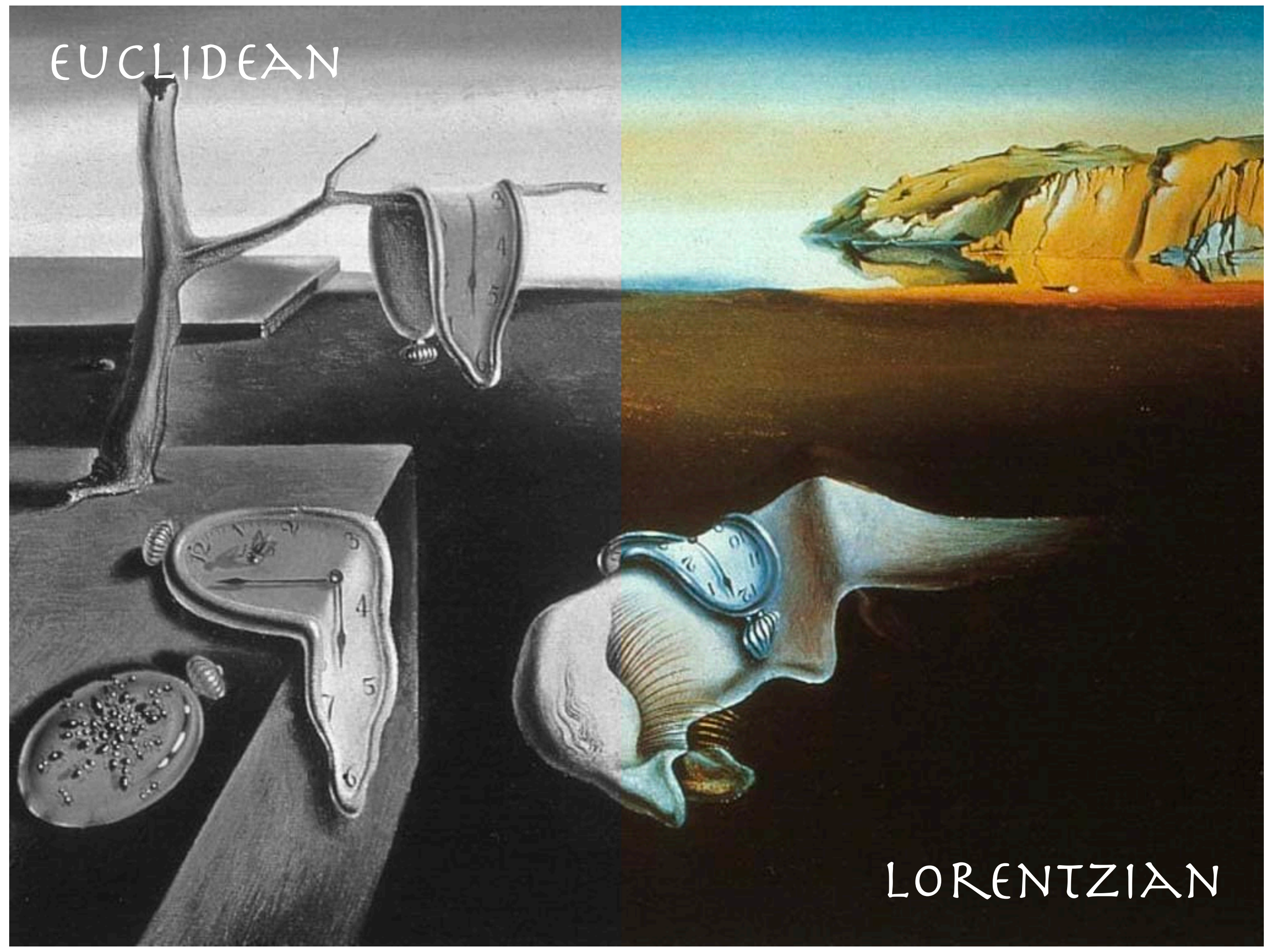
THE HEBREW UNIVERSITY OF JERUSALEM

מכון רקח
The Racah Institute
לפיסיקה
of Physics



Polychronic Tunneling

Yutaro Shoji

The Hebrew University of Jerusalem

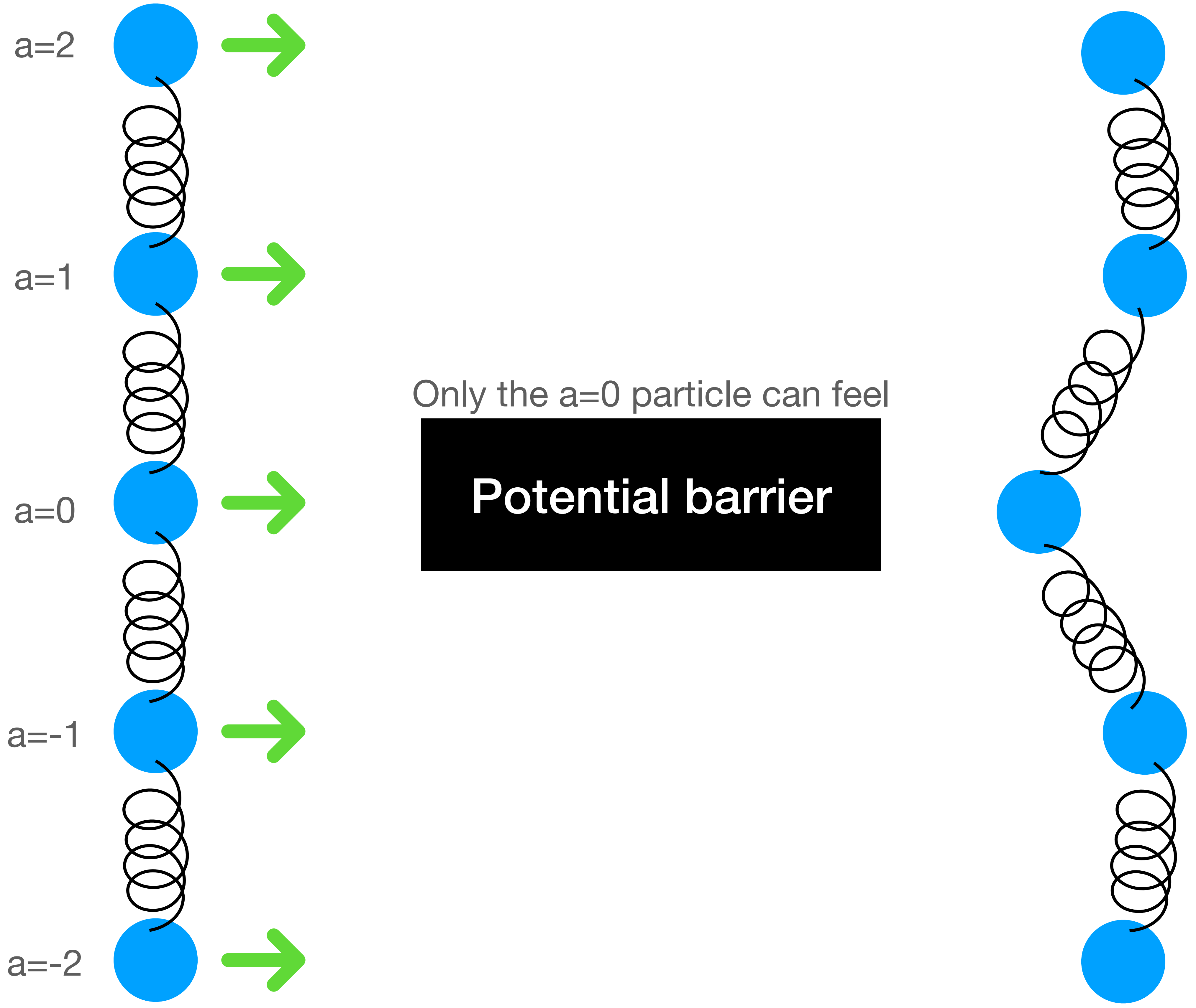
N. Oshita, YS, M. Yamaguchi, PRD 107 (2023) 4

YS, 2212.06774 [hep-th]

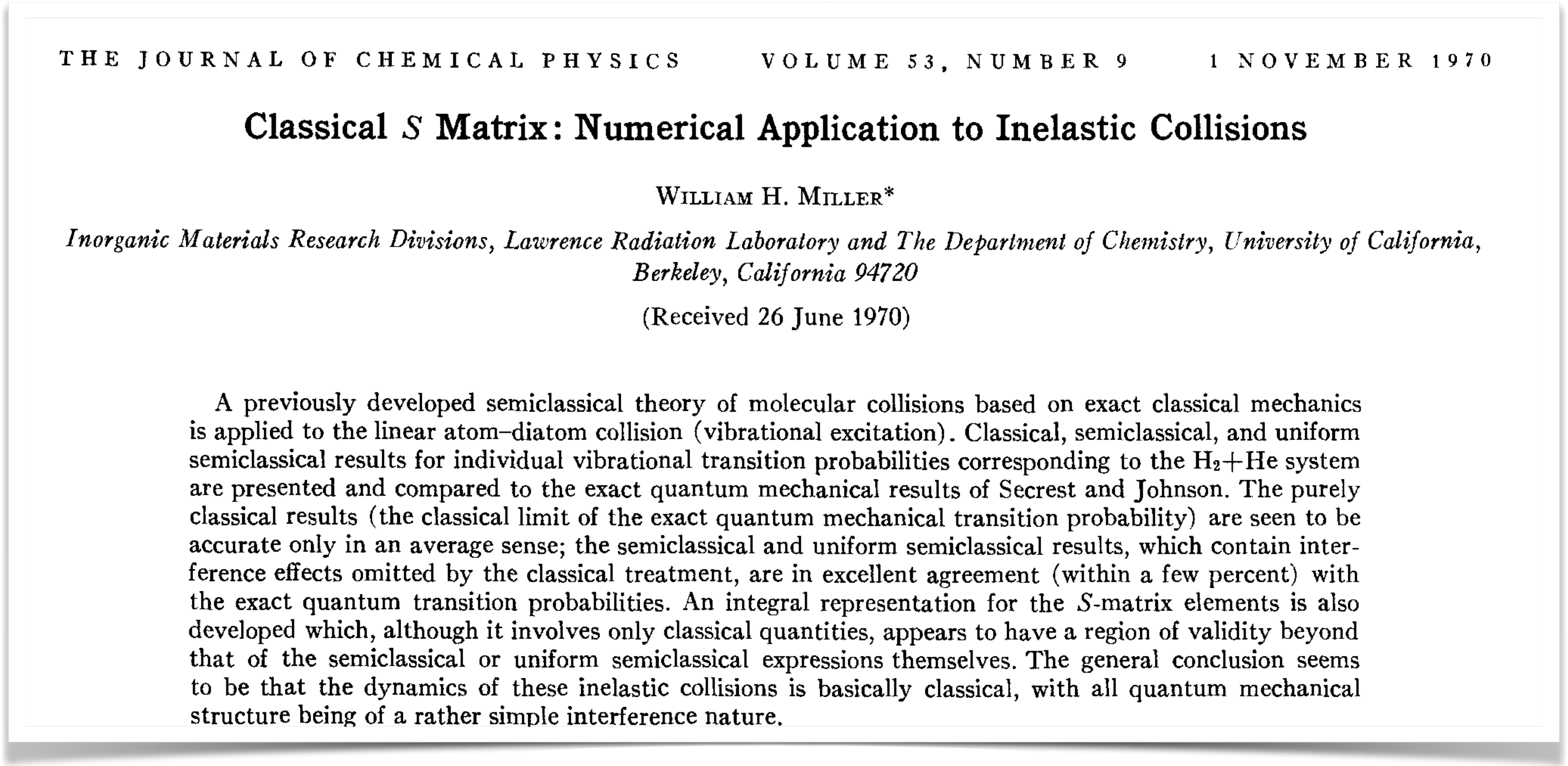
Portoroz 2023, 10-14 Apr 2023

Mixed tunneling

Mixed tunneling phenomena



This has been discussed from 1970's



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 53, NUMBER 9 1 NOVEMBER 1970

Classical S Matrix: Numerical Application to Inelastic Collisions

William H. Miller*

Inorganic Materials Research Divisions, Lawrence Radiation Laboratory and The Department of Chemistry, University of California, Berkeley, California 94720

(Received 26 June 1970)

A previously developed semiclassical theory of molecular collisions based on exact classical mechanics is applied to the linear atom–diatom collision (vibrational excitation). Classical, semiclassical, and uniform semiclassical results for individual vibrational transition probabilities corresponding to the H_2+He system are presented and compared to the exact quantum mechanical results of Secrest and Johnson. The purely classical results (the classical limit of the exact quantum mechanical transition probability) are seen to be accurate only in an average sense; the semiclassical and uniform semiclassical results, which contain interference effects omitted by the classical treatment, are in excellent agreement (within a few percent) with the exact quantum transition probabilities. An integral representation for the S-matrix elements is also developed which, although it involves only classical quantities, appears to have a region of validity beyond that of the semiclassical or uniform semiclassical expressions themselves. The general conclusion seems to be that the dynamics of these inelastic collisions is basically classical, with all quantum mechanical structure being of a rather simple interference nature.

There are a few known techniques

<u>Complex trajectories</u>

No first principle derivation

<u>Adiabatic approximation</u>

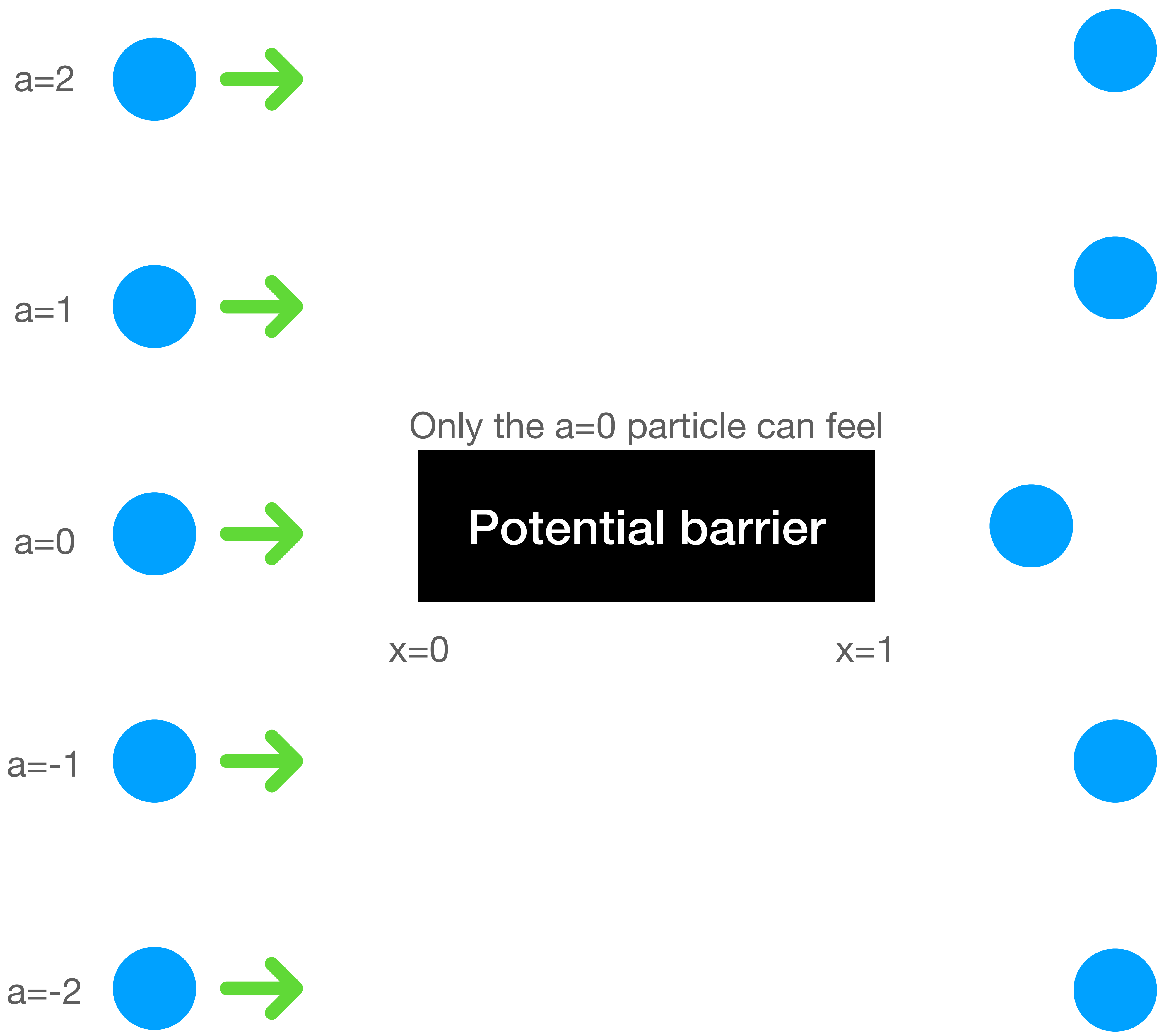
Only for adiabatic, diabatic or weak-coupling cases

Tunneling time itself has been a controversial issue of QM

<u>Huygens principle</u>

Construction of wave fronts, computationally very hard

Separable problem



Hamiltonian

There are (2N+1) independent particles

$$H = \sum_{a=-N}^{N} \frac{p_a^2}{2m} + \delta_{a0} V(x^a), \qquad V(x) = \begin{cases} V_0 & 0 < x < 1, \\ 0 & \text{otherwise} \end{cases}.$$

Initial kinetic energy

All particles have the same energy

$$\mathcal{E} < V_0$$

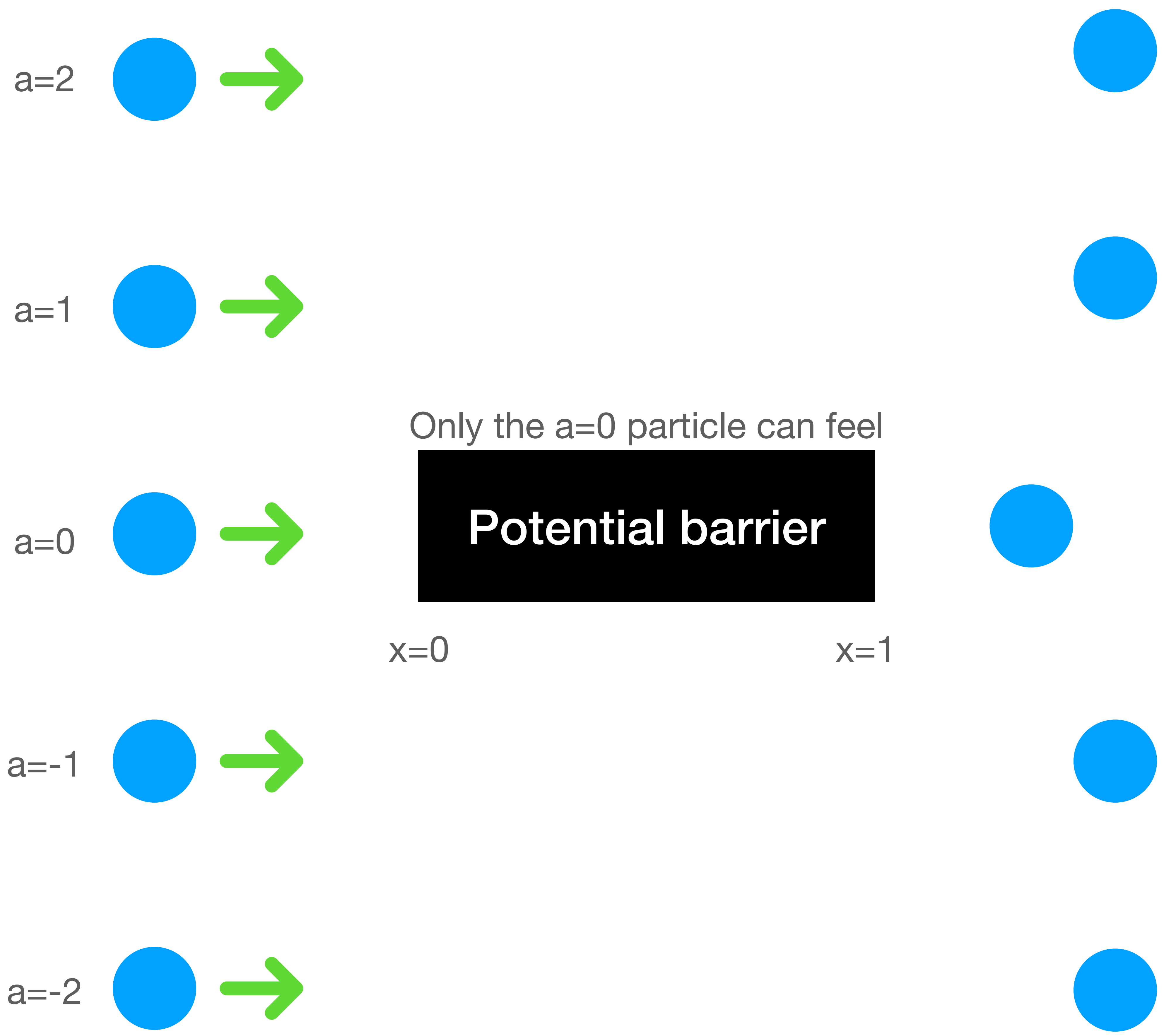
What is expected?

Only a=0 particle tunnels with probability

$$P = \frac{|\psi(s_f)|^2}{|\psi(s_i)|^2} \simeq \exp\left[-\frac{2}{\hbar}\int_0^1 \mathrm{d}x \sqrt{2m(V_0 - \mathcal{E})}\right]$$

The wrong calculation

Standard way of solving the Hamilton-Jacobi equation



Shroedinger equation

$$\hat{H}\psi = E\psi. \qquad E = (2N+1)\mathcal{E}.$$

WKB approximation

1 Semi-classical expansion

$$\psi = \exp\left[\frac{i}{\hbar}\Theta^{(0)} + \Theta^{(1)} + \dots\right]$$

2 0th-order WKB equation

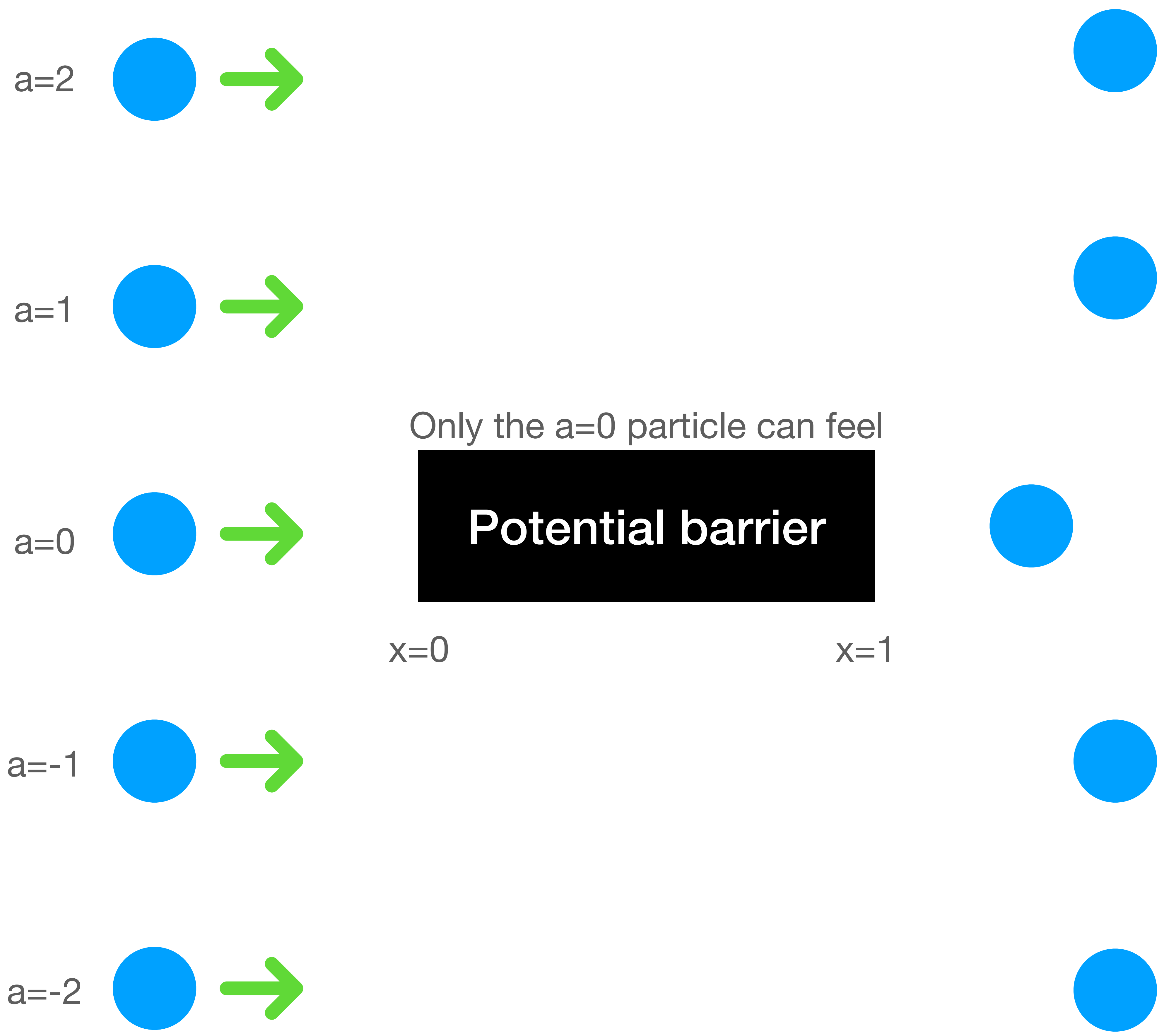
$$\frac{1}{2m}\sum_a \left(\frac{\partial\Theta^{(0)}}{\partial x^a}\right)^2 = E - V(x^0).$$

3 Solution of the Hamilton-Jacobi equation

$$\Theta^{(0)}(\{x^a(s_f)\}) - \Theta^{(0)}(\{x^a(s_i)\}) = \int_{s_i}^{s_f} \mathrm{d}s\,\sqrt{2m(E - V(x^0))}\sqrt{\sum_a \left(\frac{\mathrm{d}x^a}{\mathrm{d}s}\right)^2}.$$

The wrong calculation

Standard way of solving the Hamilton-Jacobi equation



Shroedinger equation

$$\hat{H}\psi = E\psi. \qquad E = (2N+1)\mathcal{E}.$$

WKB approximation

1 Semi-classical expansion

$$\psi = \exp\left[\frac{i}{\hbar}\Theta^{(0)} + \Theta^{(1)} + \dots\right]$$

2 0th-order WKB equation

$$\frac{1}{2m}\sum_a \left(\frac{\partial\Theta^{(0)}}{\partial x^a}\right)^2 = E - V(x^0).$$

3 Solution of the Hamilton-Jacobi equation

$$\Theta^{(0)}(\{x^a(s_f)\}) - \Theta^{(0)}(\{x^a(s_i)\}) = \int_{s_i}^{s_f} \mathrm{d}s\, \underline{\sqrt{2m(E - V(x^0))}} \sqrt{\sum_a \left(\frac{\mathrm{d}x^a}{\mathrm{d}s}\right)^2}.$$

No tunneling if $V_0 < E$???

What was wrong?

Shroedinger equation for each particle

$$\hat{\mathcal{H}}_a \psi = 0, \qquad \mathcal{H}_a = \frac{p_a^2}{2m} + \delta_{a0} V(x^a) - \mathcal{E}.$$

WKB approximation

Execute the WKB approximation for each particle

$$\Theta^{(0)}(\{x^a(s_f)\}) - \Theta^{(0)}(\{x^a(s_i)\}) = \sum_{a=-N}^{N} \int_{s_i}^{s_f} \mathrm{d}s \sqrt{2m(\mathcal{E} - \delta_{a0} V(x^a))} \sqrt{\left(\frac{\mathrm{d}x^a}{\mathrm{d}s}\right)^2}.$$

Correct result!

$$P = \frac{|\psi(s_f)|^2}{|\psi(s_i)|^2} \simeq \exp\left[-\frac{2}{\hbar}\int_0^1 \mathrm{d}x \sqrt{2m(V_0 - \mathcal{E})}\right]$$

What was wrong?

2 0th-order WKB equation

$$\frac{1}{2m}\sum_a \left(\frac{\partial \Theta^{(0)}}{\partial x^a}\right)^2 = E - V(x^0).$$

3 Solution of the Hamilton-Jacobi equation

$$\Theta^{(0)}(\{x^a(s_f)\}) - \Theta^{(0)}(\{x^a(s_i)\}) = \int_{s_i}^{s_f} \mathrm{d}s \sqrt{2m(E - V(x^0))} \sqrt{\sum_a \left(\frac{\mathrm{d}x^a}{\mathrm{d}s}\right)^2}.$$

Coupled Anharmonic Oscillators. I. Equal-Mass Case

Thomas Banks*
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Carl M. Bender†
Department of Mathematics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Tai Tsun Wu‡
Gordon McKay Laboratory, Harvard University, Cambridge, Massachusetts 02138
(Received 7 May 1973)

equation for the phase S of a wave function with energy E is[15]

$$(\vec{\nabla} S)^2 = V - E. \qquad (3.1)$$

This is just the Hamilton-Jacobi equation for a classical system with Hamiltonian $\vec{p}^2 + V$. In one dimension it reduces to $(dS/dx)^2 = V - E$, whose solution is $S = \pm\int (V-E)^{1/2}$. For the general multidimensional case it is a nonlinear partial differential equation. Of course, if the Hamiltonian has a continuous symmetry, Eq. (3.1) will be separable. However, Eq. (3.1) is nontrivial in general. The new multidimensional techniques which we have discovered simplify the problem of solving Eq. (3.1) because now we need to solve it only in a small, approximately one-dimensional region. Our technique is expressly designed to deal with problems which do *not* have continuous symmetries, and is thus *complementary* to the separation of variables idea.

Complex Hamilton-Jacobi equation

Complex exponent

$$\Theta^{(0)} = W_R + iW_I.$$

Hamilton-Jacobi equation

$$\frac{1}{2m}\sum_{a=-N}^{N}\left[\left(\frac{\partial W_R}{\partial x^a}\right)^2 - \left(\frac{\partial W_I}{\partial x^a}\right)^2\right] = E - V(x^0),$$

$$\sum_{a=-N}^{N}\left(\frac{\partial W_R}{\partial x^a}\right)\left(\frac{\partial W_I}{\partial x^a}\right) = 0.$$

Decomposition

x_R^A : contribute only to W_R

x_I^B : contribute only to W_I

$$\frac{1}{2m}\sum_A\left(\frac{\partial W_R}{\partial x_R^A}\right)^2 = E - V(x^0) + \Xi,$$

$$\frac{1}{2m}\sum_B\left(\frac{\partial W_I}{\partial x_I^B}\right)^2 = \Xi,$$

No information from
time-independent Schroedinger equation

We can solve these in the conventional way

Complex Hamilton-Jacobi equation

Complex exponent

$$\Theta^{(0)} = W_R + iW_I.$$

Hamilton-Jacobi equation

$$\frac{1}{2m}\sum_{a=-N}^{N}\left[\left(\frac{\partial W_R}{\partial x^a}\right)^2 - \left(\frac{\partial W_I}{\partial x^a}\right)^2\right] = E - V(x^0),$$

$$\sum_{a=-N}^{N}\left(\frac{\partial W_R}{\partial x^a}\right)\left(\frac{\partial W_I}{\partial x^a}\right) = 0.$$

Decomposition

x_R^A : contribute only to W_R

x_I^B : contribute only to W_I

$$\frac{1}{2m}\sum_A\left(\frac{\partial W_R}{\partial x_R^A}\right)^2 = E - V(x^0) + \Xi,$$

$$\frac{1}{2m}\sum_B\left(\frac{\partial W_I}{\partial x_I^B}\right)^2 = \Xi,$$

No information from
time-independent Schroedinger equation

We can solve these in the conventional way

Local energy conservation law

$$\hat{\mathcal{H}}_a\psi = 0,$$

$$\mathcal{H}_a = \frac{p_a^2}{2m} + \delta_{a0}V(x^a) - \mathcal{E}.$$

Uniquely determines the decomposition and Ξ

Formulation

In our formulation, the starting point is

<u>**Not the Schroedinger equation**</u>

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\psi = \hat{H}\psi$$

<u>**But the local energy conservation law**</u>

$$\hat{\mathcal{H}}_a \psi = 0,$$

$$\mathcal{H}_a = \frac{p_a^2}{2m} + \delta_{a0} V(x^a) - \mathcal{E}.$$

cf.) Hamiltonian of quantum gravity

Lagrange multiplier

Local Hamiltonian

$$H = \lambda \pi_N + \lambda_i \pi_N^i + N\mathcal{H} + N_i \mathcal{H}^i + \partial_\mu \mathcal{H}^\mu_{\mathrm{bdy}}$$

$$\mathcal{H} \approx 0$$

Hamiltonian constraint/Wheeler-deWitt equation

$$\mathcal{H} = \frac{1}{\sqrt{h}}\left[2\kappa G_{ijkl}\pi^{ij}\pi^{kl} + \frac{1}{2}\pi_\phi^2\right] + \sqrt{h}\left[-\frac{1}{2\kappa}{}^{(3)}\mathcal{R} + \frac{1}{2}h^{ij}(\partial_i\phi)(\partial_j\phi) + V(\phi)\right],$$

$$\mathcal{H}^i = (\partial^i\phi)\pi_\phi - 2\sqrt{h}\nabla_j \frac{\pi^{ij}}{\sqrt{h}},$$

$$\mathcal{H}^s_{\mathrm{bdy}} = \pi^{ij}h_{ij},$$

$$\mathcal{H}^i_{\mathrm{bdy}} = 2\pi^{ij}N_j - \pi^{kl}h_{kl}N^i + \frac{\sqrt{h}}{\kappa}\partial^i N.$$

$$G_{ijkl} = \frac{1}{2}(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}).$$

Path integral

Path integral formula

[YS; 22]

$$\int \mathcal{D}X\,\delta_\eta \exp\left[\frac{i}{\hbar}\sum_{a=-N}^{N}\int_{s_1}^{s_n} \mathrm{d}s\, 2\sqrt{\mathcal{K}^a(s)}\sqrt{-\mathcal{V}^a(s)}\right]$$

Here,

$$\mathcal{K}^a = \frac{m}{2}\left(\frac{\mathrm{d}x^a}{\mathrm{d}s}\right)^2,$$

$$\mathcal{V}^a = \delta_{a0}V(x^a) + \frac{w}{2}\frac{(x^a - x^{a+1})^2 + (x^a - x^{a-1})^2}{2} - \eta^a + \eta^{a-1}.$$

With eta satisfying

$$\frac{\mathrm{d}\eta^a(s)}{\mathrm{d}s} = \frac{w}{2}(x^{a+1}(s) - x^a(s))\left(\frac{\mathrm{d}x^{a+1}(s)}{\mathrm{d}s} + \frac{\mathrm{d}x^a(s)}{\mathrm{d}s}\right).$$

Path integral

Path integral formula [YS; 22]

$$\int \mathcal{D}X \delta_\eta \exp\left[\frac{i}{\hbar}\sum_{a=-N}^{N}\int_{s_1}^{s_n} \mathrm{d}s\, 2\sqrt{\mathcal{K}^a(s)}\sqrt{-\mathcal{V}^a(s)}\right]$$

Here,

$$\mathcal{K}^a = \frac{m}{2}\left(\frac{\mathrm{d}x^a}{\mathrm{d}s}\right)^2,$$

$$\mathcal{V}^a = \delta_{a0}V(x^a) + \frac{w}{2}\frac{(x^a - x^{a+1})^2 + (x^a - x^{a-1})^2}{2} - \eta^a + \eta^{a-1}.$$

With eta satisfying

$$\frac{\mathrm{d}\eta^a(s)}{\mathrm{d}s} = \frac{w}{2}(x^{a+1}(s) - x^a(s))\left(\frac{\mathrm{d}x^{a+1}(s)}{\mathrm{d}s} + \frac{\mathrm{d}x^a(s)}{\mathrm{d}s}\right).$$

$\mathcal{V}^a < 0$

Lorentzian path integral

$$= \int \mathcal{D}X \exp\left[i\int_{s_1}^{s_n} \mathrm{d}s\, L(\{x^a\},\{\dot{x}^a\})\right]$$

$\mathcal{V}^a > 0$

Euclidean path integral

$$= \int \mathcal{D}X \exp\left[-\int_{s_1}^{s_n} \mathrm{d}s\, L_E(\{x^a\},\{\dot{x}^a\})\right]$$

Mixed

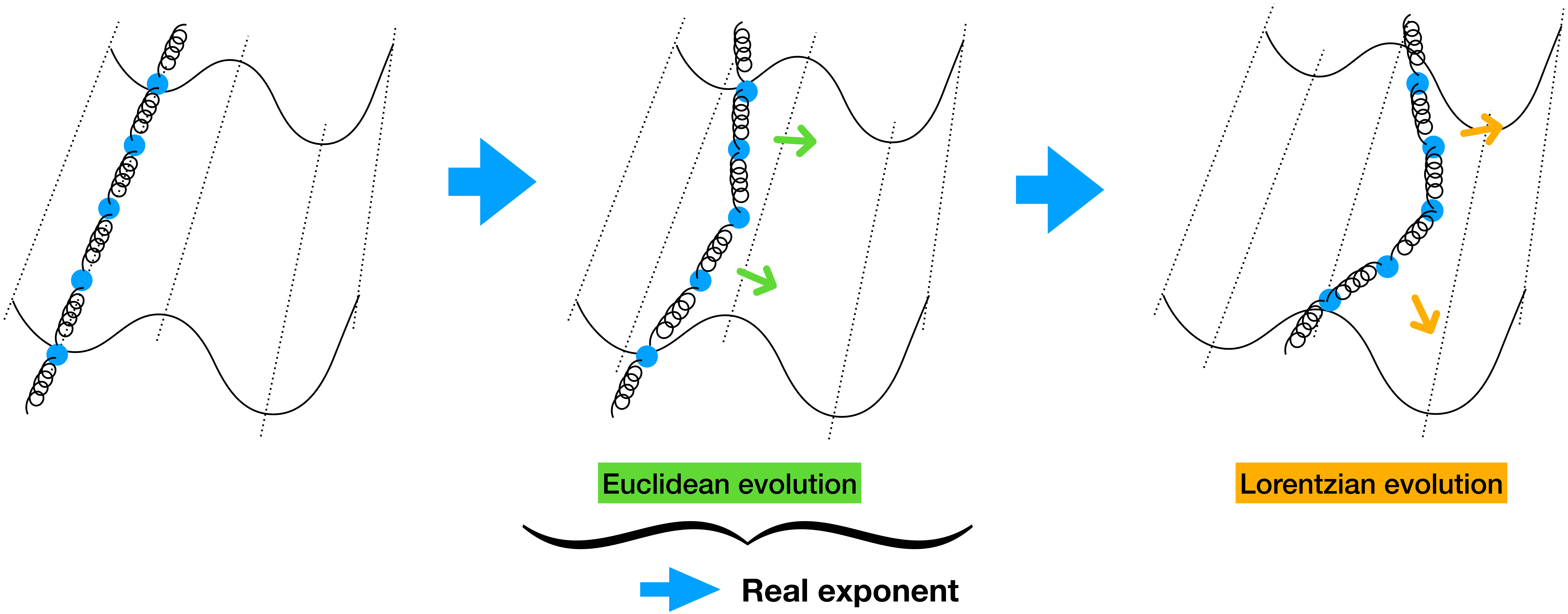
Separable example

$$\sum_{a=-N}^{N}\int_{s_i}^{s_f} \mathrm{d}s\,\sqrt{2m(\mathcal{E} - \delta_{a0}V(x^a))}\sqrt{\left(\frac{\mathrm{d}x^a}{\mathrm{d}s}\right)^2}.$$

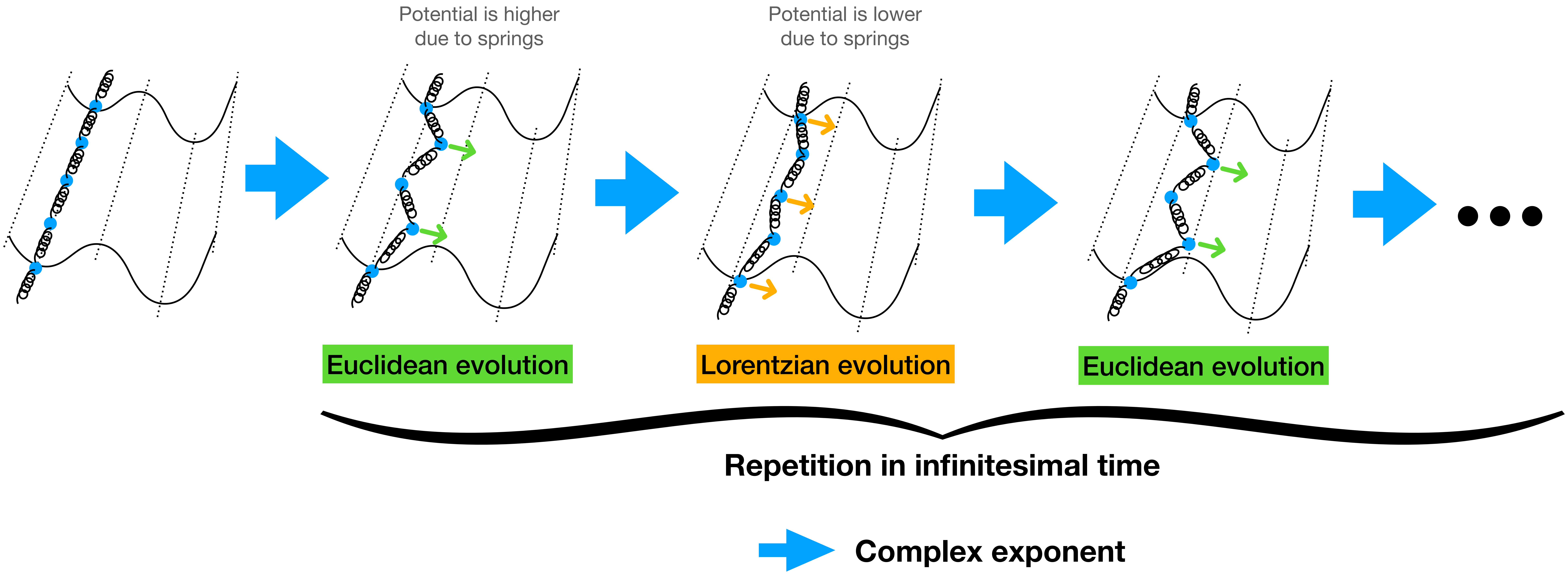
Polychronic tunneling
~ new tunneling process in QFT ~

One-dimensional chain explanation

CDL tunneling



One-dimensional chain explanation
Polychronic tunneling

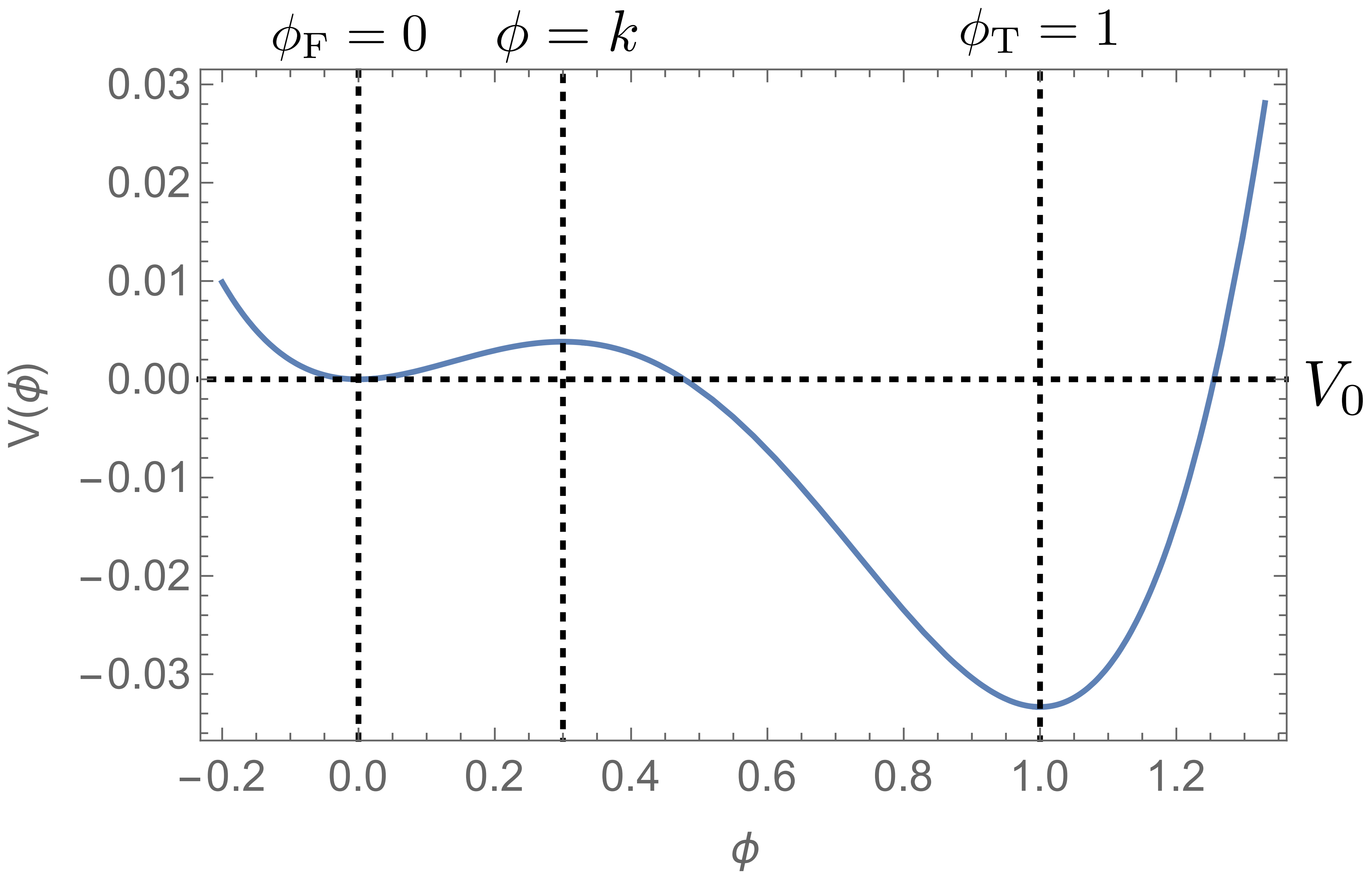


Numerical analysis

Setup

Potential

$$V(\phi) = \frac{\phi^4}{4} - \frac{k+1}{3}\phi^3 + \frac{k}{2}\phi^2 + V_0,$$



SO(3) x R Ansatz

$$\phi = \phi(s, r),$$

$$h_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j = e^{\eta(s,r)}\,\mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2),$$

False vacuum

$$\phi(0, r) = \phi_{\mathrm{F}},$$

$$\eta(0, r) = -\ln\left(1 - \frac{\kappa r^2}{3}V(\phi_{\mathrm{F}})\right).$$

=> Search for a complex saddle point

Unit of parameters are set by $\kappa = 8\pi G$

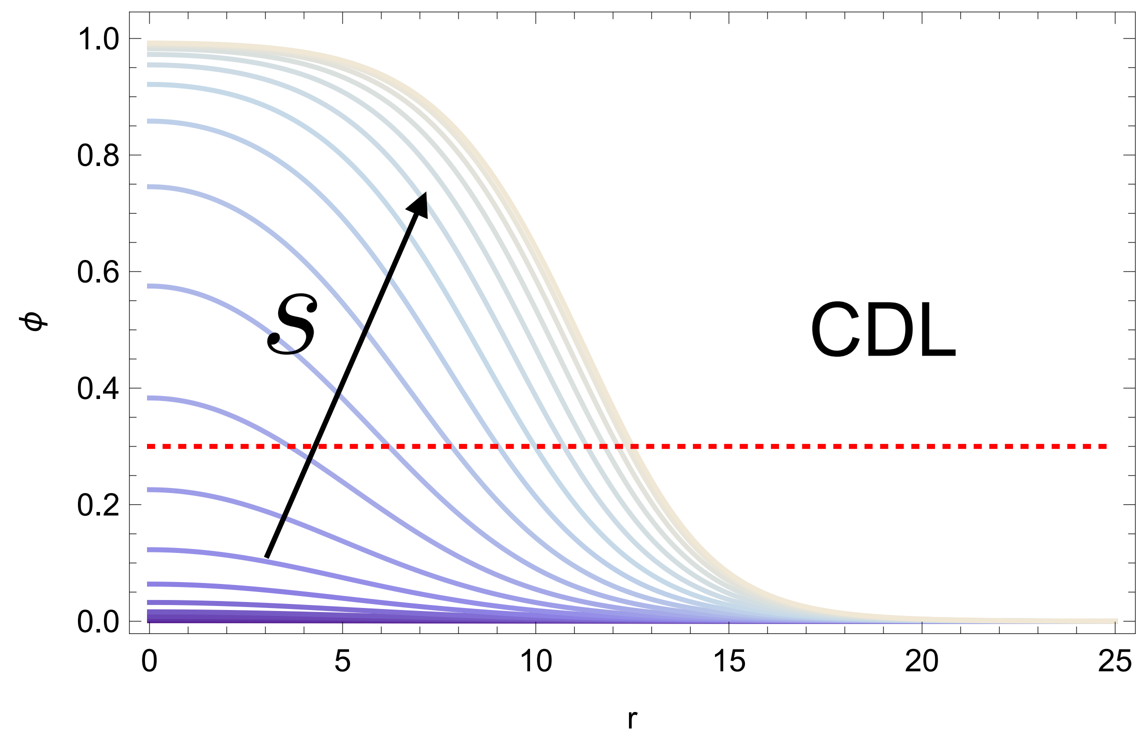
Numerical analysis

[N. Oshita, YS, M. Yamaguchi, '23]

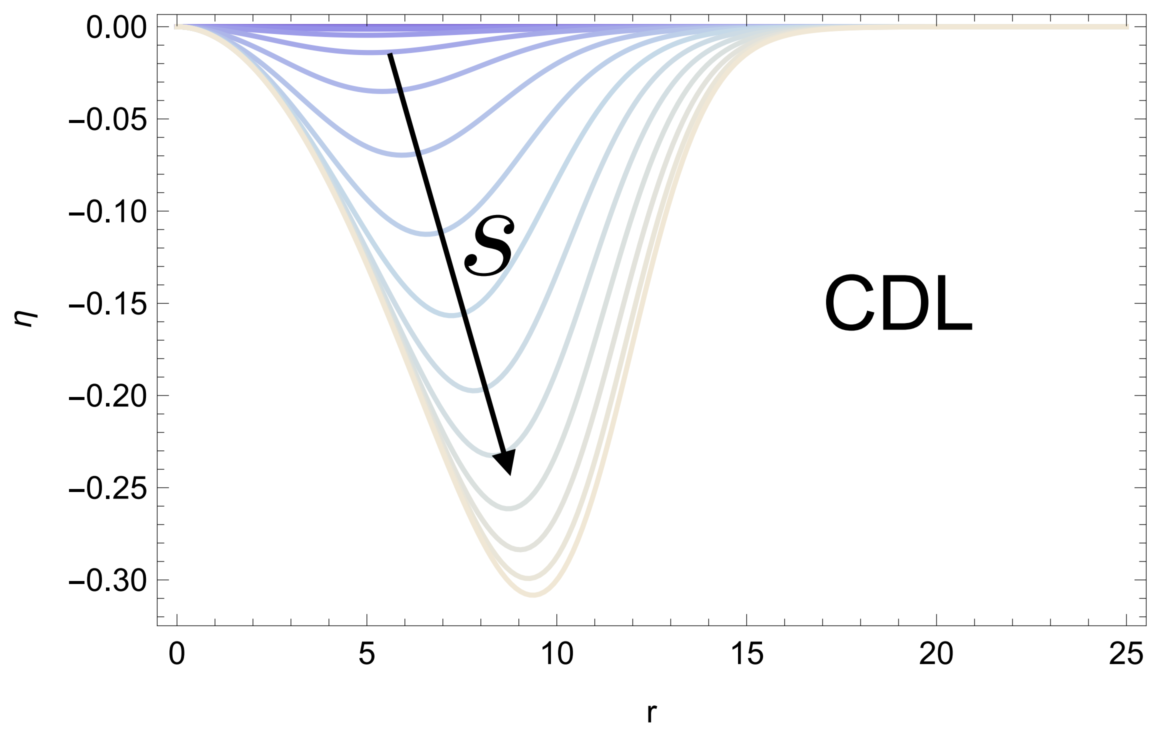
CDL vs PT

$$(\kappa, k, V_0) = (0.5, 0.3, 0)$$

ϕ



η

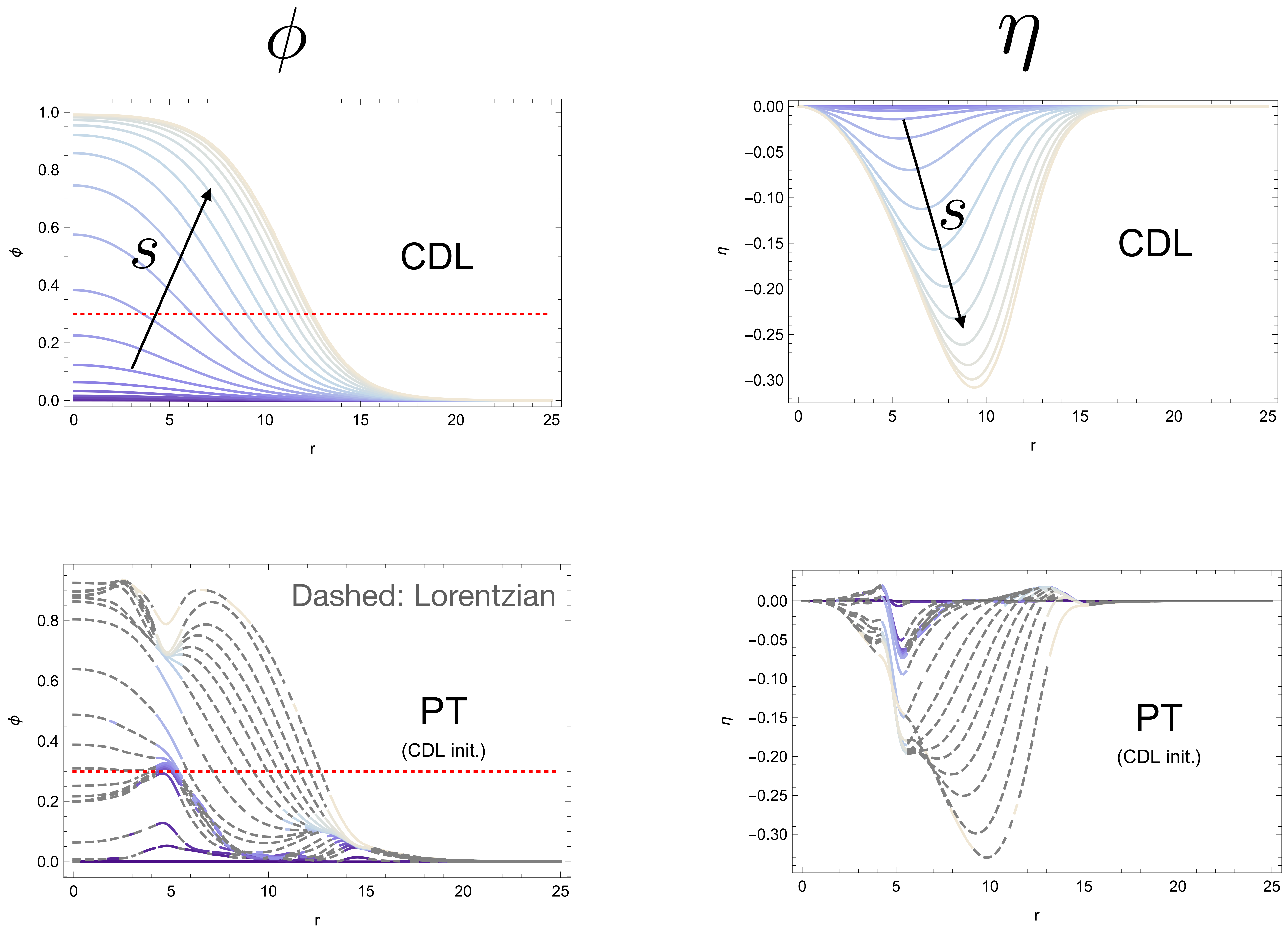


Numerical analysis

[N. Oshita, YS, M. Yamaguchi, ’23]

CDL vs PT

$(\kappa, k, V_0) = (0.5, 0.3, 0)$



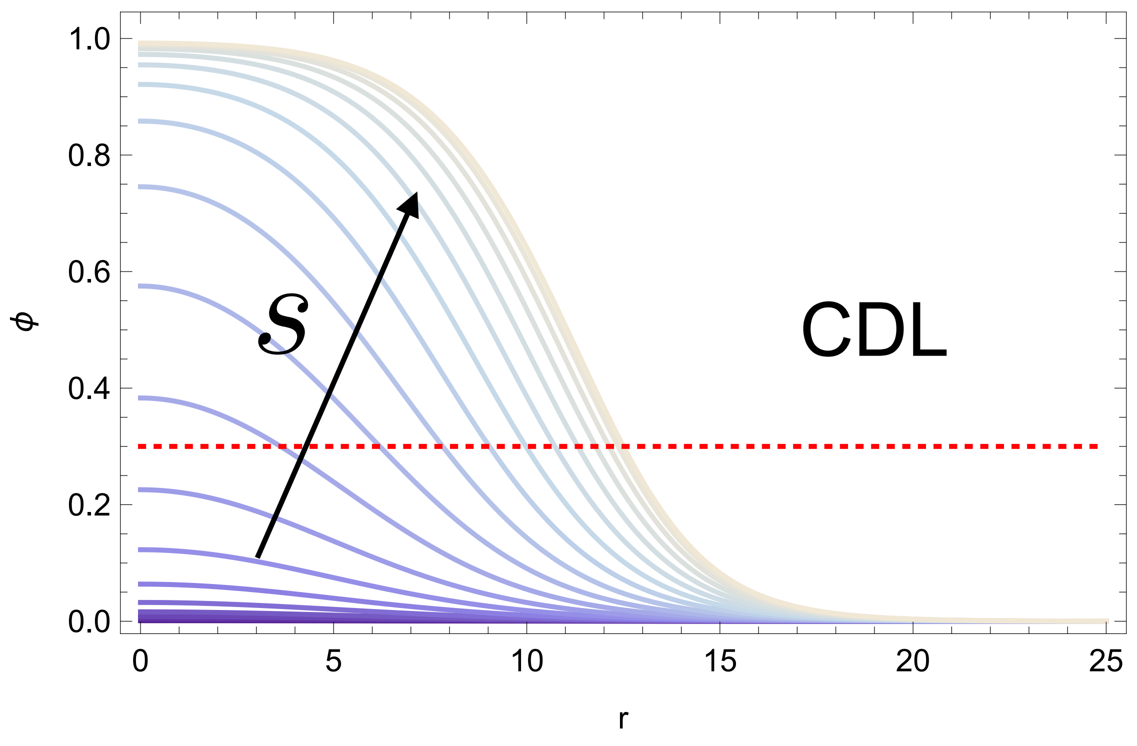
Numerical analysis

CDL vs PT

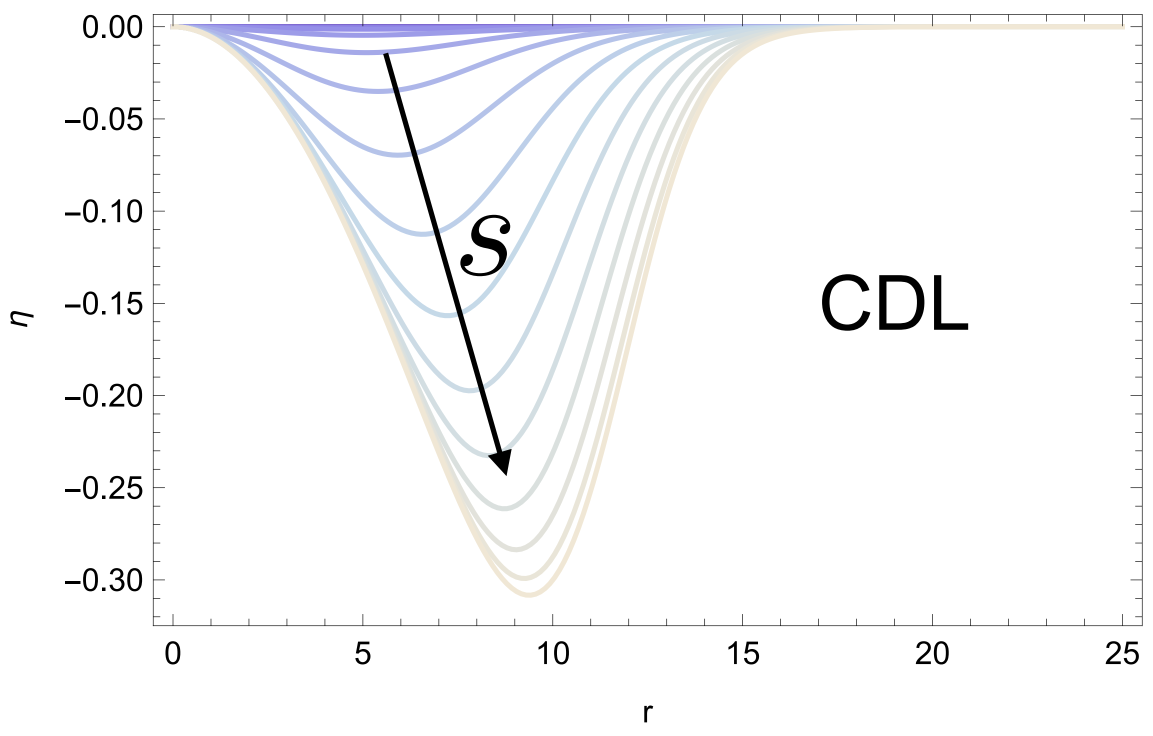
[N. Oshita, YS, M. Yamaguchi, ’23]

$$(\kappa, k, V_0) = (0.5, 0.3, 0)$$

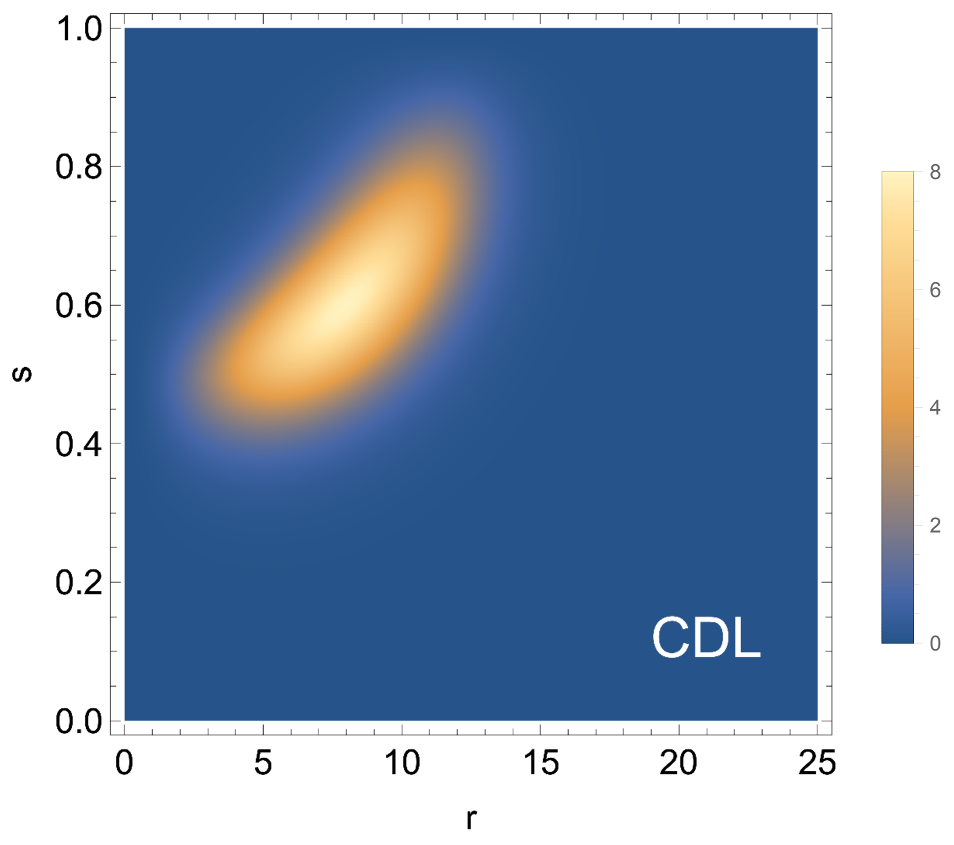
ϕ



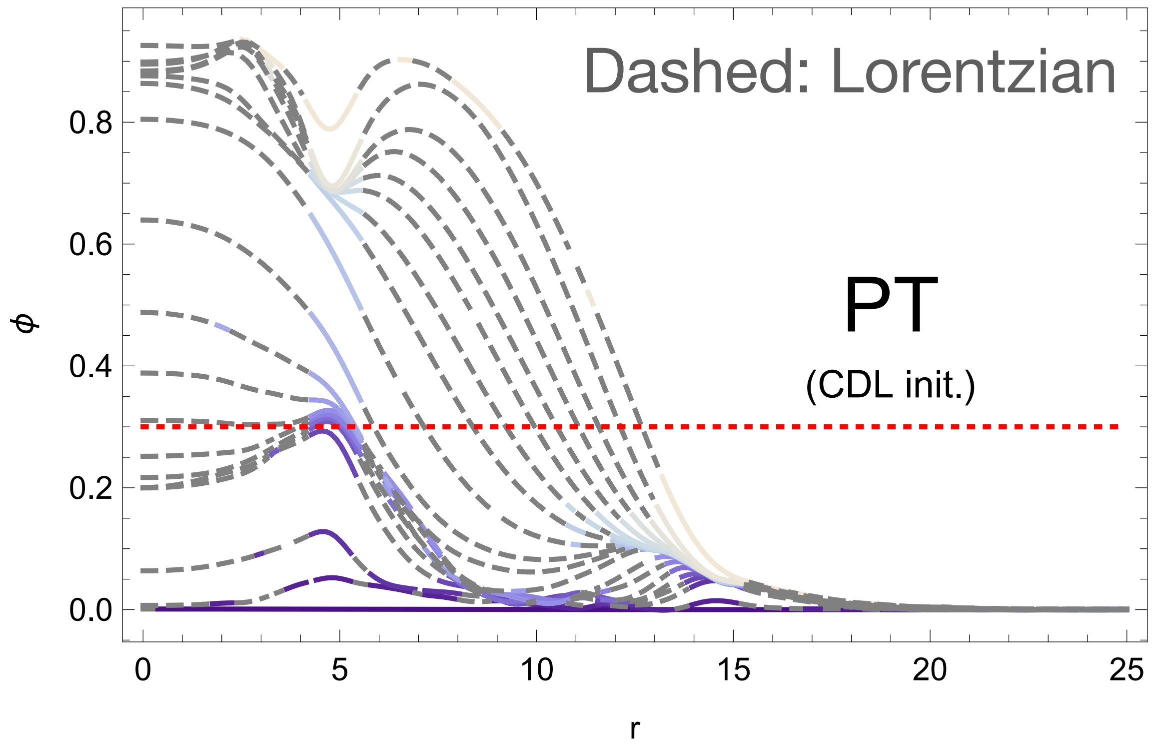
η

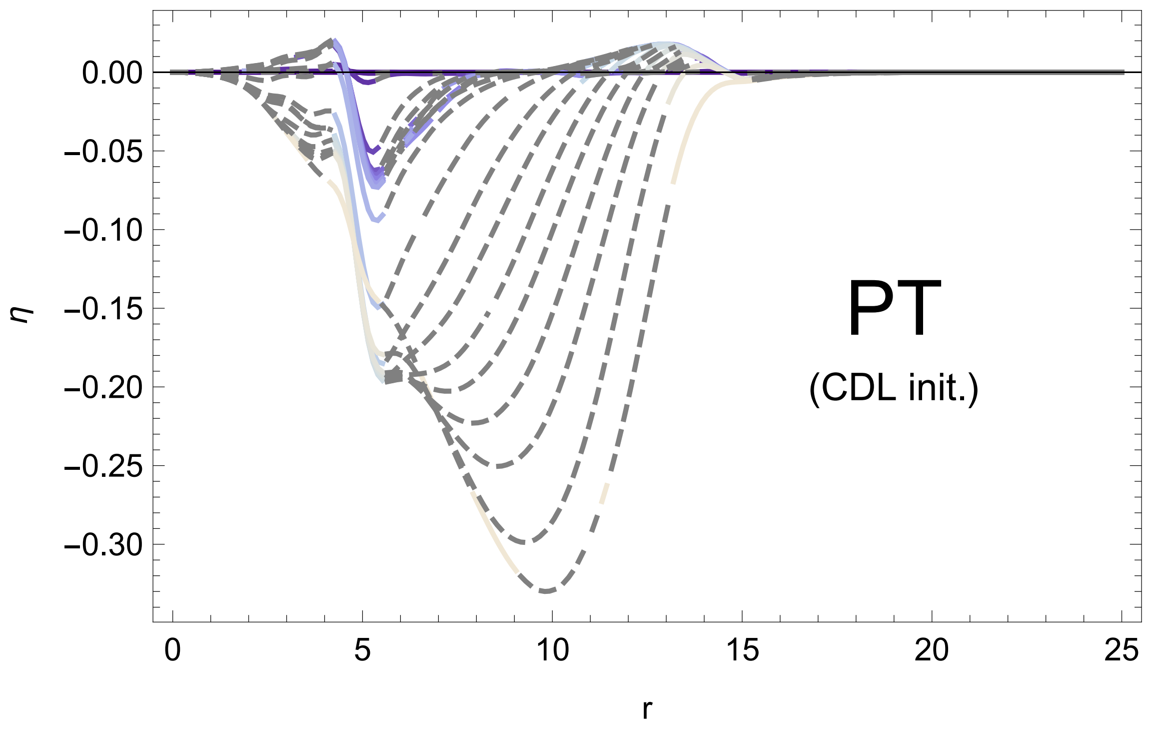


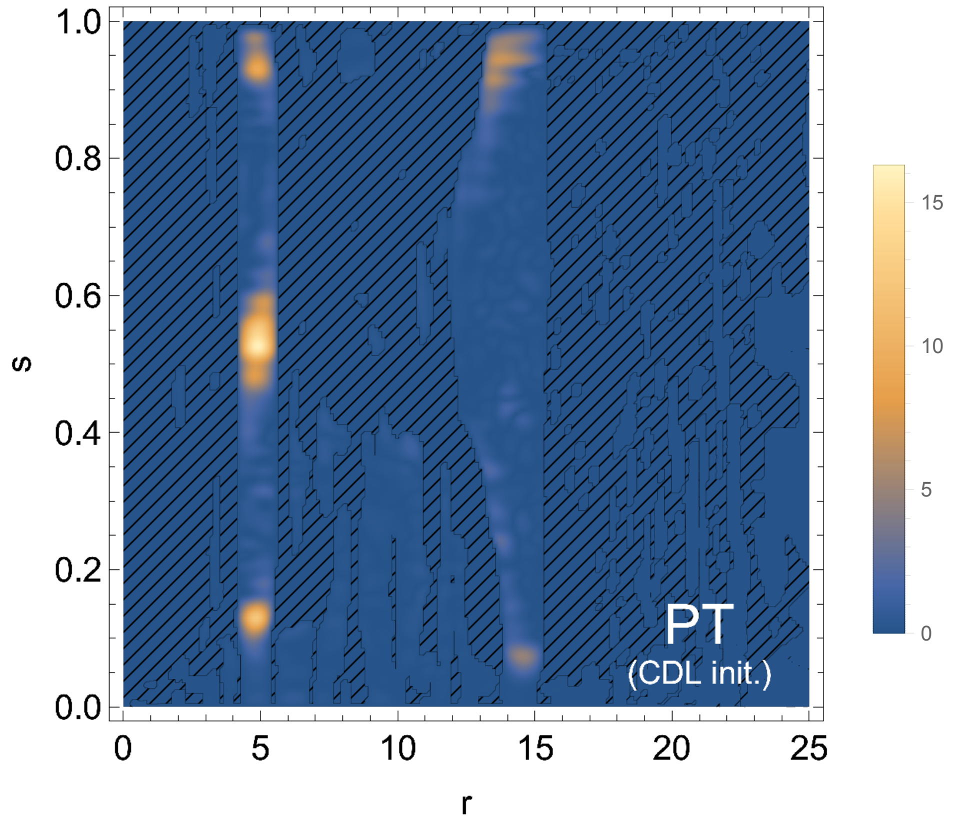
I



$$\ln \gamma^{(0)} \simeq -710$$

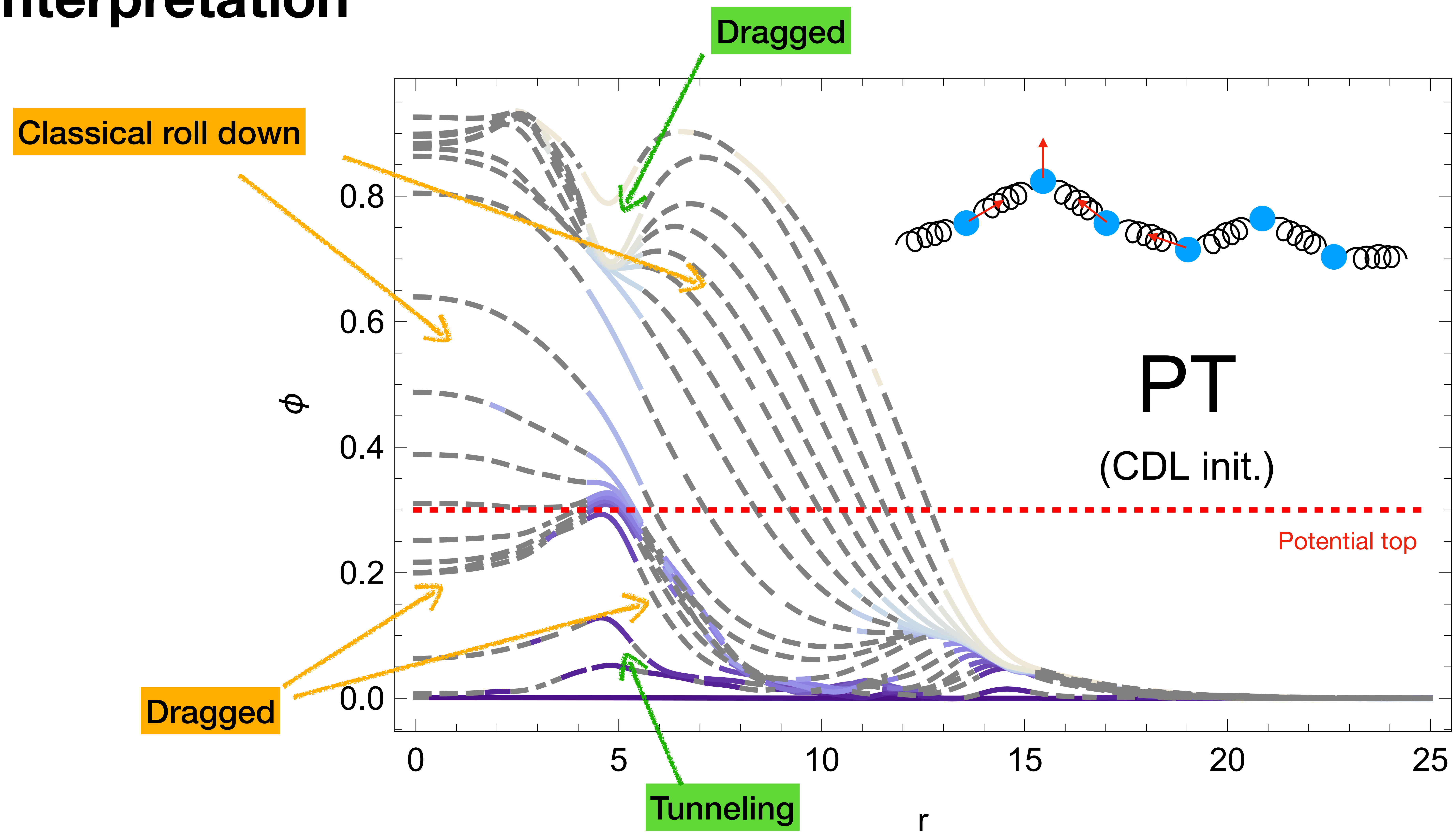






$$\ln \gamma^{(0)} \simeq -232$$

Numerical analysis
Interpretation



Summary

- Quantum tunneling in a many-body system is non-trivial and the conventional techniques sometimes fail to give the correct results
- Our starting point is not the Schroedinger equation, but the local energy conservation law
- We have formulated path-integral for mixed tunneling and polychronic tunneling
- In QFT, we have found faster tunneling processes than the CDL one