}{2}M\omega_{\mathrm{r}}^2(x^2 - \tilde{x}^2) - \gamma(x - \tilde{x})\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial \tilde{x}}\right) - \frac{2M\gamma}{\beta}(x - \tilde{x})^2$$

The effect of decoherence is $\propto \frac{\gamma}{\beta}$

Quantum decoherence is captured by complex saddles in the real-time path integral.

5. Summary and discussions

Summary

- Quantum time-evolution includes many interesting physics.
  - quantum tunneling
  - beginning of the Universe
  - quantum decoherence

- Real-time path integral : very useful in studying these things.
  - Oscillating integral can be dealt with by the Picard-Lefschetz theory.
  - These phenomena can be captured by relevant (complex) saddle points.
  - Monte Carlo simulation is possible by using the generalized thimble method.

- Various applications are waiting for us!
  - Quantum-to-classical transition (How does the classical world emerge?)
  - Measurement problems (Schrödinger's cat)
  - Instability problem of the Vilenkin's saddle (smooth beginning of the Universe)
  - Matrix model (emergence of (3+1)-expanding Universe from superstring theory)
  - Quantum chaos (and its relation to blackholes through holography)
  - Quantum information (and its relation to AdS/CFT) etc.