# A collection of fun numerical methods that [might] lead us to Lattice QCD yes i think they're fun

Based on: Lattice QCD: a practical guide; SUPA lecture series by Christine Davies, and G. P. Lepage, Lattice QCD for Novices, hep-lat/0506036

Vithyaban Anjelo Narendran @ Graduate Symposium 2024

Assume you know of QCD

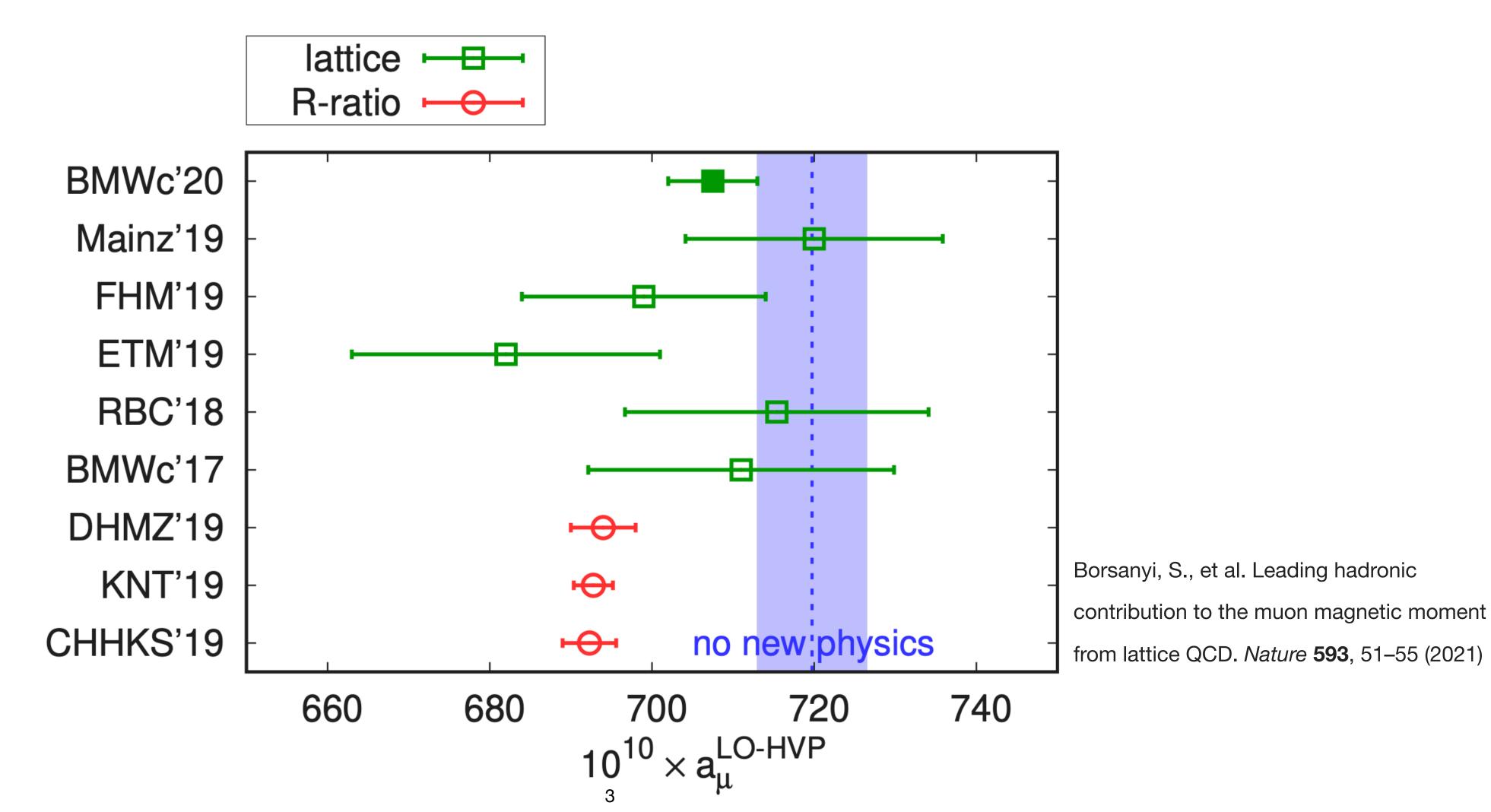
- Assume you know of QCD
- Problems when doing perturbation theory
  - Power series expansion in  $\alpha_{s}$ , the QCD coupling constant.

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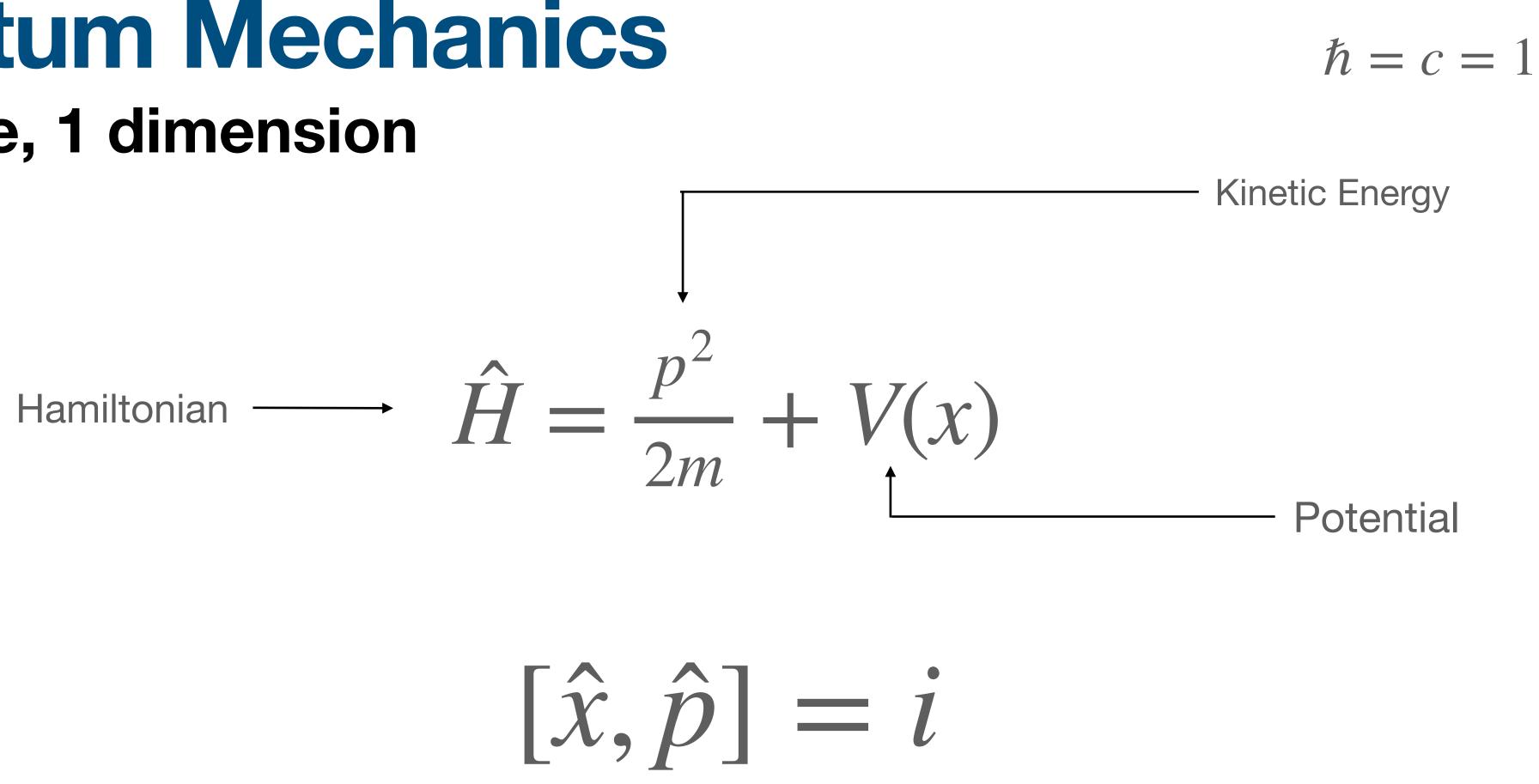
- Assume you know of QCD
- Problems when doing perturbation theory
  - Power series expansion in  $\alpha_{\rm s}$ , the QCD coupling constant.
    - Blows up if  $\alpha_s$  is large.
- and properties of the bound states.

Calculate numerically the properties we want to know about in QCD - masses

### Muon g-2 Houston, we have a result!







Position and Momentum Operators don't commute

$$\hat{H} = \frac{p^2}{2m} + V(x) [\hat{x}, \hat{p}] = i$$

### Solve Schrödinger's equation.

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# Solve Schrödinger's equation. Find Eigenfunctions, Eigenvalues Partv!

### **Path Integral Formulation Transition Amplitude and Action**

# $K(x,t;x_i,t_i) = \langle x(t) \mid x_i(t_i) \rangle = \int \mathscr{D}x(t)e^{iS[x]}$

### **Path Integral Formulation Transition Amplitude and Action**

# Possible Path $K(x,t;x_i,t_i) = \left\langle x(t) \mid x_i(t_i) \right\rangle = \int \mathscr{D}x(t)e^{iS[x]}$

## **Path Integral Formulation Transition Amplitude and Action** Possible Path $K(x,t;x_i,t_i) = \left\langle x(t) \mid x_i(t_i) \right\rangle = \int \mathscr{D}x(t)e^{iS[x]}$ Weighted by exponential

of classical action

### Path Integral Formula Transition Amplitude and Action

 $K(x,t;x_i,t_i) = \langle x(t)$ 

 $S[x] \equiv \int_{t_i}^t dt L(x, \dot{x})$ 

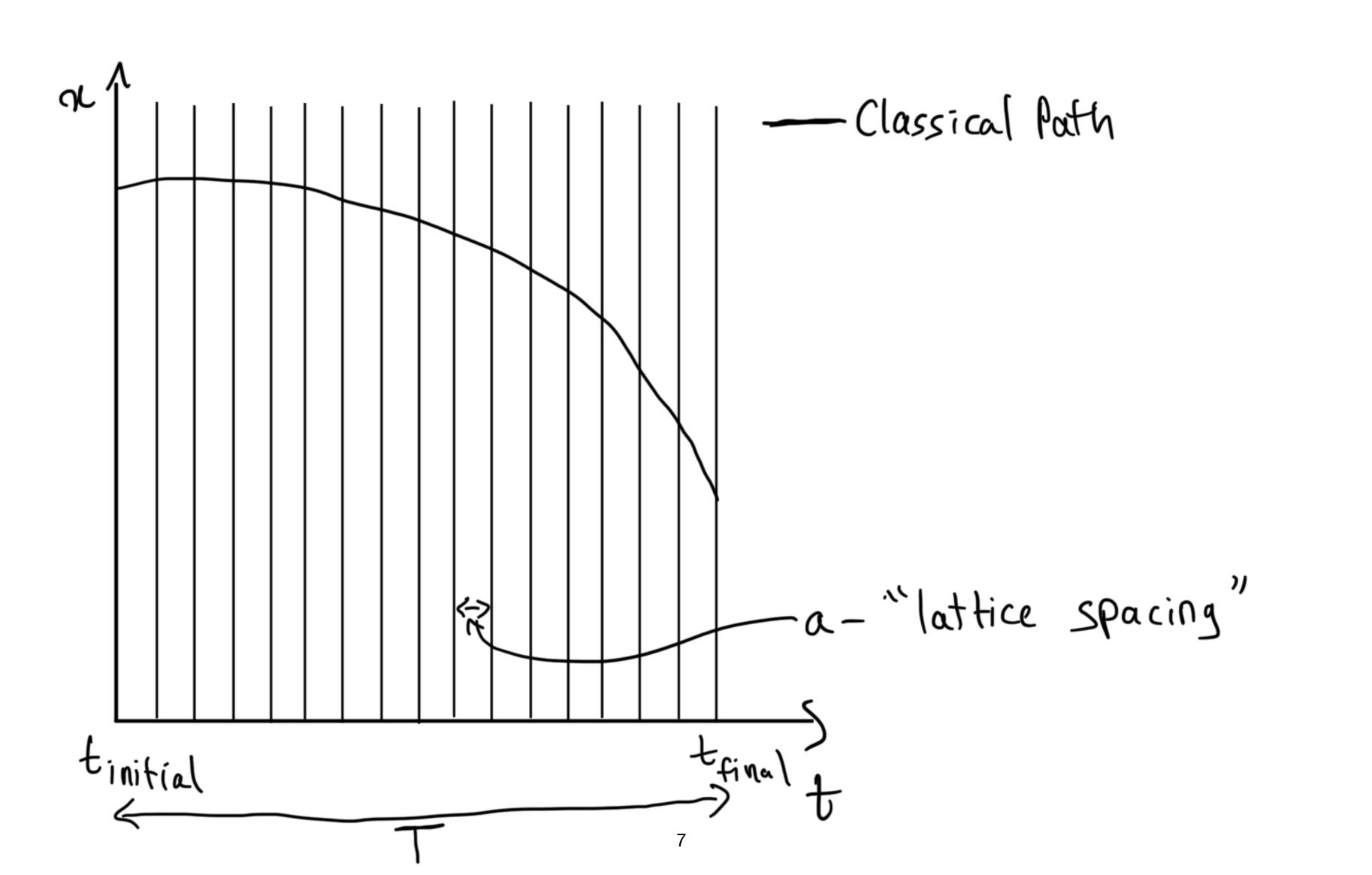
**ation**  
Possible Path  

$$|x_{i}(t_{i})\rangle = \int \mathscr{D}x(t)e^{iS[x]}$$
Weighted by exponent  
of classical action  
Weighted by exponent  
of classical action

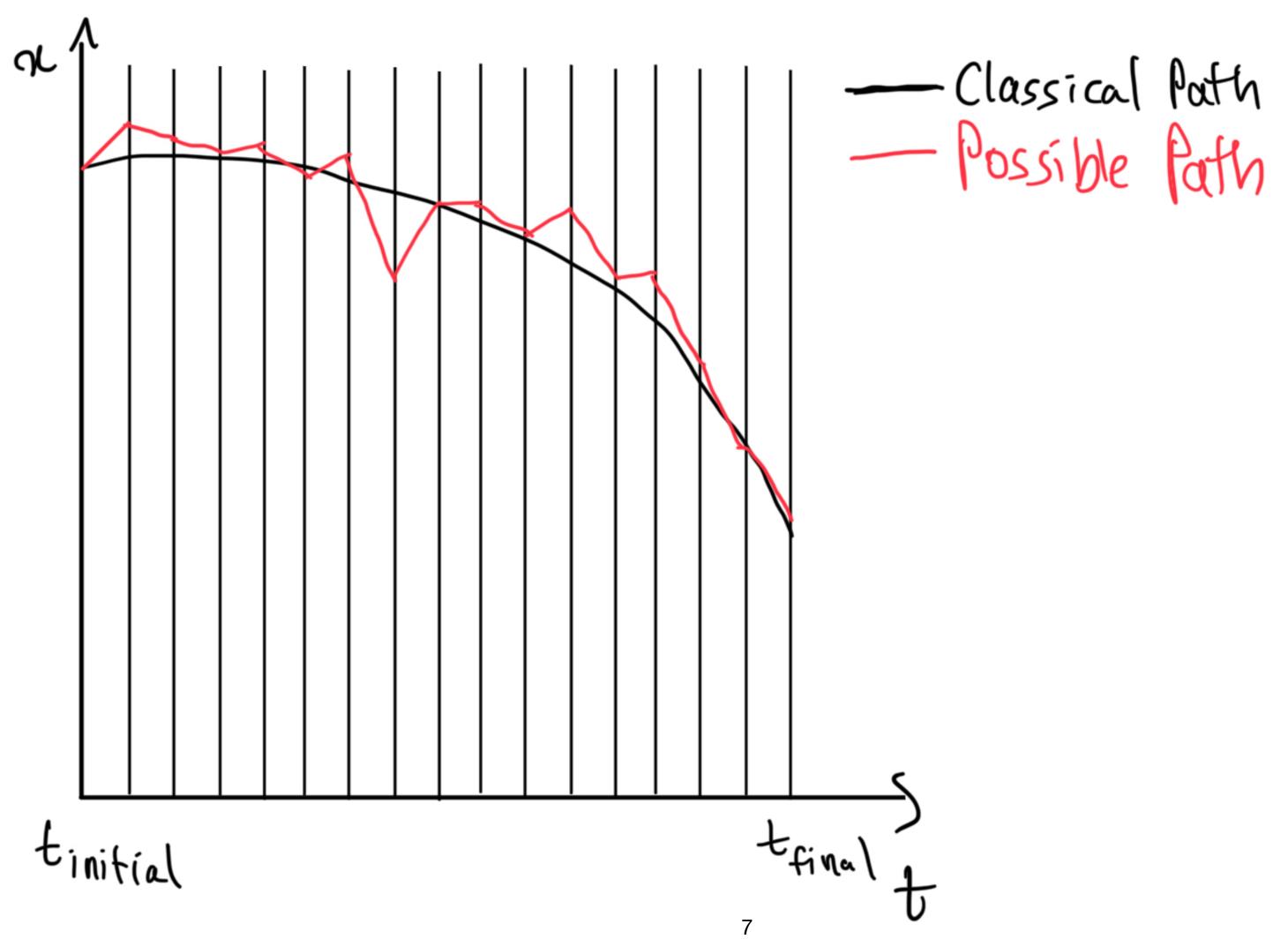
Lagrangian

tial

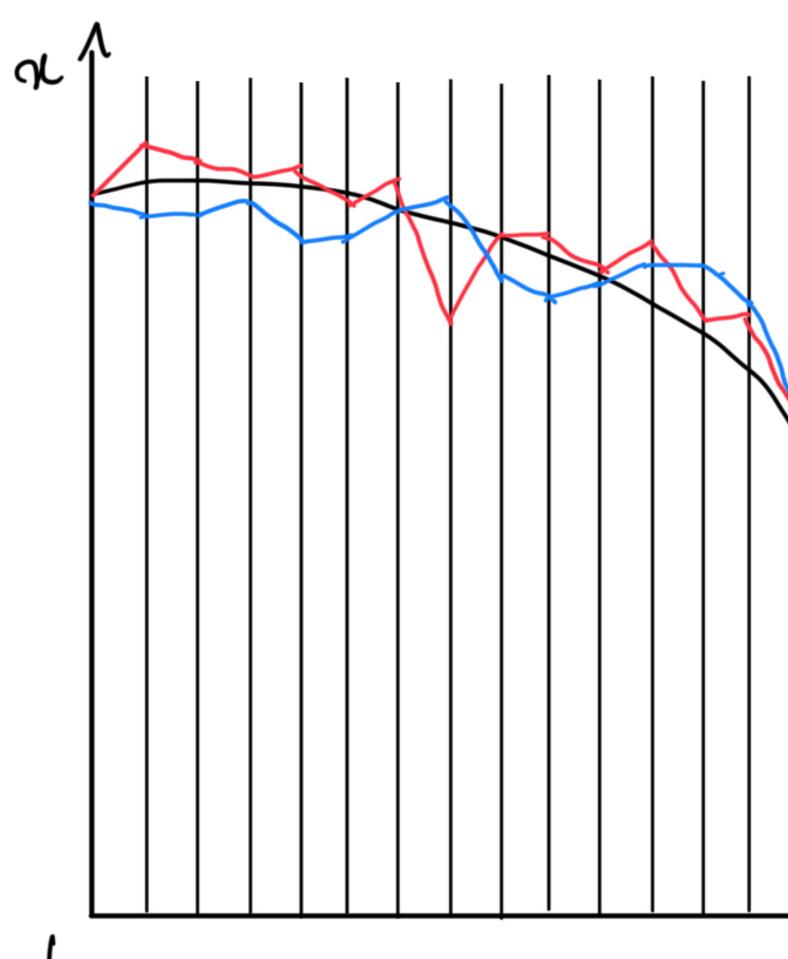
### **Classical Paths and Quantum Fluctuations**



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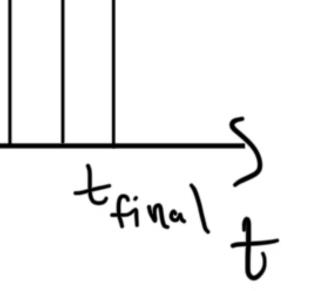


## **Classical Paths and Quantum Fluctuations**



tinitial

Classical Path Possible Path Possible Path 2



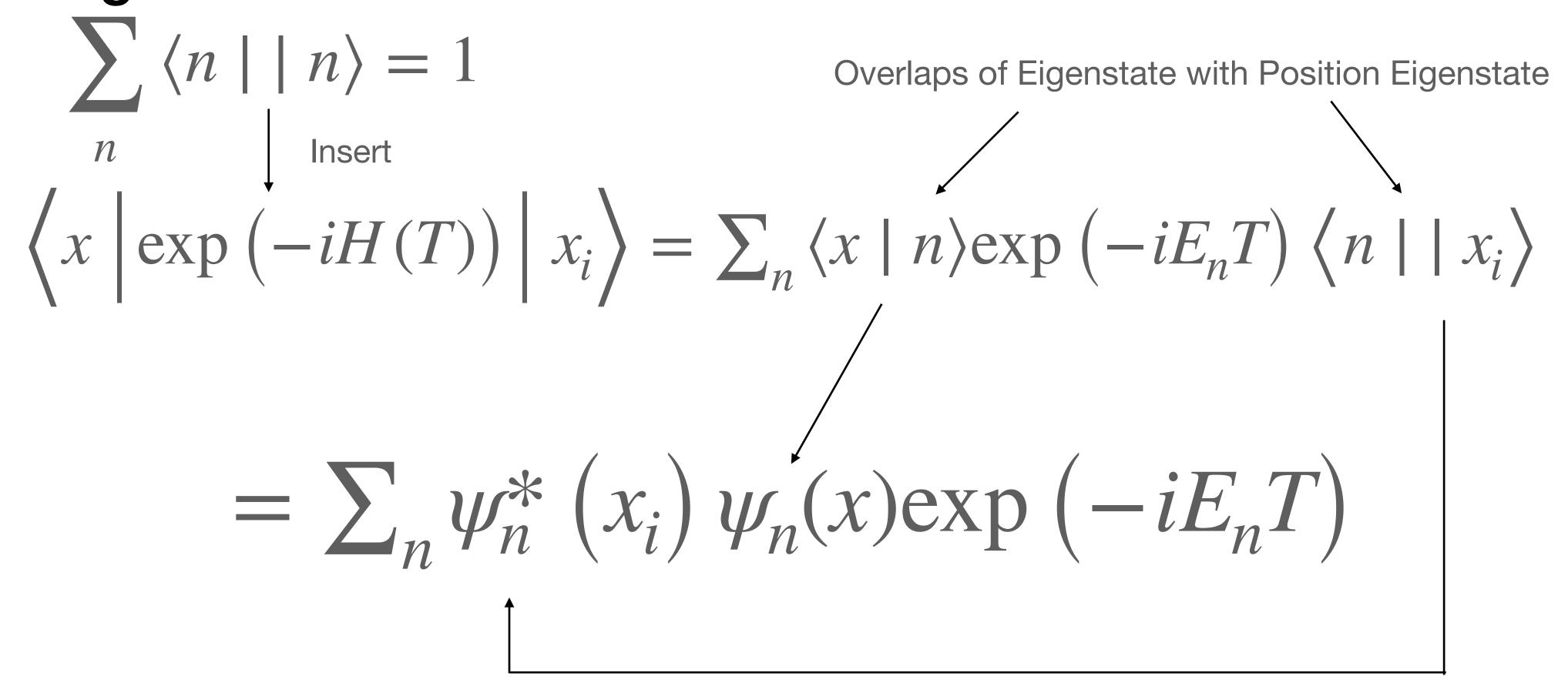
# $\left\langle x \left| \exp\left(-iH(T)\right) \right| x_i \right\rangle = \sum_n \langle x \mid n \rangle \exp\left(-iE_nT\right) \langle n \mid | x_i \rangle$

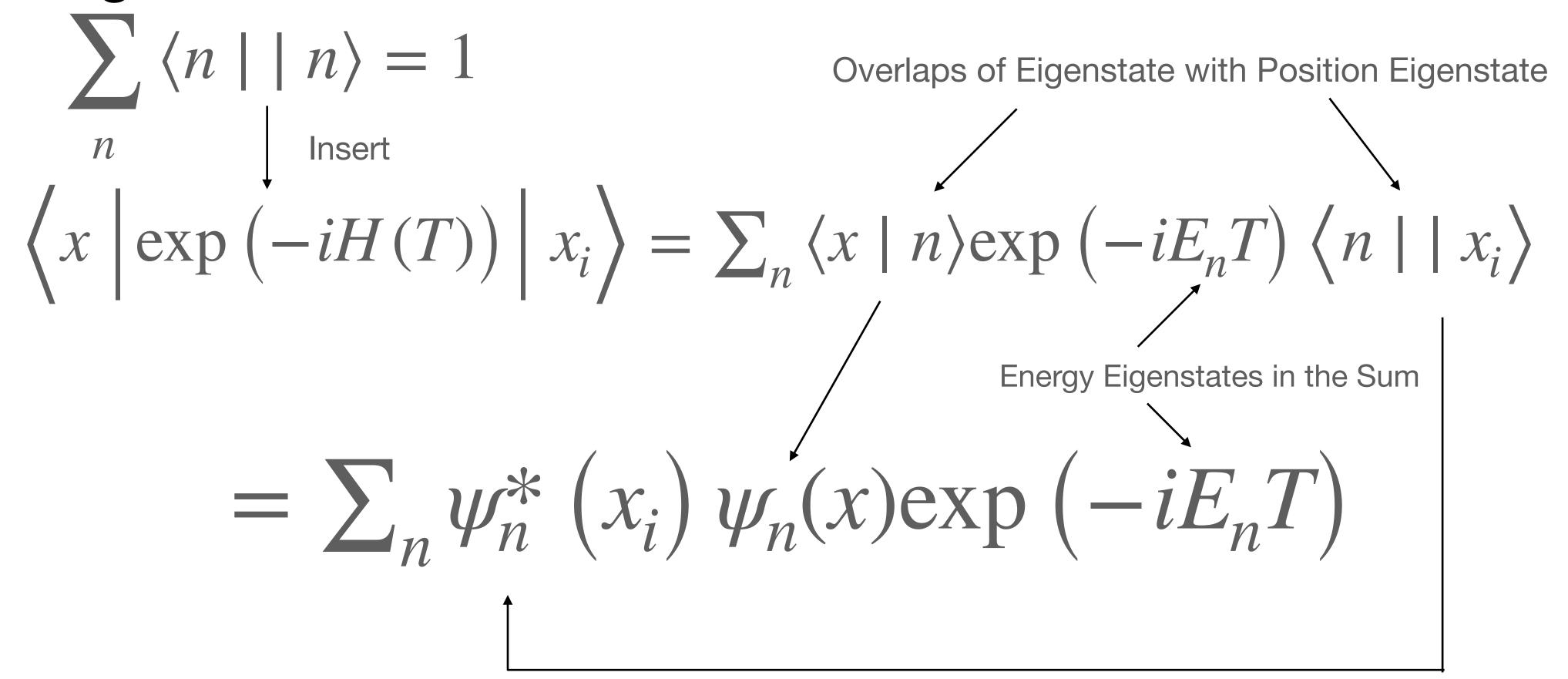
# $\sum_{n}^{\infty} \langle n \mid | n \rangle = 1$ $\lim_{n \to \infty} | \text{Insert}$ $\left\langle x \left| \exp\left(-iH(T)\right) \right| x_i \right\rangle = \sum_{n} \langle x \mid n \rangle \exp\left(-iE_nT\right) \left\langle n \mid | x_i \right\rangle$

# $\sum_{n} \langle n \mid n \rangle = 1$ $\lim_{n \to \infty} |n| = 1$ $\int_{\text{Insert}} |n| = 1$ $\int_{\text{Insert}} |x_i| = 2$

**Overlaps of Eigenstate with Position Eigenstate** 

$$\sum_{n} \langle x \mid n \rangle \exp\left(-iE_{n}T\right) \left\langle n \mid x_{i} \right\rangle$$





### $x_i = x_f = x$

New Transition Amplitude
$$\left\langle x \mid e^{-H(T)} \mid x \right\rangle = \int \mathscr{D} x e^{-S[x]}$$

### $x_i = x_f = x$

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# $S[x] \equiv \int_0^T dt L(x, \dot{x}) \equiv \int dt \left| \frac{m \dot{x}(t)^2}{2} + V(x(t)) \right|$

Weighting is  $\Re$  valued



New Transition Amplitude  

$$\left\langle x \mid e^{-H(T)} \mid x \right\rangle = \int \mathscr{D} x e^{-S[x]} \qquad S[x] \equiv \int_{0}^{T} dt L(x, \dot{x}) \equiv \int dt \left[ \frac{m \dot{x}(t)^{2}}{2} + V(x(t)) \right] dt$$
Weighting is  $\mathscr{B}$  valued

Inserting Eigenstates as before:

$$\left\langle x \mid e^{-H(T)} \mid x \right\rangle =$$

 $x_i = x_f = x$ 

vergnung is *s* valued

 $= \sum_{n} \psi_n^*(x) \psi_n(x) e^{-E_n T}$ 



New Transition Amplitude  

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Inserting Eigenstates as before:

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If we have large T, smallest E gets picked out -> Extract  $E_0$ 

 $x_i = x_f = x$ 

verynning is 21 valueu

Decaying Exponential of all E Eigenstates  $= \sum_{n} \psi_n^*(x) \psi_n(x) e^{-E_n T}$ 



Transition Amplitudes -> Eigenstates of the Hamiltonian -> Physics

 $\left\langle x(T) \left| x(t_2) x(t_1) \right| x(0) \right\rangle \qquad \int \mathcal{Q}$  $\langle x(T) \mid x(0) \rangle$ 

$$\mathscr{D}xx(t_2)x(t_1)e^{-S[x]}$$
$$\int \mathscr{D}xe^{-S[x]}$$

 $\left\langle x(T) \left| x(t_2) x(t_1) \right| x(0) \right\rangle$  $\langle x(T) \mid x(0) \rangle$ 



Average 
$$x(t_1)x(t_2)$$
  
on each path

$$\mathscr{D}xx(t_2)x(t_1)e^{-S[x]} \\ \int \mathscr{D}xe^{-S[x]}$$

Average over all paths generated

$$\frac{\left\langle x(T) \left| x(t_2) x(t_1) \right| x(0) \right\rangle}{\left\langle x(T) \mid x(0) \right\rangle} = \frac{\int \mathscr{D} x x(t_2) x(t_1) e^{-S[x]}}{\int \mathscr{D} x e^{-S[x]}}$$

Plug a complete set of Eigenstates in as before:

$$= \left| \left\langle E_0 | x | E_1 \right\rangle \right|^2 e^{-(E_1 - E_0)(t_2 - t_1)}, t_2 - t_1 \to \infty$$



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Matrix Element



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Matrix Element Excitation Energy between ground and f



Average 
$$x(t_1)x(t_2)$$
  
on each path

Average over all paths generated

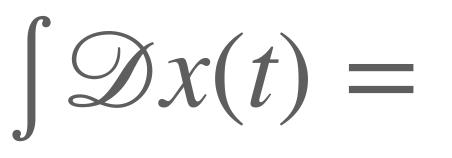
first excited state

### **Calculating the Path Integral Numerically Discretise Time**

Divide up the line from  $t_i \rightarrow t_f$  to a set of points

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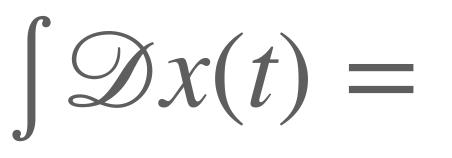
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 $\int \mathscr{D}x(t) = \int dx_1 dx_2 \dots dx_n$ 

## **Calculating the Path Integral Numerically Discretise Time**

Divide up the line from  $t_i \rightarrow t_f$  to a set of points



Value of x at  $t_n$  $\int \mathscr{D}x(t) = \int dx_1 dx_2 \dots dx_n$ 

## **Calculating the Path Integral Numerically Discretise Time**

Divide up the line from  $t_i \rightarrow t_f$  to a set of points

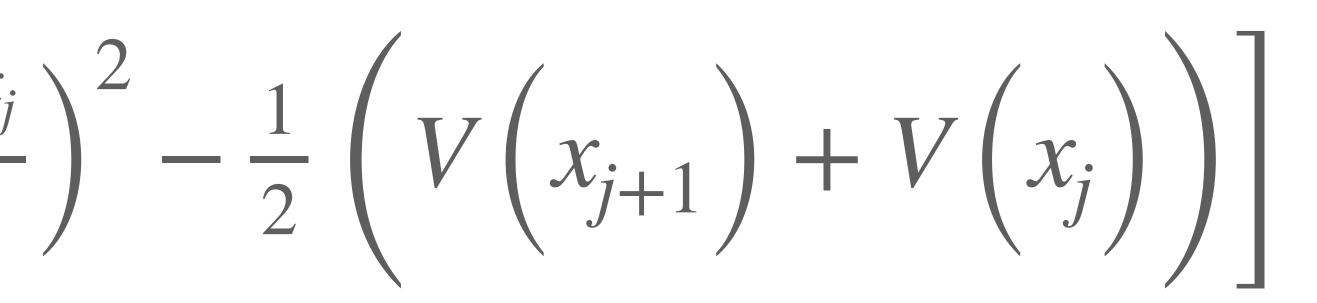
Integrate over all the possible values of x for each  $x_i$ 

n-dimensional integral

Value of x at  $t_n$  $\int \mathscr{D}x(t) = \int dx_1 dx_2 \dots dx_n$ 

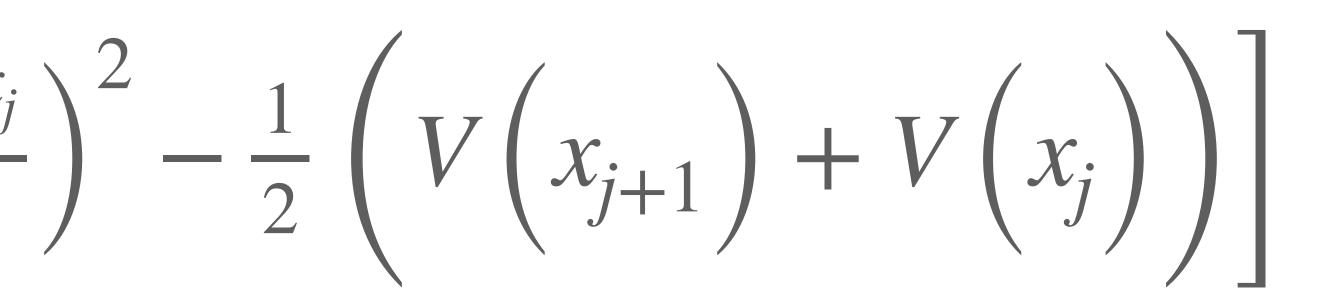
Call  $t_{j+1} - t_j = a$ , the lattice spacing

$$\int_{t_j}^{t_{j+1}} dt L \approx a \left[ \frac{m}{2} \left( \frac{x_{j+1} - x_j}{a} \right) \right]$$



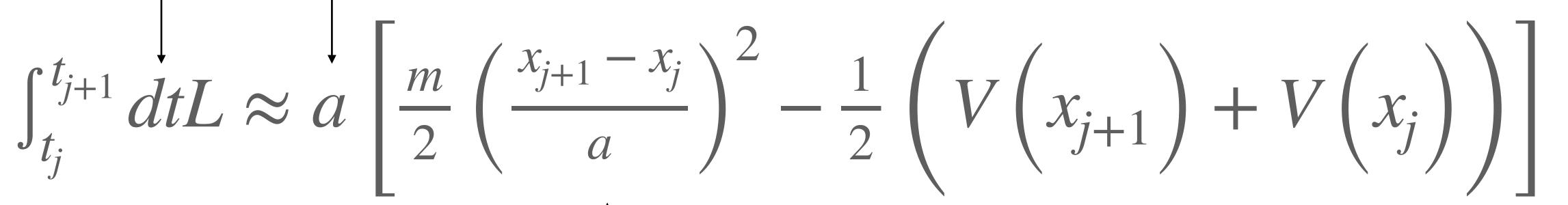
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 $\dot{x}(t)^2$  between  $t_{i+1}$  and  $t_i$ **Euler Method** 

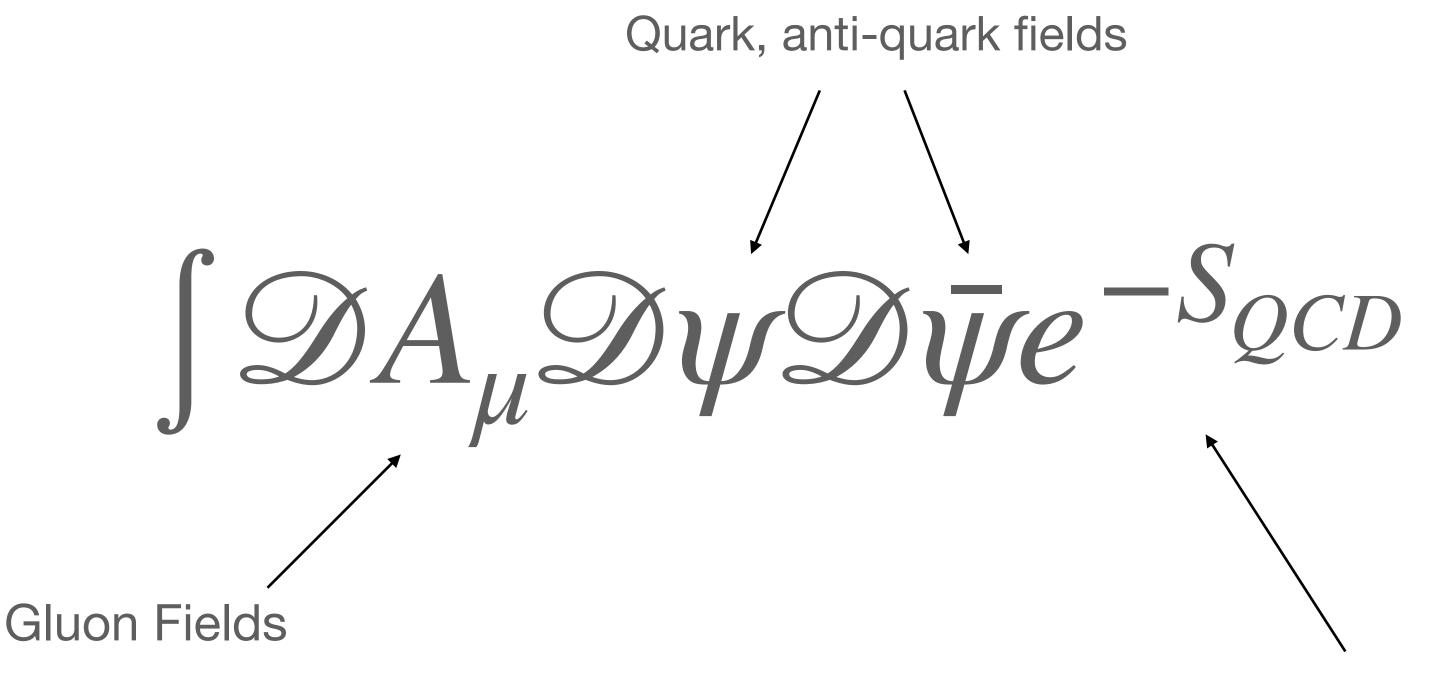


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 $\int_{t_i}^{t_{j+1}} dt L \approx a \left[ \frac{m}{2} \left( \frac{x_{j+1} - x_j}{a} \right)^2 - \frac{1}{2} \left( V\left(x_{j+1}\right) + V\left(x_j\right) \right) \right]$  $\dot{x}(t)^2$  between  $t_{i+1}$  and  $t_i$ **Euler Method** 

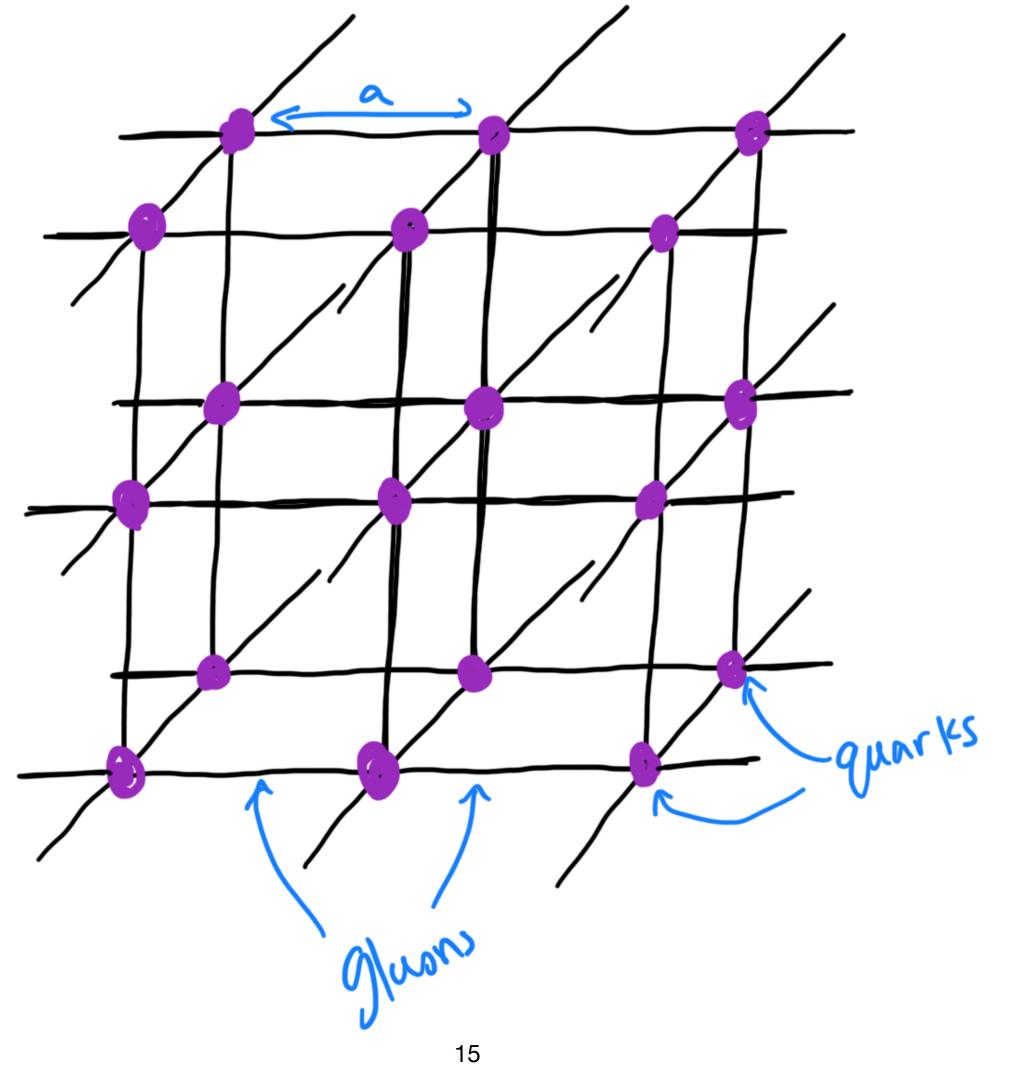
A discretisation of the potential

## **Moving to QCD** The Path Integral in QCD

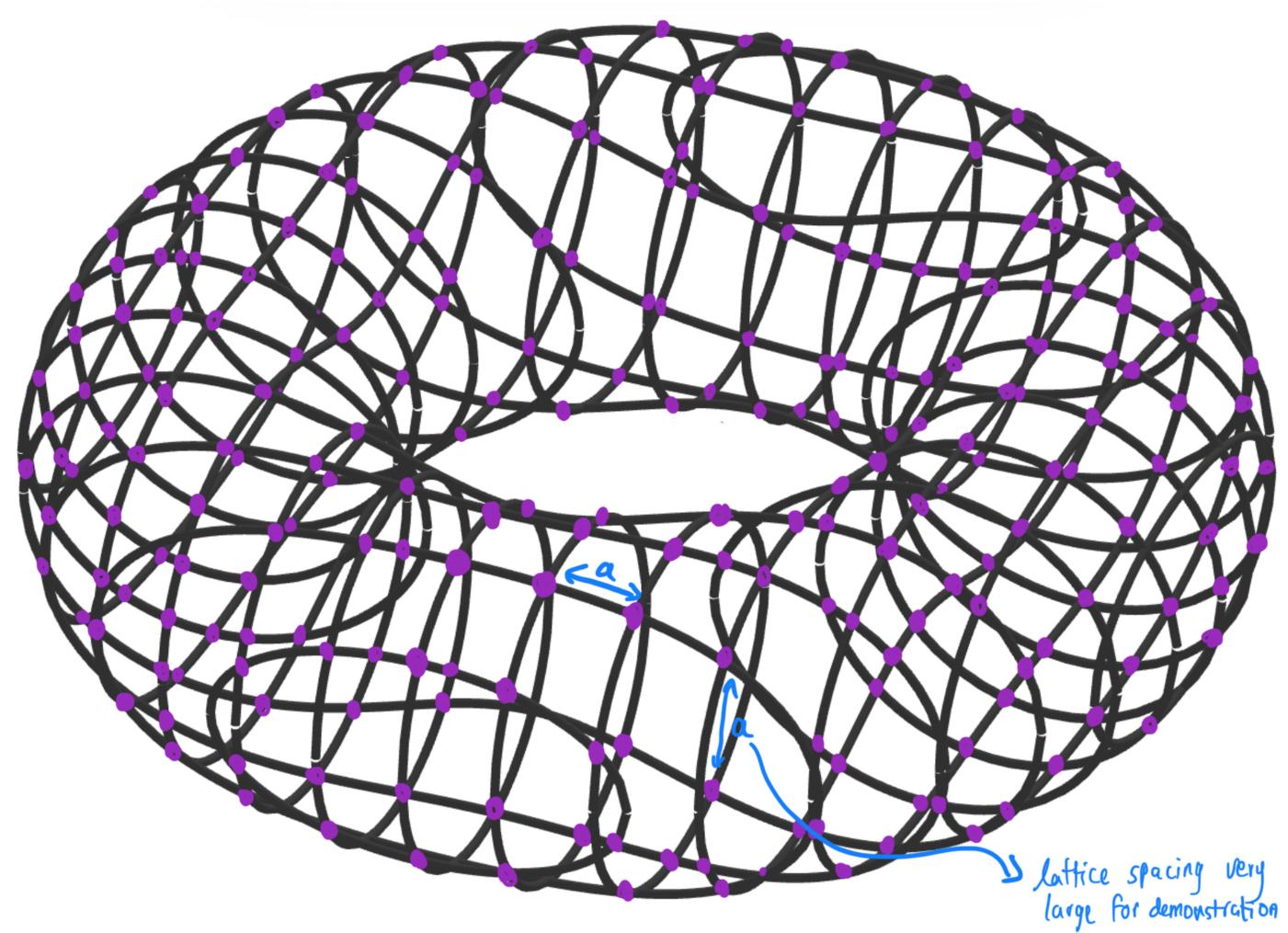


Weighted by the exponential of the QCD action

### **Moving to QCD Build a Lattice**



## **Moving to QCD** Impose Periodic Boundary Conditions







# 4D Doughnut?

Rendering error: Try installing additional dimensions via: sudo apt-get xtra-dims

## Finishing Up

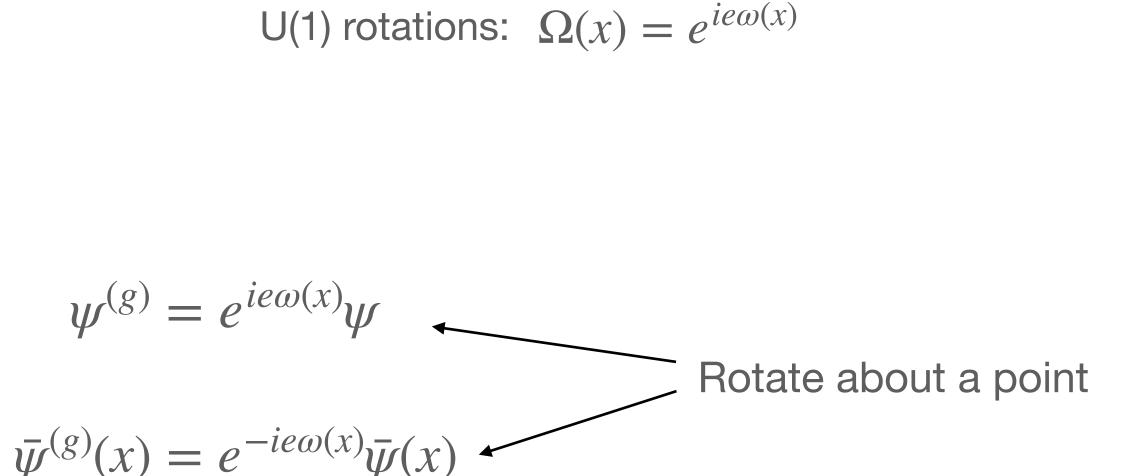
- Path Integrals for Eigenstates, and useful physics
- Calculating excited states (particles)
- Discretisation
- Make-up of the lattice
- There are so very many cool things in this field
- Big thanks to Christine Davies Physicist in Lattice QCD

#### **More on the Lattice** Local Gauge Invariance of QFTs

 $\mathscr{L}_{OED}(x) = -\frac{1}{4}F_{\mu\nu}(x)F^{\mu\nu}(x) + \bar{\psi}(x)(\gamma \cdot D + m)\psi(x)$  $F_{\mu\nu}(x) = \partial_{\mu}A_{\nu}(x) - \partial_{\nu}A_{\mu}(x)$  $D_{\mu} = \partial_{\mu} + ieA_{\mu}(x)$ 

 $A_{\mu}^{(g)} = A_{\mu} - \partial_{\mu}\omega(x)$ 

Photon field 'picks up' the difference of the gauge transformation - at the ends of a 'Link'



### **More on the Lattice** QCD Lagrangian

# $\mathscr{L}_{QCD}(x) = -\frac{1}{4} F^a_{\mu\nu}(x) F^{\mu\nu,a}(x) + \bar{\psi}(x)(\gamma \cdot D + m)\psi(x)$

#### **More on the Lattice** Local Gauge Invariance of QFTs

$$\mathscr{L}_{QED}(x) = -\frac{1}{4}F_{\mu\nu}(x)$$

 $F_{\mu\nu}(x) =$ 

 $D_{\mu}$  =

 $\psi^{(g)} = e^{ie\omega(x)}\psi$ 

 $A^{(g)}_{\mu}$ 

 $F^{\mu\nu}(x) + \bar{\psi}(x)(\gamma \cdot D + m)\psi(x)$ 

$$= \partial_{\mu}A_{\nu}(x) - \partial_{\nu}A_{\mu}(x)$$

$$= \partial_{\mu} + ieA_{\mu}(x)$$

$$\Omega(x) = e^{ie\omega(x)}$$

$$\psi, \bar{\psi}^{(g)}(x) = e^{-ie\omega(x)}\bar{\psi}(x)$$

$$= A_{\mu} - \partial_{\mu}\omega(x)$$