Thimble simulations of real-time quantum tunneling

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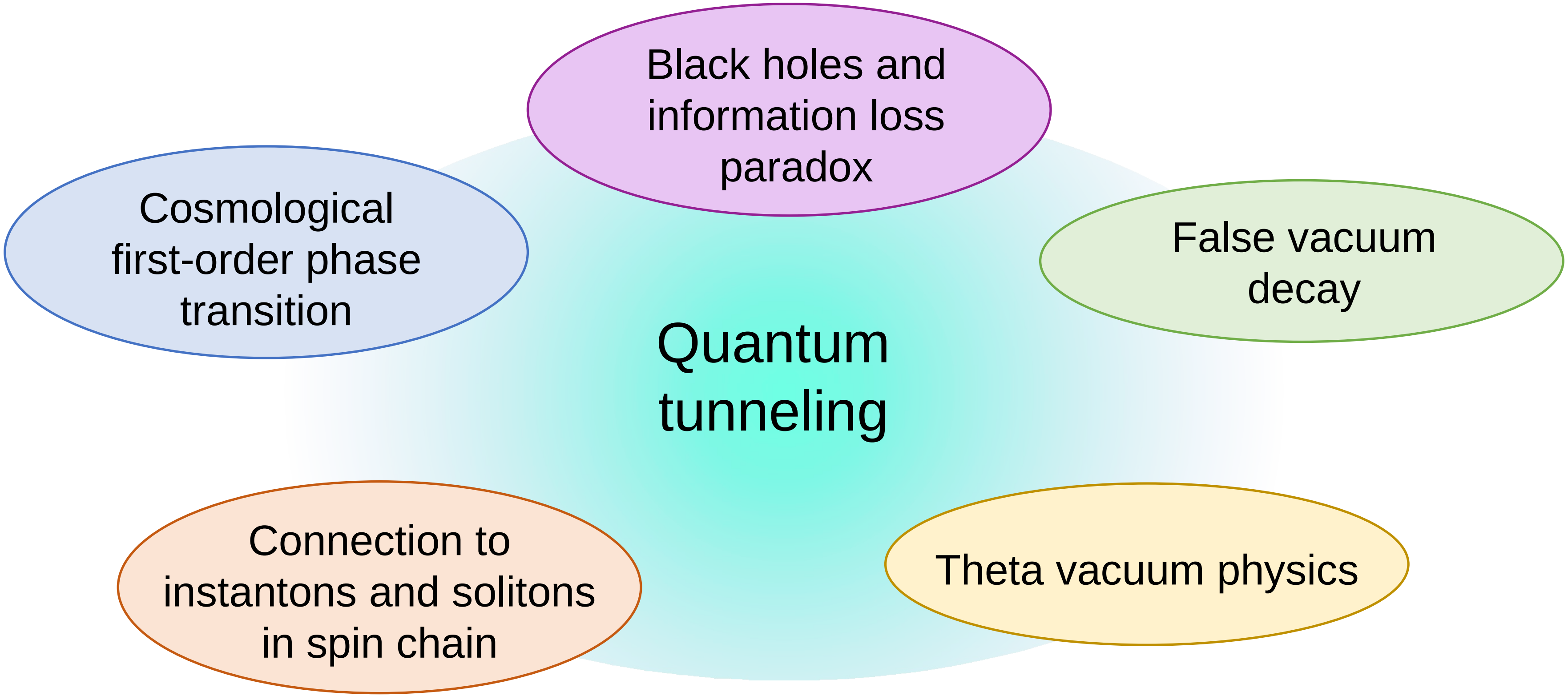
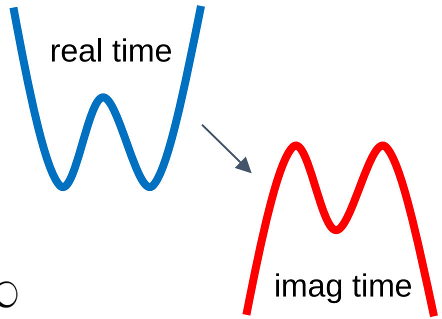
Quantum tunneling is an important concept that appears in many topics of theoretical physics.



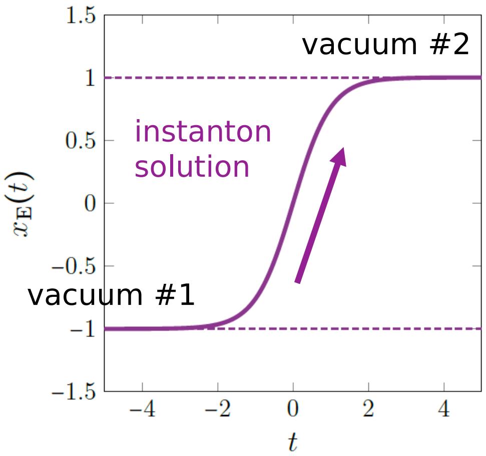
Tunneling amplitude computation

It is standard to compute tunneling amplitude via imaginary-time formalism (Coleman'77)



1. Use imaginary time $t = -i\tau$ (= flip the potential)
2. Send (imaginary) time interval to infinity $-\infty < \tau < \infty$
3. Amplitude can be approximated via the saddle points (instantons)

$$\Gamma \sim \sum_n \exp(-S_{\text{instantons}})$$



Although calculated in imaginary time, this gives the real-time amplitude!

Imaginary-time vs Real-time

Imaginary-time formalism is a convenient tool.
But it prevents us from studying time evolution!

→ real-time formalism is essential

On the other hand, real-time partition function is a highly-oscillating integral…

$$G(x_1, x_2; t) = \int_{x(0)=x_1}^{x(t)=x_2} Dx \; e^{iS_{\mathrm{QM}}[x]/\hbar}$$

This complex phase prevents us from performing a Monte Carlo simulation → sign problem

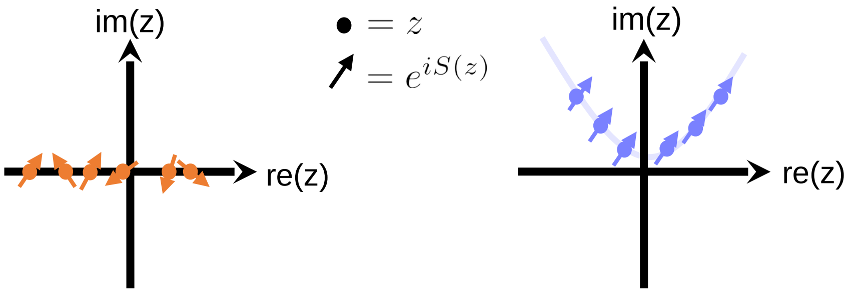
a very serious problem that occurs in various subjects in theoretical physics
(e.g., finite density QCD, supersymmetry, theta term, etc.)

The Lefschetz thimble method

Highly-oscillating integral can be made non-oscillating via contour deformation

$$G(x_1, x_2; t) = \int_{x(0)=x_1}^{x(t)=x_2} Dx(t)\ e^{iS[x]} \underset{\text{Cauchy's theorem}}{=} \int_{z(0)=x_1}^{z(T)=x_2} Dz(t)\ e^{iS[z]}$$

z → complex path



Original integral suffers from the sign problem.

This is resolved on the deformed contour.

the deformed path is defined via the gradient flow

$$z(\sigma) : x \in \mathbb{R}^N \longrightarrow z \in \mathcal{M}$$

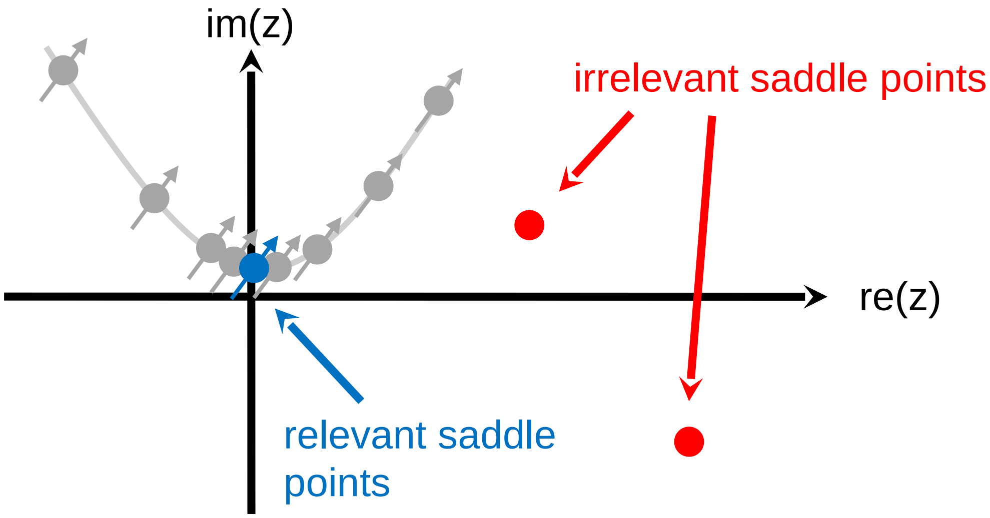
$$\frac{dz}{d\sigma} = \overline{\frac{\partial S(z)}{\partial z}}; \quad z(0) = x$$

$$\sigma : \text{ flow time}$$

Significance of saddle points

Integration along the deformed path ≈ fluctuations around saddle points.

But not all saddle points are relevant!



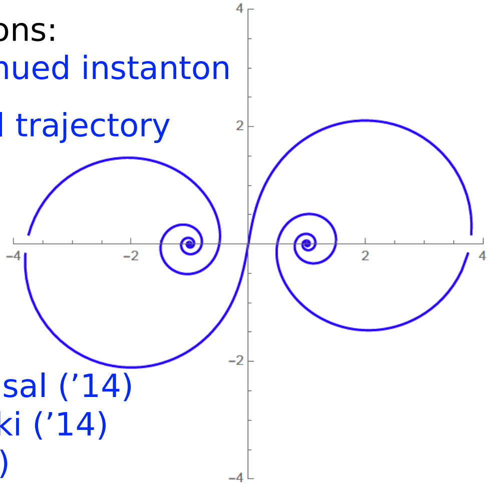
difficult question:

Which saddle points are relevant for real-time quantum tunneling?

Previous discussions:

analytically continued instanton

= complex spiral trajectory



- Cherman-Unsal ('14)
- Koike-Tanizaki ('14)
- Ai et al. ('19)

Monte Carlo simulation

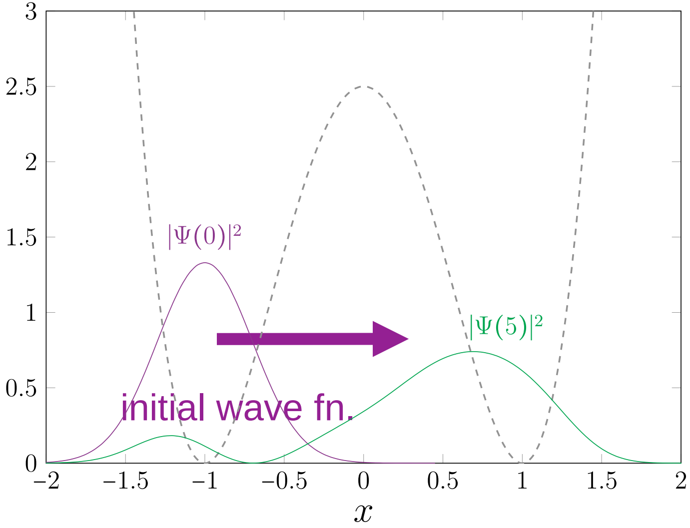
This puzzle can be answered explicitly using the Monte Carlo methods.
perform the sampling dynamically

Previously, the simulation is known to suffer from various problems.
But they are all resolved in recent developments.

- ergodicity problem at large flow time
  → worldvolume formulation (Fukuma-Matsumoto; ’21)
- high computational cost for calculating ‘force’ in the HMC methods
  → backpropagating Monte Carlo (Fujisawa-Nishimura-Sakai-A.Y.; ’22)
- divergence problem near the saddles
  → optimized flow equation (Nishimura-Sakai-A.Y; to be published)

The setups

We compute the tunneling of the initial Gaussian wave fn. through the barrier.



$$V(x) = \frac{\lambda}{2}(x^2 - 1)^2$$

calculated observables:
weakly-measured trajectory

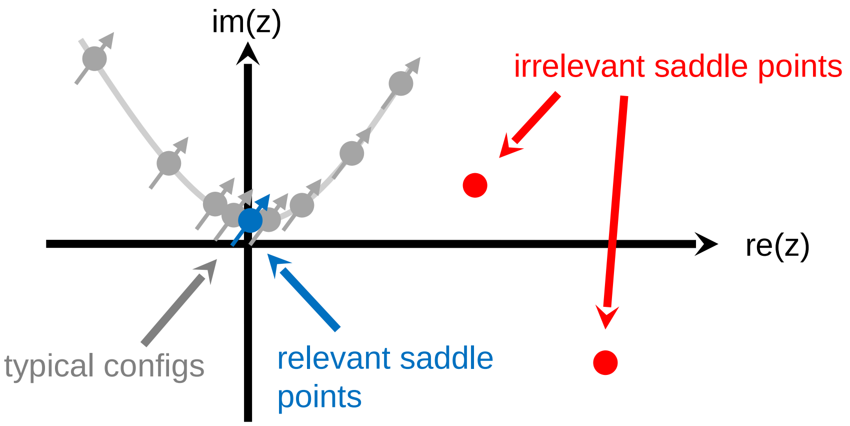
state-operator definition:

$$\langle x(t) \rangle_{\mathrm{WM}} = \frac{\langle x_{\mathrm{f}} | e^{-iH(T-t)} \hat{x}(t) e^{-iHt} | \Psi_0 \rangle}{\langle x_{\mathrm{f}} | e^{-iHT} | \Psi_0 \rangle}$$

path-integral definition:

$$\langle x(t) \rangle_{\mathrm{WM}} = \frac{1}{Z} \int Dx(t') x(t) e^{-iS[x(t')]} \Psi_0(x(0))$$

Observing the saddle points

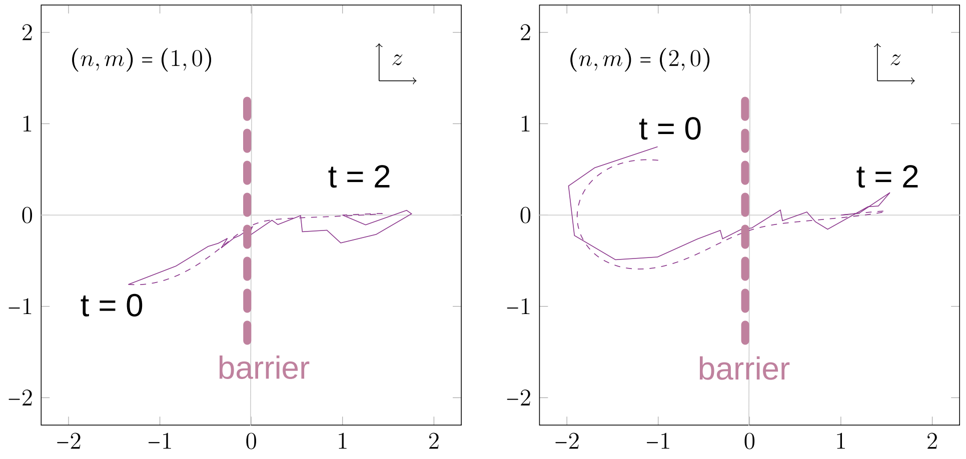


Saddle points can be observed by looking at typical trajectories at large flow time.

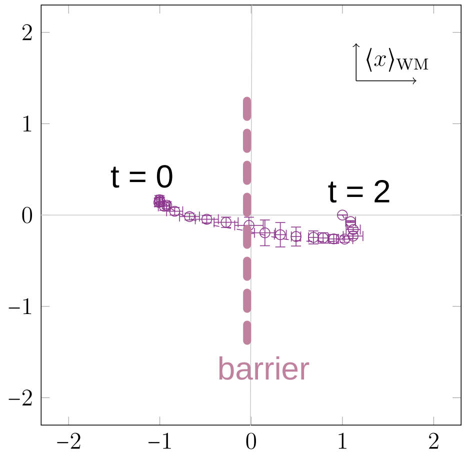
One of a few examples where individual configurations are physically meaningful!

Highlighted results: Quantum tunneling

Complex saddle points are observed!



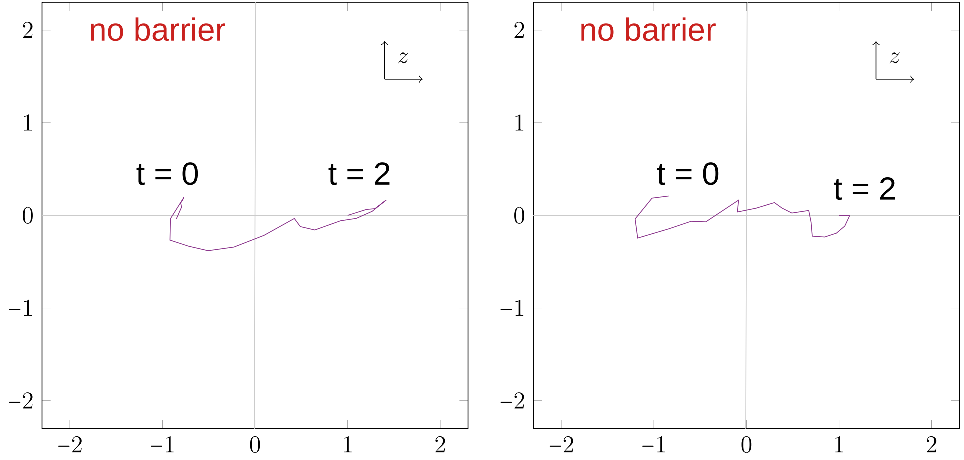
typical trajectories in the complex plane
(dashed line = classical soln.)



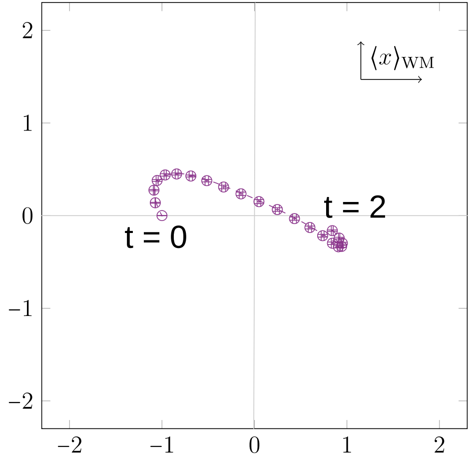
Weak values in agreement
with solving Schrodinger eq.

Highlighted results: No tunneling

Complex saddles disappear when the barrier is removed.

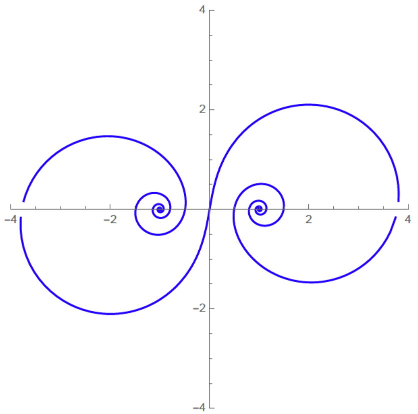


Typical trajectories under
The quartic action ($V(x) = x^4$)

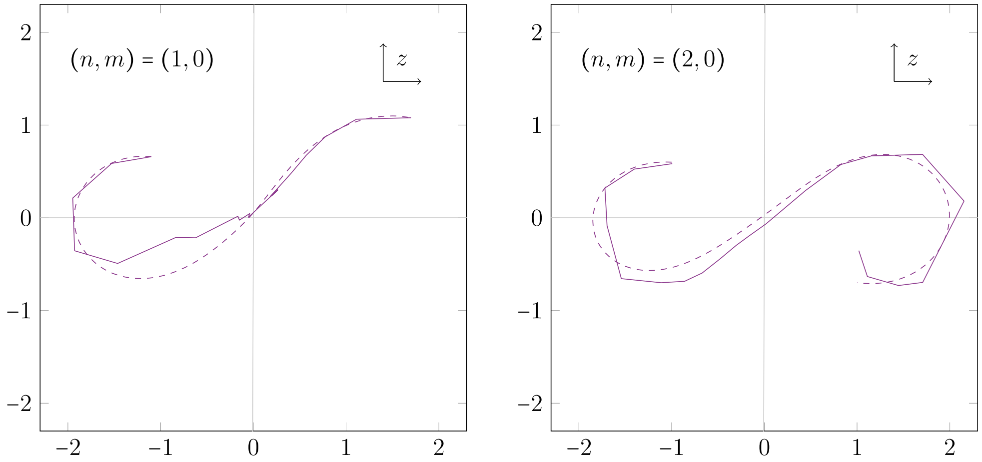


Weak values in agreement
with solving Schrodinger eq.

Highlighted results: complex instanton?



complexified instanton (infinite T)



our simulation at $T = 2$
(having wave fn. On both ends)

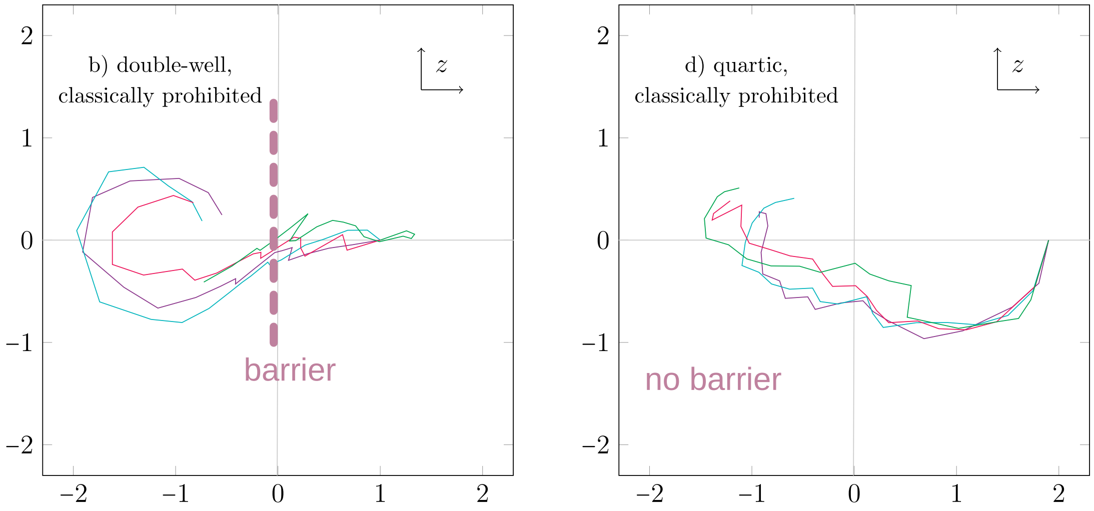
Our result supports the hypothesis that complexified
instanton is a saddle point for quantum tunneling at infinite T

Highlighted results: classical limit

Computation with hbar = 0.5

We find that complex saddle points appear for any classically prohibited processes.

Even if there is no potential barrier!



Quantum tunneling is not specific to the double-well systems.

Summary and discussions

- To get detailed information of the dynamics, it is important to consider quantum tunneling in real time.

- The real-time path integral can be made convergent via the Lefschetz thimble method.

- We perform the Monte Carlo simulation and successfully identified the relevant saddle points.
    - Complex saddle points are shown to be responsible for quantum tunneling.

- The thimble method is a powerful tool for studying real-time dynamics.