Monte Carlo studies of quantum time-evolution based on the real-time path integral

Workshop “High Energy Physics in the Quantum Era”

KEK Theory Center, Tsukuba, Japan

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

Progress in real-time path integral

- quantum mechanics :

$$\Psi(x_f, t_f) = \int_{x(t_f)=x_f} \mathcal{D}x(t)\, \Psi(x(t_i), t_i)\, e^{iS[x(t)]/\hbar}$$

- 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.

⇨ Lefschetz thimble method

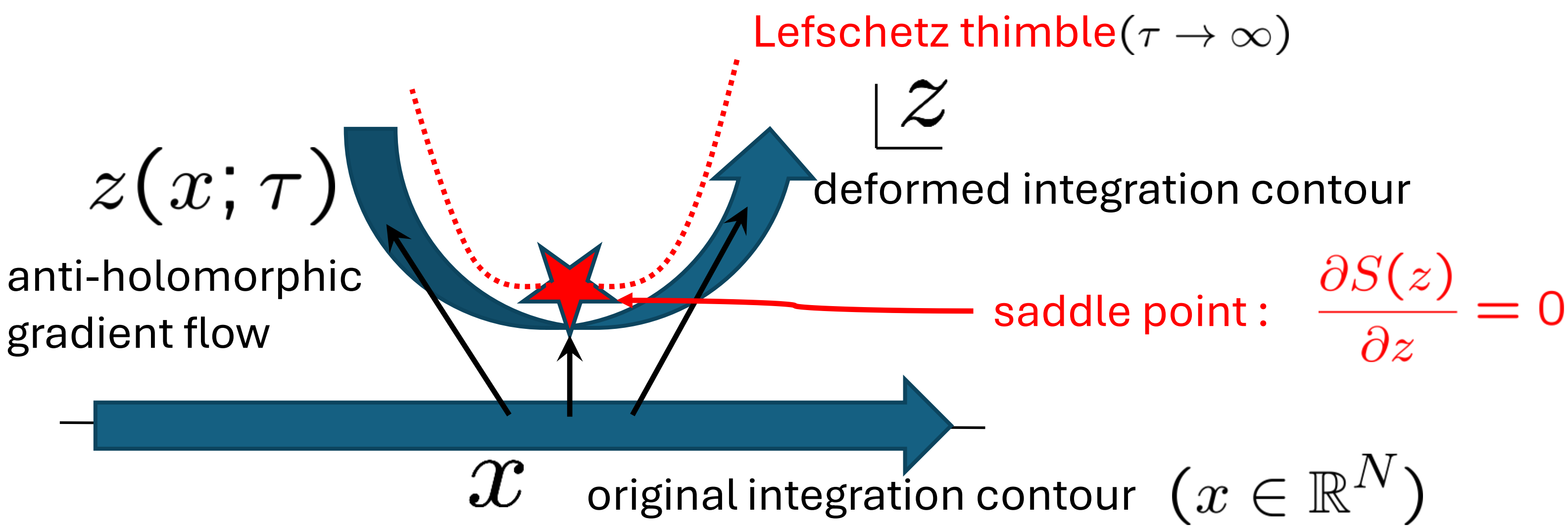
Plan of the talk

1. Lefschetz thimble method and the Picard-Lefschetz theory

Lefschetz thimble method

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

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



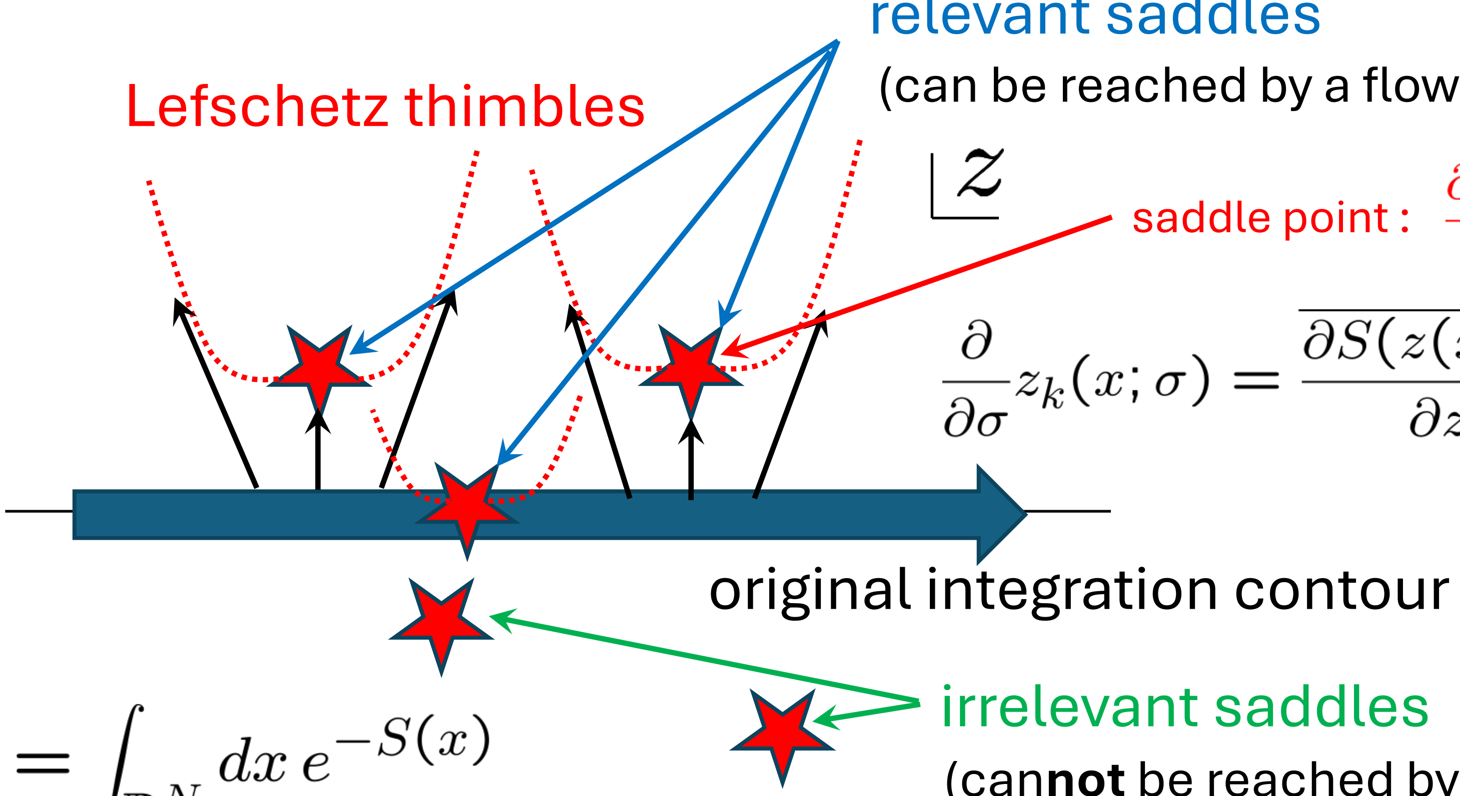
Solve $\frac{\partial}{\partial \sigma} z_k(x;\sigma) = \overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$ from $\sigma = 0$ to $\sigma = \tau$

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)

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

multi-dimensional version of steepest descent method



saddle point : $\dfrac{\partial S(z)}{\partial z} = 0$

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

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

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, arXiv: 2307.11199 [hep-th]

Time-evolution of the wave function

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

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

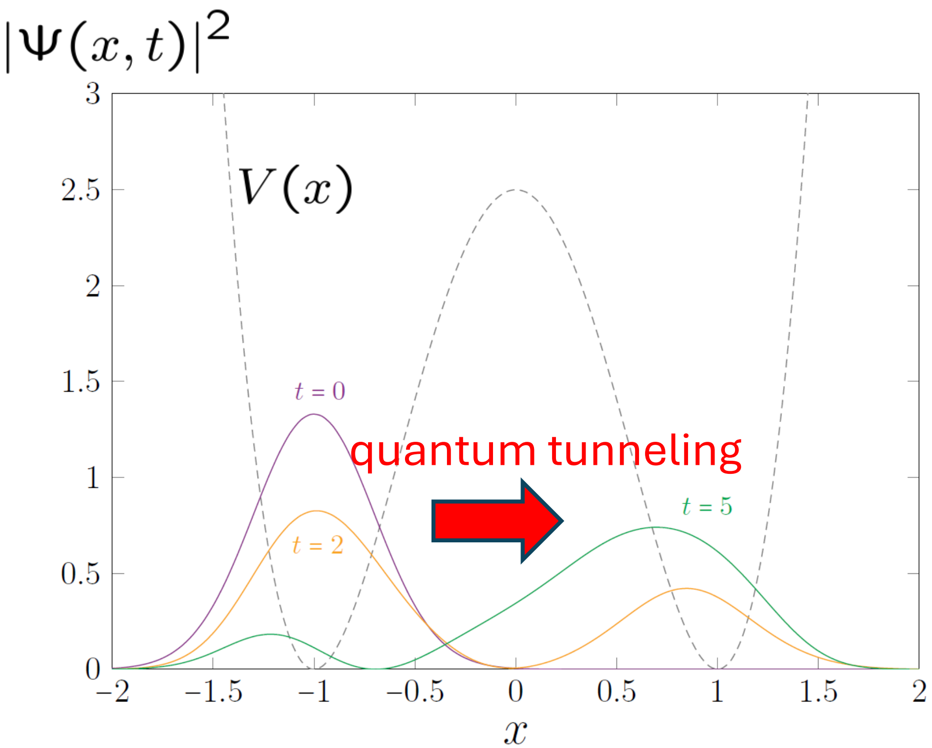
$$V(x) = \alpha (x^2 - 1)^2 \qquad \alpha = 2.5$$

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

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

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

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



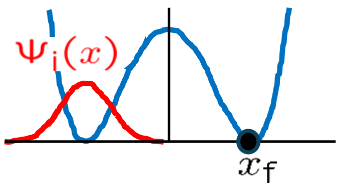
Discretize the time as:

$$x_n = x(t_n)$$

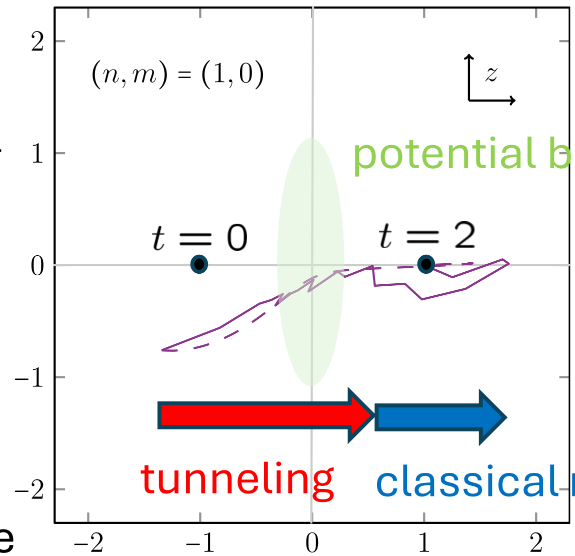
$$t_n = \frac{n}{N} T \qquad (n = 0, \cdots, N)$$

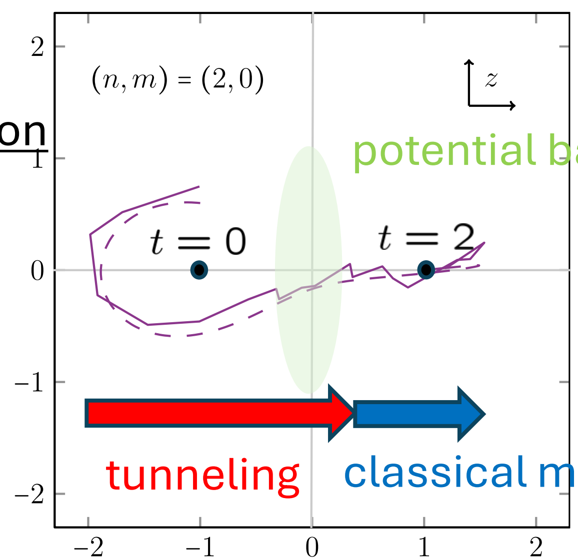
$$N = 20$$

Results of Lefschetz thimble method



typical config $z(t)$ at large τ





(Rem)
The dashed line represents the closest complex solution of the EOM.

↑

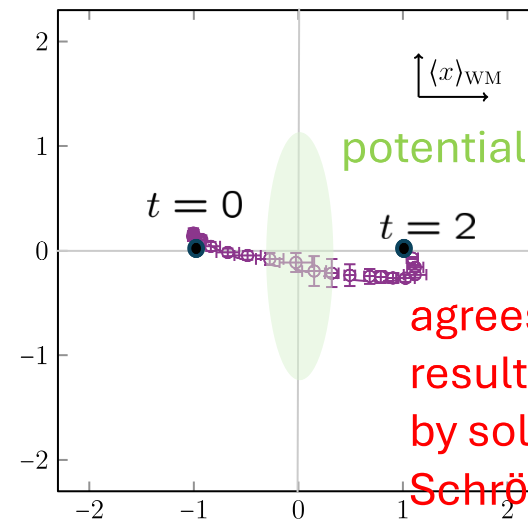
Koike-Tanizaki ('14)

$N_\tau = 10$, $0.2 < \tau < 4$

$t_{\mathrm{HMC}} = 1.0$, $N_{\mathrm{HMC}} = 10$

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

$$\frac{\langle x_f | e^{-i\hat{H}(T-t)} \hat{x} e^{-i\hat{H}t} | \Psi_i \rangle}{\langle x_f | e^{-i\hat{H}(T-t)} e^{-i\hat{H}t} | \Psi_i \rangle}$$



agrees with results obtained by solving Schrödinger eq.

Quantum tunneling is represented by complex trajectories.

A new understanding of quantum tunneling

$$\Psi(x_f, t_f) = \int_{x(t_f)=x_f} \mathcal{D}x(t)\, \Psi(x(t_i), t_i)\, e^{iS[x(t)]/\hbar}$$

initial wave function $\quad \Psi(x, t_i) = \varphi(x)\, e^{ipx/\hbar}$

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

$\hbar \to 0$

Classical EOM

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

Boundary condition

$$x(t_i) \in \Delta\,, \quad \dot{x}(t_i) = \frac{p}{m}$$
$$x(t_f) = x_f$$

- 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

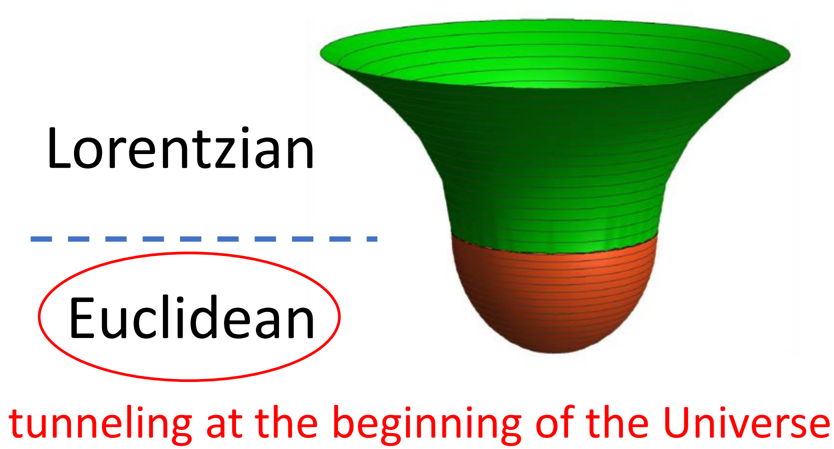
Can be observed by using the weak measurement

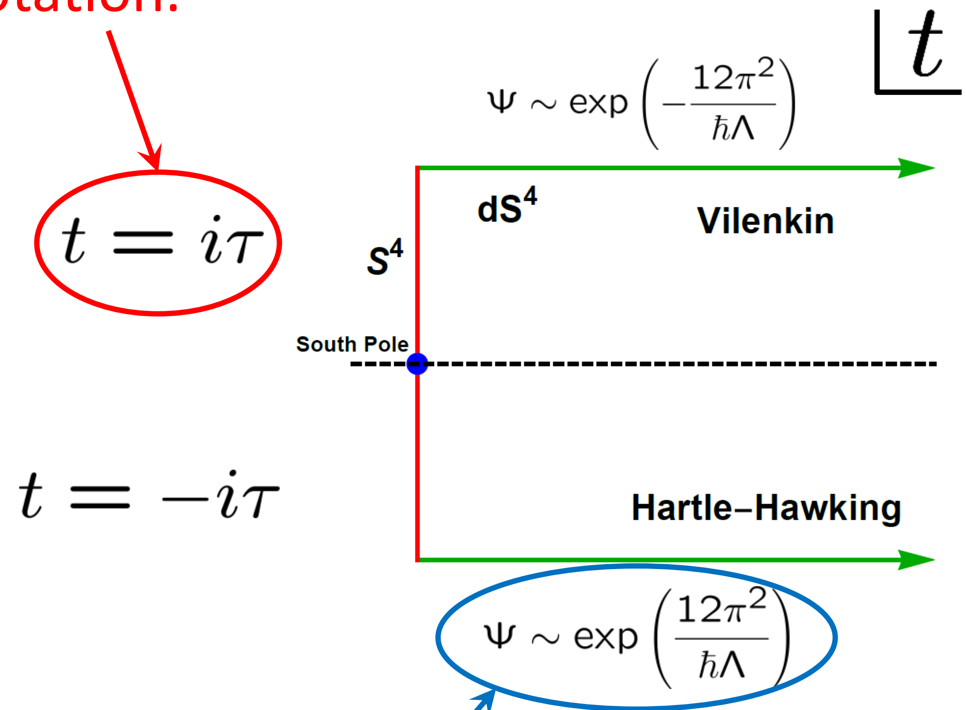
3. Quantum tunneling at the beginning of the universe

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

Issues in quantum cosmology

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





- 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

$$ds^2 = a^2(\eta)(-N(\eta)^2 d\eta^2 + d\Omega_3{}^2) \qquad \eta : \text{conformal time}$$

scale factor lapse function

Einstein-Hilbert action

$$S_{\mathrm{EH}}[a, N] = 6\pi^2 \int d\eta \left\{ -\frac{1}{N}\left(\frac{da}{d\eta}\right)^2 + NV(a) \right\} \qquad V(a) = a^2 - \frac{\Lambda}{3}a^4$$

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

$$ds^2 = -\frac{N^2}{q(t)}dt^2 + q(t)\, d\Omega_3{}^2 \qquad N = \text{const.} \quad (\text{reparam. inv.})$$

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

$q(t)$ 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]

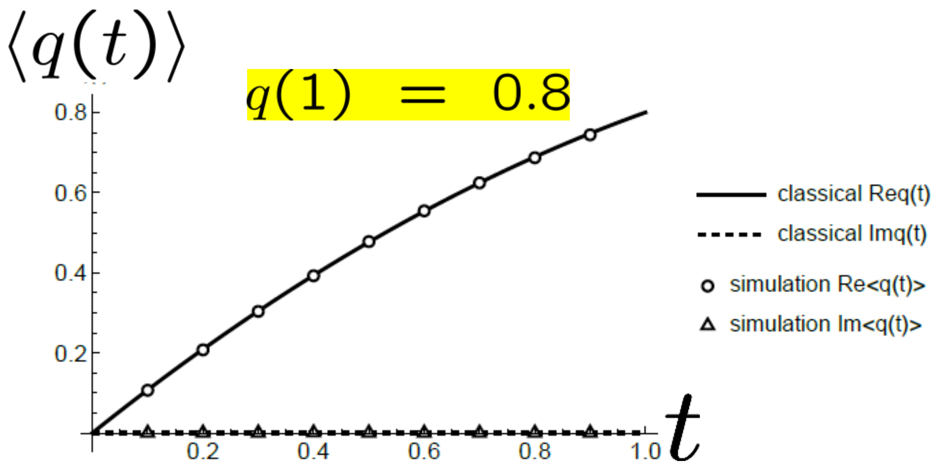
Simulating quantum cosmology

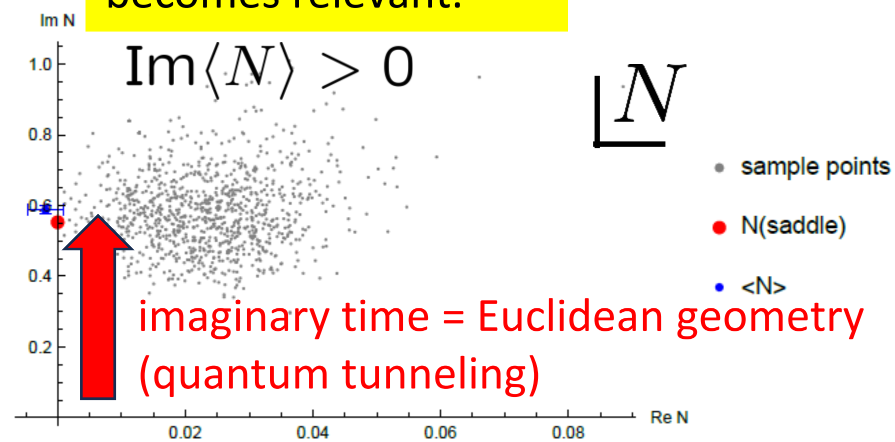
$q(0) = 0$ "no boundary" condition

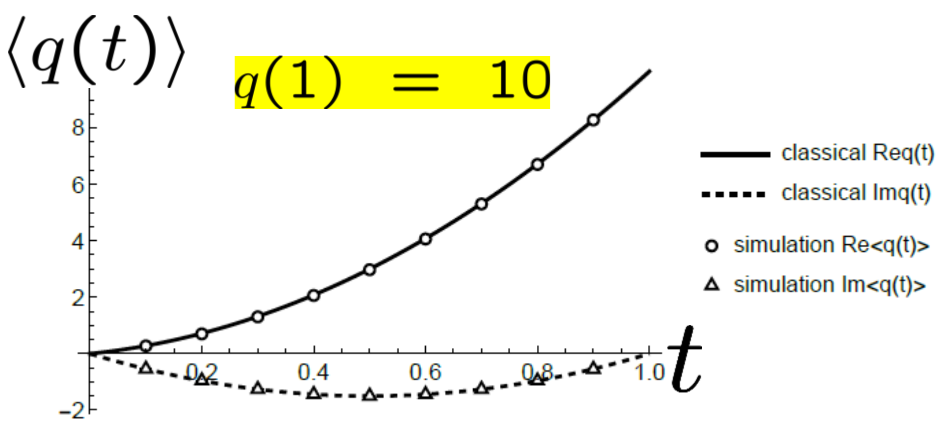
$\Lambda = 3$

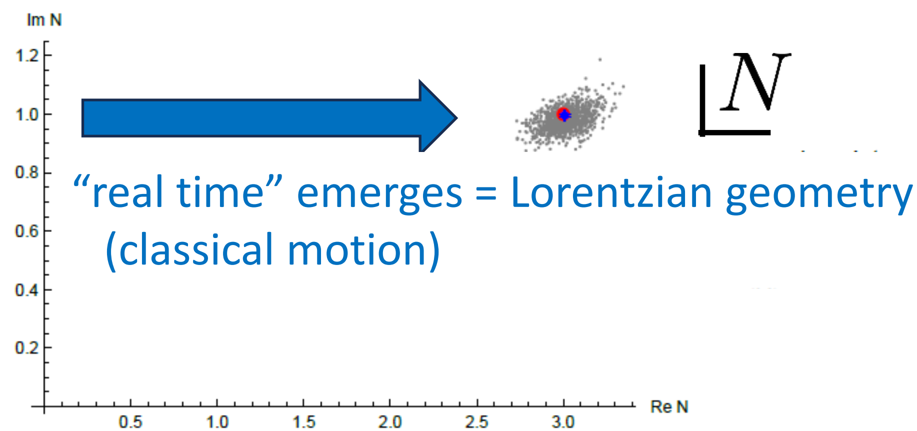
Chou-JN, 2407.17724 [gr-qc]

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”
arXiv: 2408.16627 [quant-ph]

Couple the system to an environment

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

Caldeira-Leggett ('83)

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

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

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

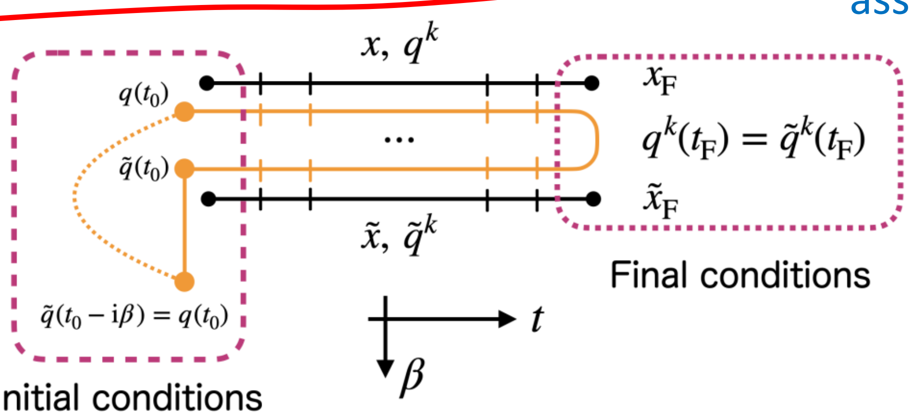
reduced density matrix after tracing out the environment

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

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

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, arXiv: 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,

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

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

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

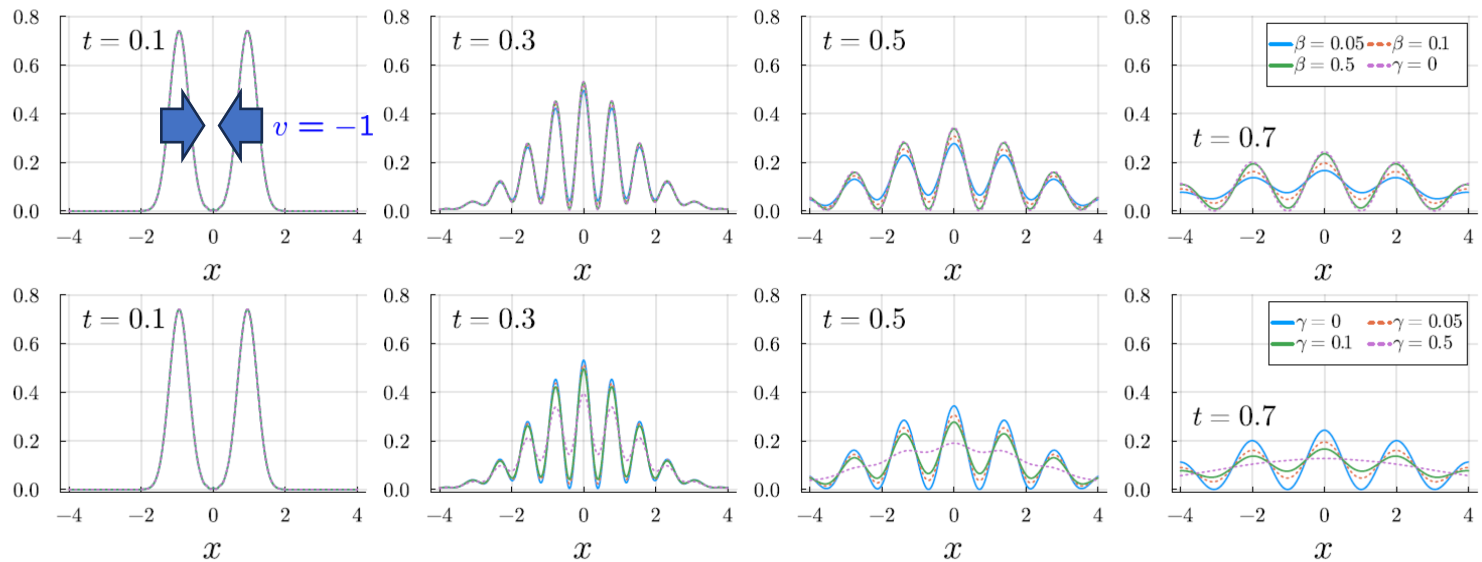
$(N_{\mathcal{E}} = 64,\ \omega_{\rm cut} = 2.0,\ \omega_{\rm r} = 0,\ \sigma = 0.1)$

$\rho_S(x, x; t)$

$t = 0$ $t = 0.3$ $t = 0.5$ $t = 0.7$

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

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



Master eq. (with Born and Markov approximations)

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

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

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 Lefschetz thimble method.

- Various applications are waiting for us!
  - Measurement problems (Schrödinger's cat)
  - Instability problem of Vilenkin's saddle (smooth beginning of the Universe)
  - Matrix model (emergence of (3+1)D spacetime from superstring theory)
  - Quantum chaos (calculations of out-of-time-order correlators)
  - Quantum information (and its relation to AdS/CFT) etc.