Simulating Quantum Physics with Computers

ZUCCMAP

Juan Fernandez

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1D Schrödinger's equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) \right] \psi(x,t)$$

1D Schrödinger's equation

$$i \frac{\partial \psi(x,t)}{\partial t} = \left[-\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x,t) \right] \psi(x,t)$$

$$(\hbar = m = 1)$$

1D Schrödinger's equation

Space discretization

$$x \in \mathbb{R} \mapsto x_n := -\frac{L}{2} + n\,h, \quad n = \{0, 1, 2, 3, \ldots, N-1\}$$

$$h = \frac{L}{2}$$

1D Schrödinger's equation

Vector representation

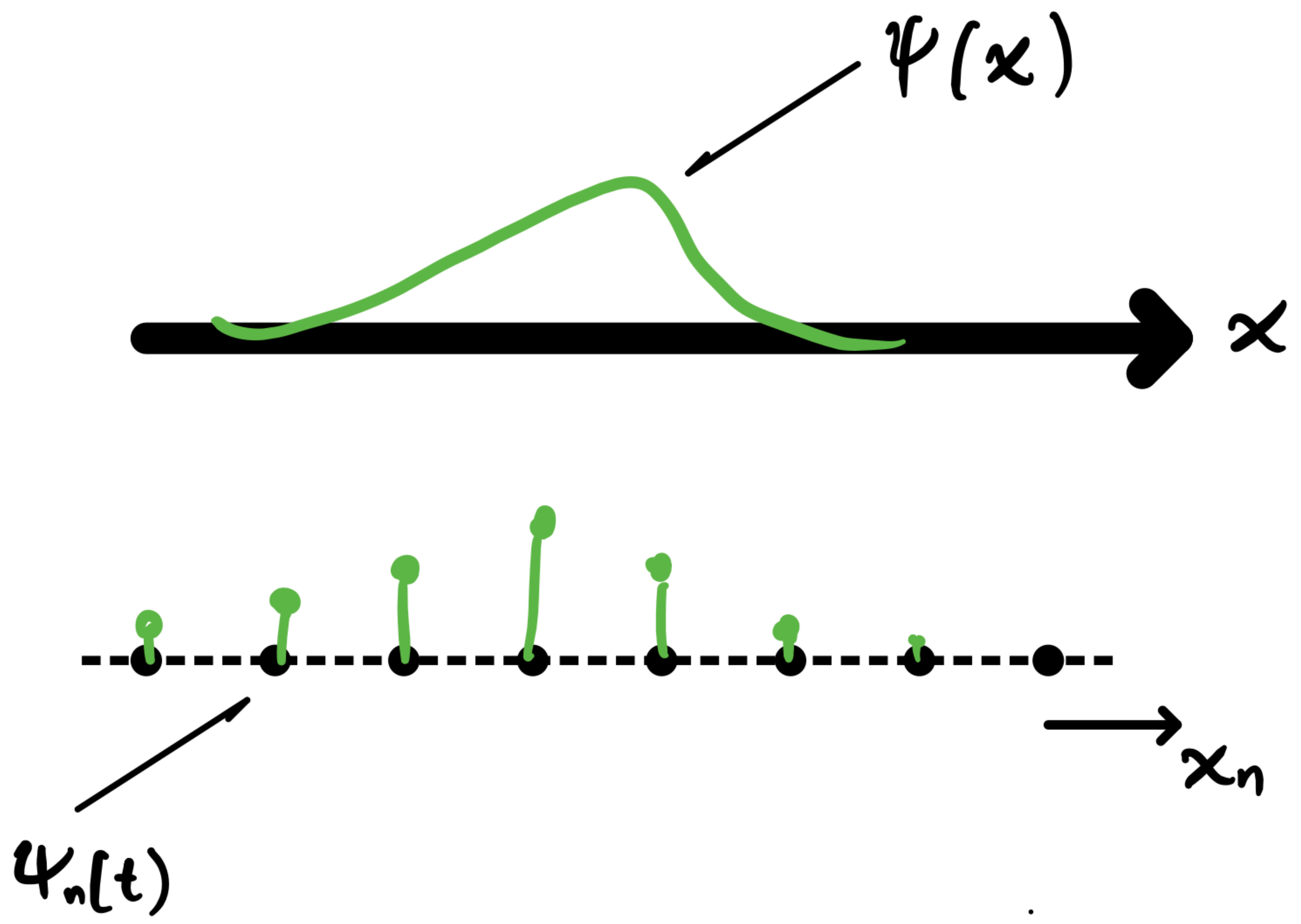
$$\psi(x,t) \mapsto \psi_n(t) = \psi(x_n, t)$$

$$\equiv \overrightarrow{\psi}(t) = \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \\ \psi_2(t) \\ \vdots \\ \psi_{N-1}(t) \end{pmatrix}$$

1D Schrödinger's equation

Vector representation

$$\overrightarrow{\psi}(t) = \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \\ \psi_2(t) \\ \vdots \\ \psi_{N-1}(t) \end{pmatrix}$$



1D Schrödinger's equation

Time discretization

$$t \in \mathbb{R} \mapsto t = \{t_0, t_0 + \tau, t_0 + 2\tau, \ \dots\} = \{t_0, t_1, t_2, \dots, t_{Nt}\}$$

$$\psi(x, t_j + \tau) = \hat{U}(t_j + \tau \,|\, t_j)\, \psi(x, t_j)$$

$$\hat{U}(t_j + \tau \,|\, t_j) \approx \exp\left(-i\tau \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V\left(x, t_j + \tau/2\right) \right] \right)$$

1D Schrödinger's equation

Separation of Kinetic and Potential sectors

$$\exp\left(-i\tau\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V\left(x,t_j+\tau/2\right)\right]\right)$$

$$\neq \exp\left(\frac{i\tau}{2}\frac{\partial^2}{\partial x^2}\right)\exp\left(-i\tau V(x,t_j+\tau/2)\right) \quad \text{!!}$$

Baker–Campbell–Hausdorff

$$\exp\left(\hat{A}+\hat{B}\right) = \exp(\hat{A}/2)\ \exp(\hat{B})\ \exp(\hat{A}/2) + \mathcal{O}([\hat{A},\hat{B}]^3)$$

1D Schrödinger's equation

Split step method

$$\hat{U}(t_j + \tau \,|\, t_j) \approx \hat{U}_K \cdot \hat{U}_{V(t_j+\tau/2)} \cdot \hat{U}_K$$

$$U_K := \exp\left(\frac{i\tau}{4}\frac{\partial^2}{\partial x^2}\right)$$

$$U_{V(t)} := \exp\left(-i\tau V(x,t)\right)$$

1D Schrödinger's equation

Potential step

$$U_{V(t)} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \\ \psi_2(t) \\ \vdots \\ \psi_{N-1}(t) \end{pmatrix}$$

1D Schrödinger's equation

Potential step

$$\begin{pmatrix} \exp[-i\tau V(x_0, t)] & & \\ & \ddots & \\ & & \exp[-i\tau V(x_{N-1}, t)] \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \vdots \\ \psi_{N-1}(t) \end{pmatrix}$$

1D Schrödinger's equation

Potential step

$$\begin{pmatrix} \exp[-i\tau V(x_0, t)] & & \\ & \ddots & \\ & & \exp[-i\tau V(x_{N-1}, t)] \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \vdots \\ \psi_{N-1}(t) \end{pmatrix}$$

$O(N)$

1D Schrödinger's equation

Kinetic step

$$\psi(x) = \int \frac{dk}{2\pi} e^{ikx}\, \tilde{\psi}(k) \qquad\qquad \tilde{\psi}(k) = \int dx\, e^{-ikx}\, \psi(x)$$

$$\implies \; U_K\, \psi(x) = \int \frac{dk}{2\pi} \exp\left(-\frac{i\tau}{4} k^2\right) e^{ikx}\, \tilde{\psi}(k)$$

DFT Interlude

$$x_n = -\frac{L}{2} + n\,h$$

$$h = \frac{L}{N}$$

$$\Longrightarrow$$

$$k_n = -\frac{K}{2} + n\,p$$

$$p = \frac{2\pi}{N\,h} = \frac{2\pi}{L}$$

$$K = N\,p = \frac{2\pi}{h}$$

DFT Interlude

$$\psi_n \approx \sum_{m=0}^{N-1} \frac{p}{2\pi} e^{ik_m x_n} \tilde{\psi}_m$$

$$\Longrightarrow$$

$$(U_K \psi)_n \approx \sum_{m=0}^{N-1} \frac{p}{2\pi} \exp\left(-\frac{i\tau}{4} k_m^2\right) e^{ik_m x_n} \tilde{\psi}_m$$

DFT Interlude

DFT/IDFT definitions in Scipy

$$DFT[\overrightarrow{\phi}] := \sum_{n=0}^{N-1} \overrightarrow{\phi} \exp\left(\frac{-2\pi i m n}{N}\right)$$

$$IDFT[\overrightarrow{\tilde{\phi}}] := \frac{1}{N} \sum_{n=0}^{N-1} \overrightarrow{\tilde{\phi}} \exp\left(\frac{2\pi i m n}{N}\right)$$

1D Schrödinger's equation

Kinetic step

$$(U_K \psi)_n \approx (-1)^n \, IDFT \left[\exp\left(-\frac{i\tau}{4} k_m^2 \right) DFT \left[(-1)^l \psi_l \right]_m \right]_n$$

1D Schrödinger's equation

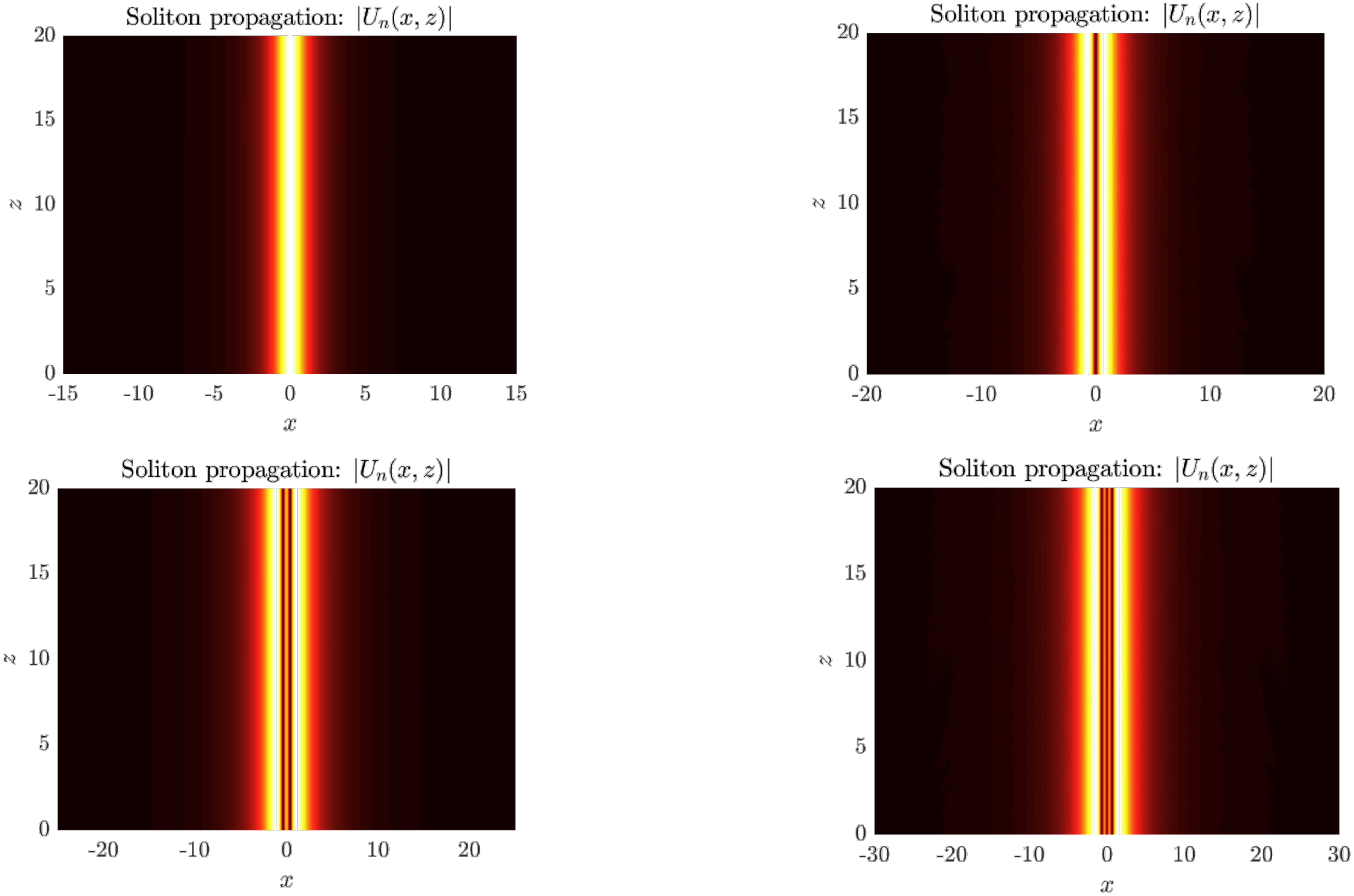
Kinetic step

$$(U_K \psi)_n \approx (-1)^n \, IDFT \left[\exp\left(-\frac{i\tau}{4} k_m^2 \right) DFT \left[(-1)^l \psi_l \right]_m \right]_n$$

$O(N \log N)$

Non-linear Schrödinger equation

$$\left[i\frac{\partial}{\partial z} + \frac{1}{2}\frac{\partial^2}{\partial x^2} + |\,U(x,z)\,|^2 + V(x,z) \right] U(x,z) = 0$$



Soliton propagation: $|U_n(x,z)|$
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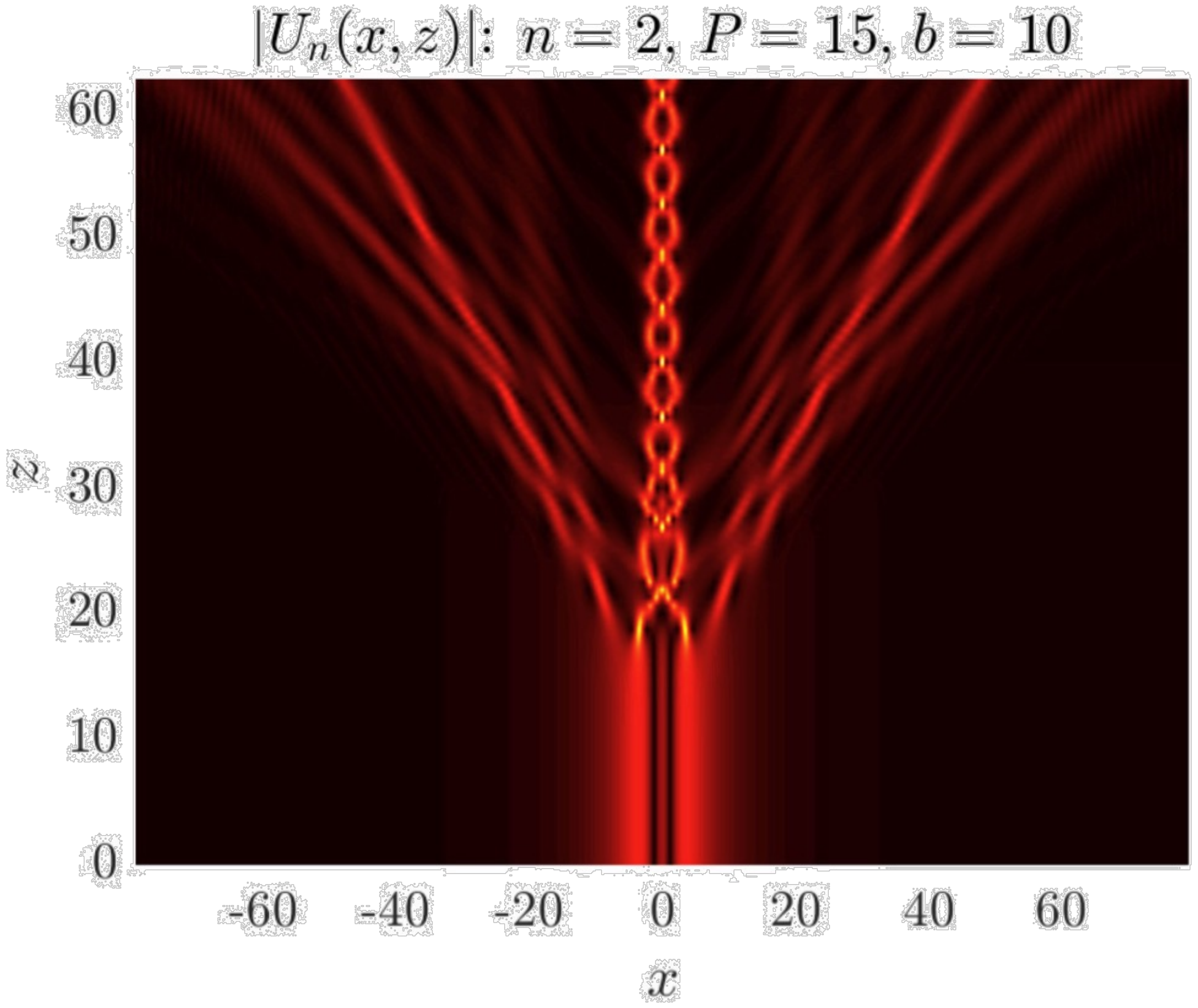
Soliton propagation: $|U_n(x,z)|$
x
z


$|U_n(x,z)|$: $n=2$, $P=15$, $b=10$
z
x
60
50
40
30
20
10
0
-60
-40
-20
0
20
40
60

Extra

$$\boxed{U_n(x,z) = \sqrt{\frac{P_{out}}{\Pi_n}}\,(b+x^2)^{1/2}\,\left[\mathrm{T}_2^{n+3}\left(\frac{x}{\sqrt{b}}\right)\right]\,e^{i\lambda z}}$$

$$\boxed{V_n(x) = \lambda - \frac{P_{out}}{\Pi_n}\,(b+x^2)\left[\mathrm{T}_2^{n+3}\left(\frac{x}{\sqrt{b}}\right)\right]^2 + \frac{b\left(n^2+6n+2\right)-6x^2}{2\left(b+x^2\right)^2}}$$

Partition function methods

Definitions

$$\rho = e^{-\beta \hat{H}} \qquad \beta = 1/T \qquad \hat{H} = \hat{T} + \hat{V} \qquad \left[\hat{T}, \hat{V}\right] \neq 0$$

Partition function methods

Definitions

$$\rho = e^{-\beta \hat{H}} \qquad \beta = 1/T \qquad \hat{H} = \hat{T} + \hat{V} \qquad \left[\hat{T}, \hat{V}\right] \neq 0$$

$$Z = Tr\left[e^{-\beta \hat{H}}\right]$$

$$\rho(x, x', \beta) = \langle x \,|\, e^{-\beta \hat{H}} \,|\, x' \rangle$$

Partition function methods

Definitions

$$Z = Tr\left[e^{-\beta\hat{H}}\right] = \int dx\, \rho(x, x, \beta)$$

Partition function methods

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$$e^{-\beta\hat{H}} = \left(e^{-\tau\hat{H}}\right)^M \qquad \tau = \beta/M$$

Partition function methods

Definitions

$$\rho(x_0, x_M, \beta) = \int dx_1 \ldots dx_{M-1}\, \rho(x_0, x_1, \tau)\, \rho(x_1, x_2, \tau)\ \ldots\ \rho(x_{M-1}, x_M, \tau)$$

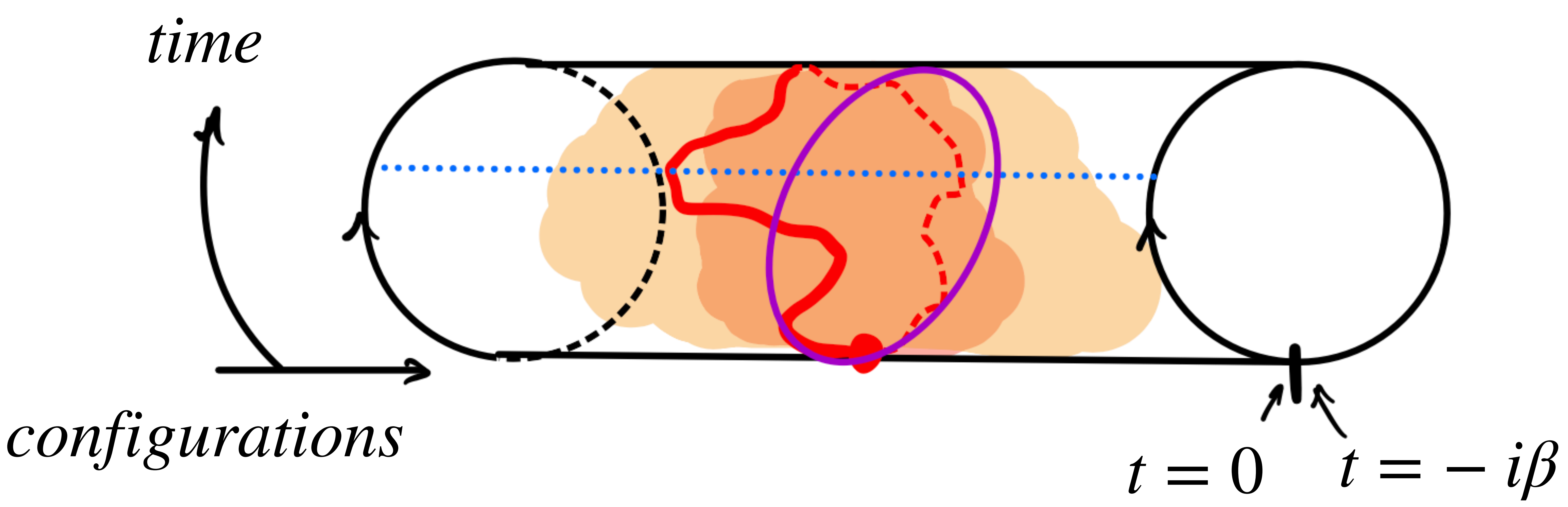
Partition function methods

Definitions

$$\rho(x_0, x_M, \beta) = \int dx_1 \ldots dx_{M-1}\, \rho(x_0, x_1, \tau)\, \rho(x_1, x_2, \tau) \;\ldots\; \rho(x_{M-1}, x_M, \tau)$$

$$\rho(x_i, x_j, \tau) = \langle x_i \,|\, e^{-\tau \hat{H}} \,|\, x_j \rangle$$

Partition function methods



Partition function methods

What's $$\rho(x_i, x_j, \tau) = \langle x_i | e^{-\tau \hat{H}} | x_j \rangle$$ **?**

Partition function methods

$$e^{-\tau\hat{H}} = e^{-\tau(\hat{T}+\hat{V})} \approx e^{-\tau\hat{V}} e^{-\tau\hat{T}}$$

Partition function methods

Potential term

$$e^{-\tau \hat{H}} = e^{-\tau(\hat{T}+\hat{V})} \approx e^{-\tau \hat{V}} e^{-\tau \hat{T}}$$

$$\langle x \,|\, e^{-\tau \hat{V}} \,|\, x' \rangle = e^{-\tau V(x)} \delta(x - x')$$

Partition function methods

Kinetic term

$$e^{-\tau\hat{H}} = e^{-\tau(\hat{T}+\hat{V})} \approx e^{-\tau\hat{V}} e^{-\tau\hat{T}}$$

$$\langle x \,|\, e^{-\tau\hat{T}} \,|\, x' \rangle = \int dp \int dp' \langle x \,|\, p \rangle \langle p \,|\, e^{-\tau\hat{T}} \,|\, p' \rangle \langle p' \,|\, x' \rangle$$

$$= \sqrt{\frac{1}{2\pi\tau}} e^{-\frac{1}{2\tau}(x-x')^2}$$

$\hat{T} = \hat{p}^2/2$

Partition function methods

$$Z = \int dx\, \rho(x, x, \beta)$$

$$= \int dx_0\, dx_1 \ldots dx_{M-1}\, \rho(x_0, x_1, \tau)\, \rho(x_1, x_2, \tau) \;\ldots\; \rho(x_{M-1}, x_0, \tau)$$

$$= \int \left(\prod_{i=0}^{M-1} dx_i \right) \prod_{i=0}^{M-1} \left[(2\pi\tau)^{-Nd/2} \exp\left(-\frac{|x_i - x_{i+1}|^2}{2\tau} - \tau V(x_i) \right) \right]$$

Metropolis Algorithm in a Nutshell

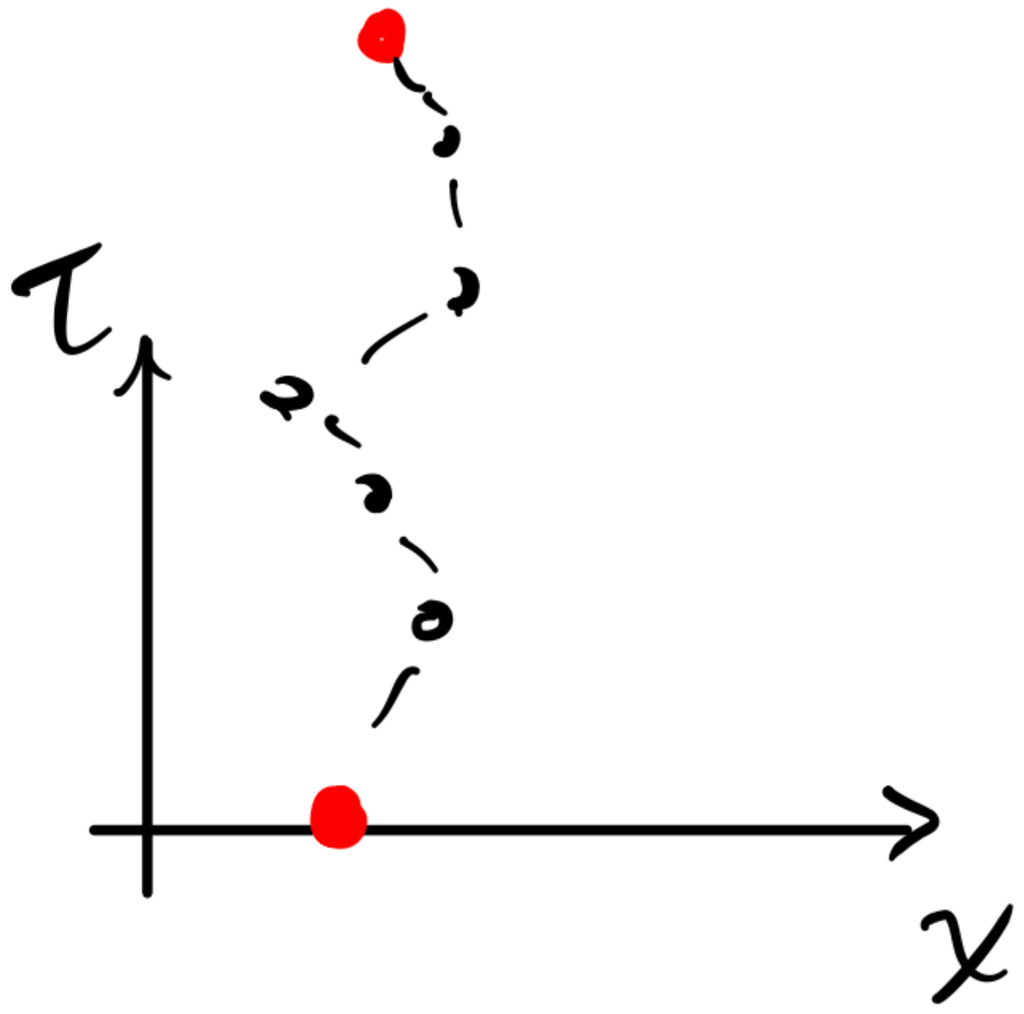
$$T(X \to X') = T(X' \to X) \sim Uniform$$

$$A(X \to X') = min\left(1, \frac{e^{-\tau \hat{H}(X')}\, T(X' \to X)}{e^{-\tau \hat{H}(X)}\, T(X \to X')}\right)$$

Metropolis Algorithm in a Nutshell

$$T(X \to X') = T(X' \to X) \sim Uniform$$

$$A(X \to X') = min\left(1, \frac{e^{-\tau \hat{H}(X')}\,\cancel{T(X' \to X)}}{e^{-\tau \hat{H}(X)}\,\cancel{T(X \to X')}}\right)$$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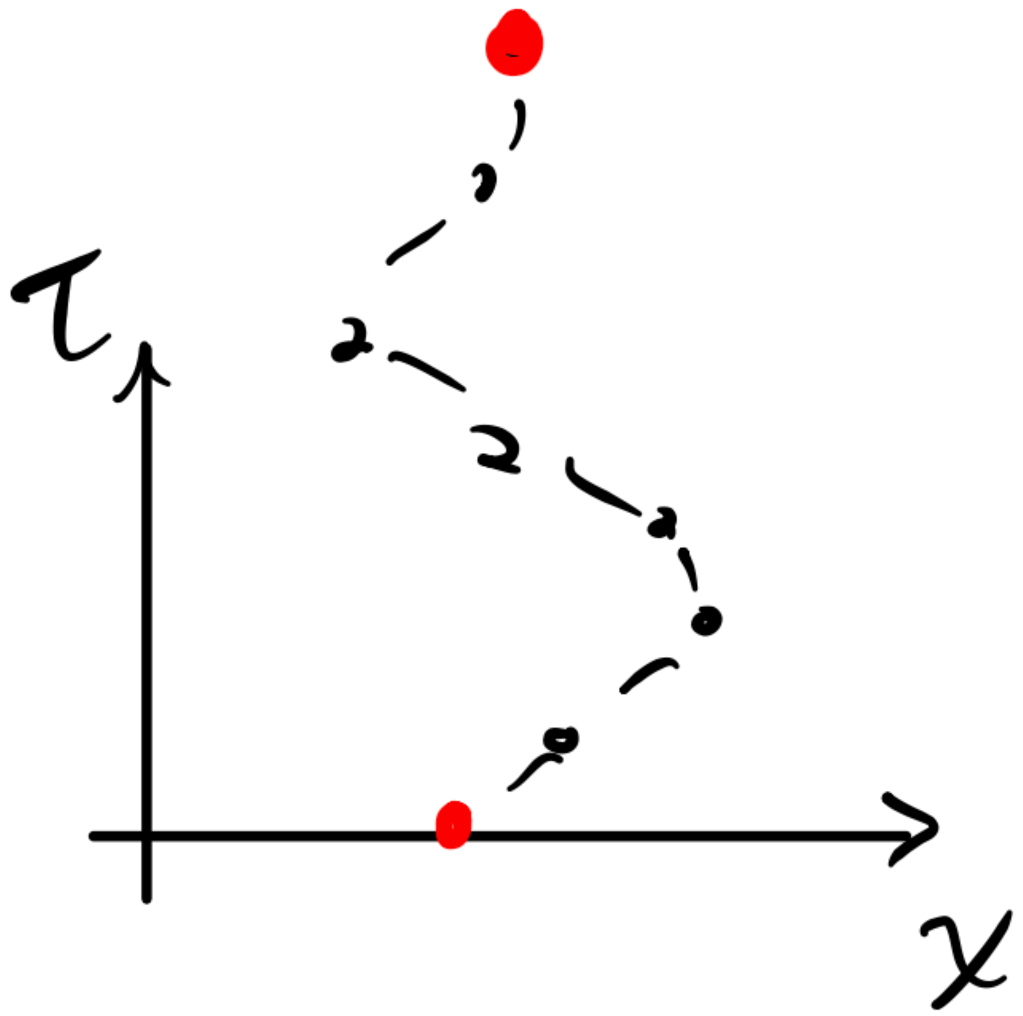
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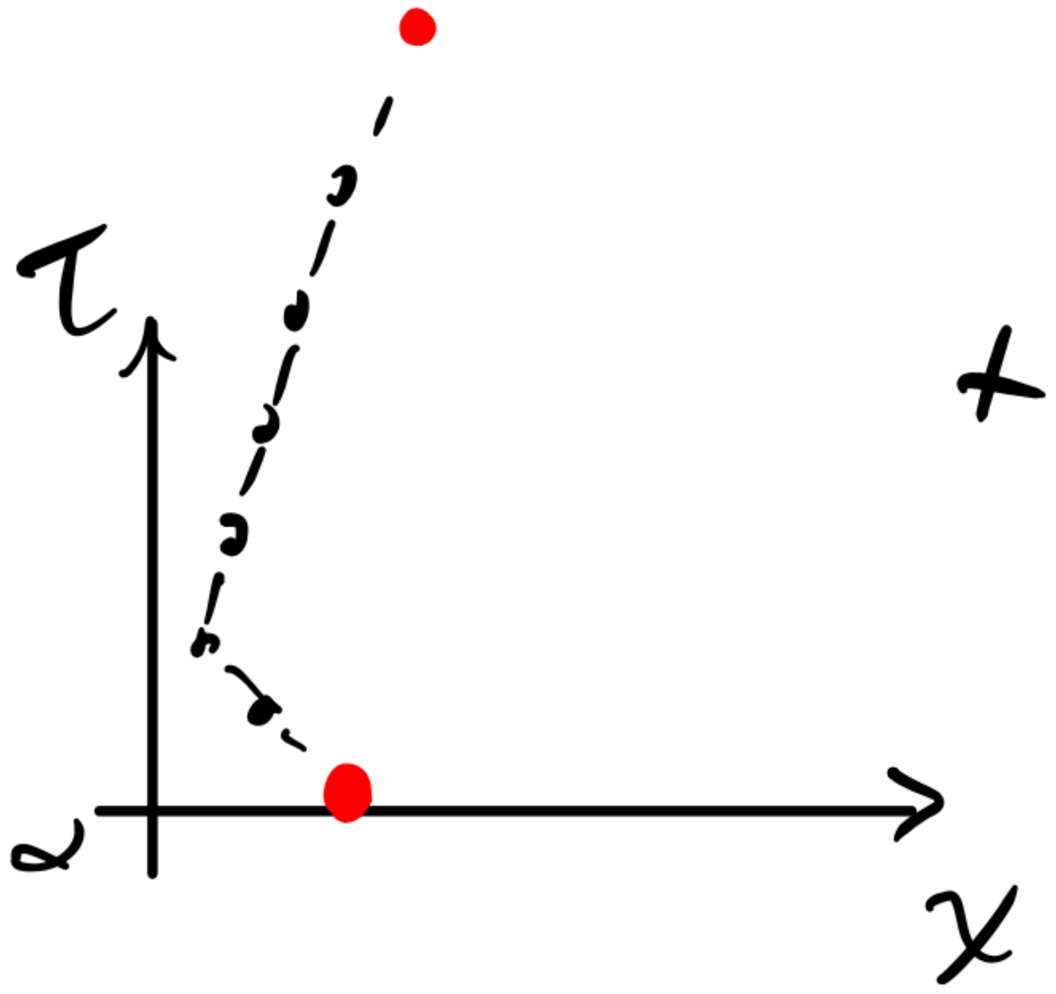
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Q ? A :

Thank you!