Towards a Configuration-space Interaction with the Quantum Potential as its Continuum limit

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Nanometric System Simulation
Nanoscience and Nanotechnology
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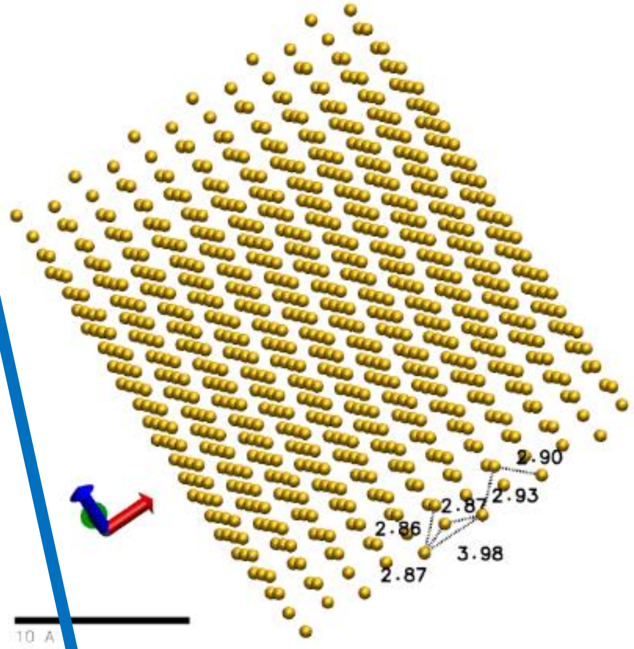

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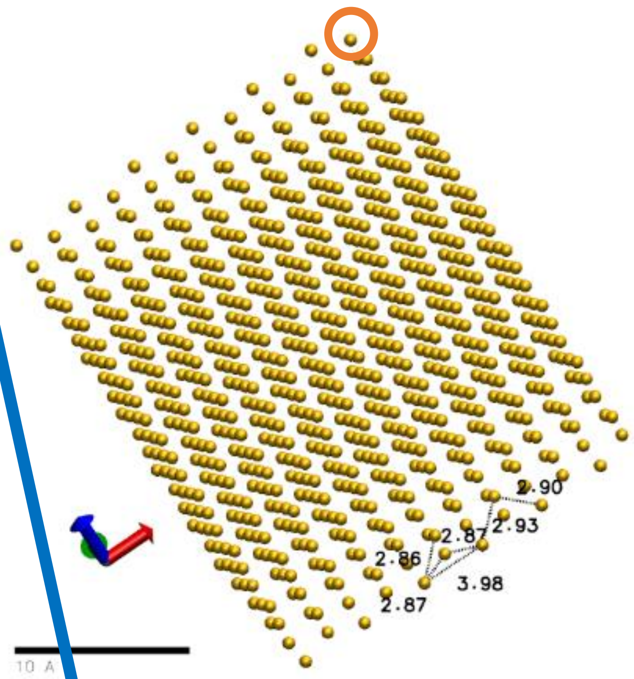

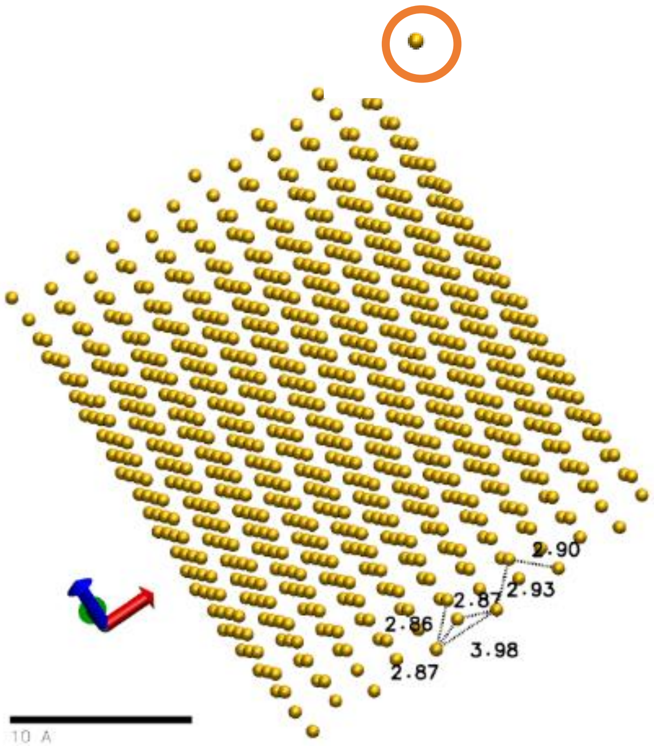

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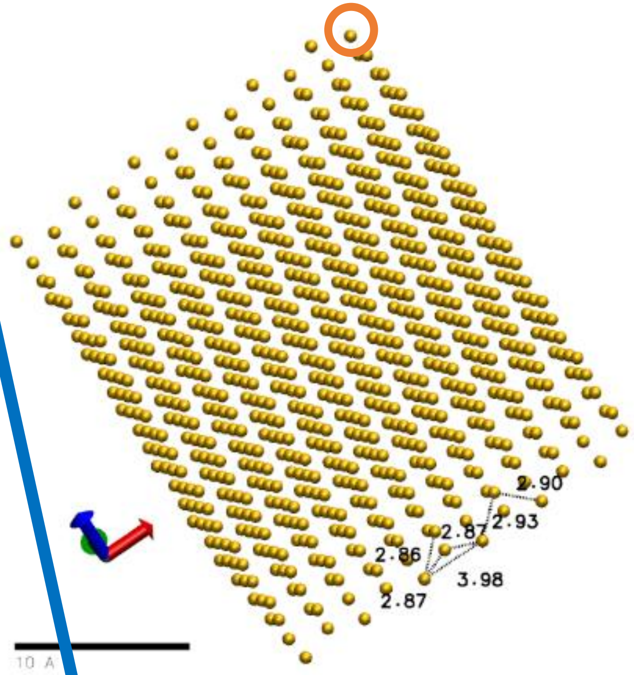

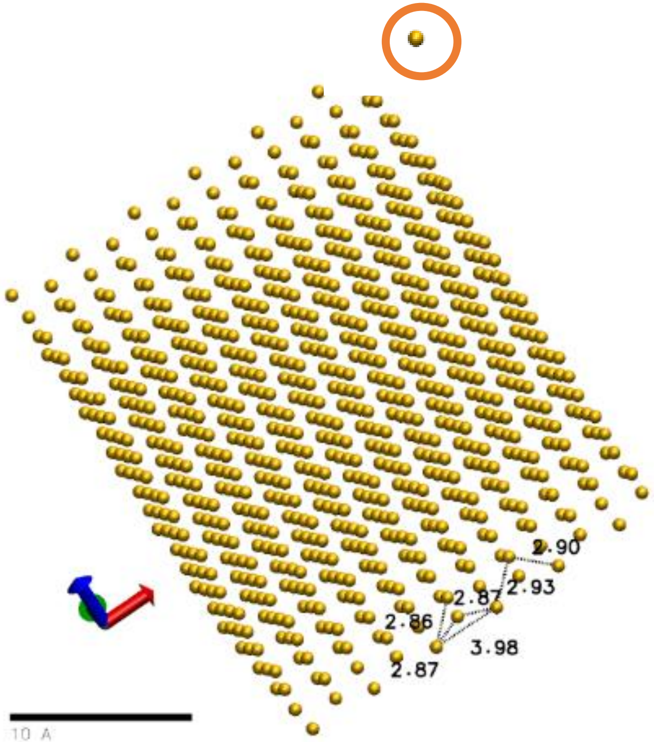

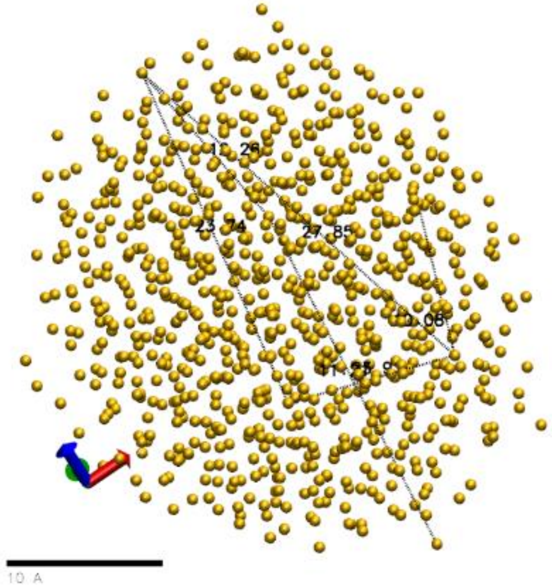

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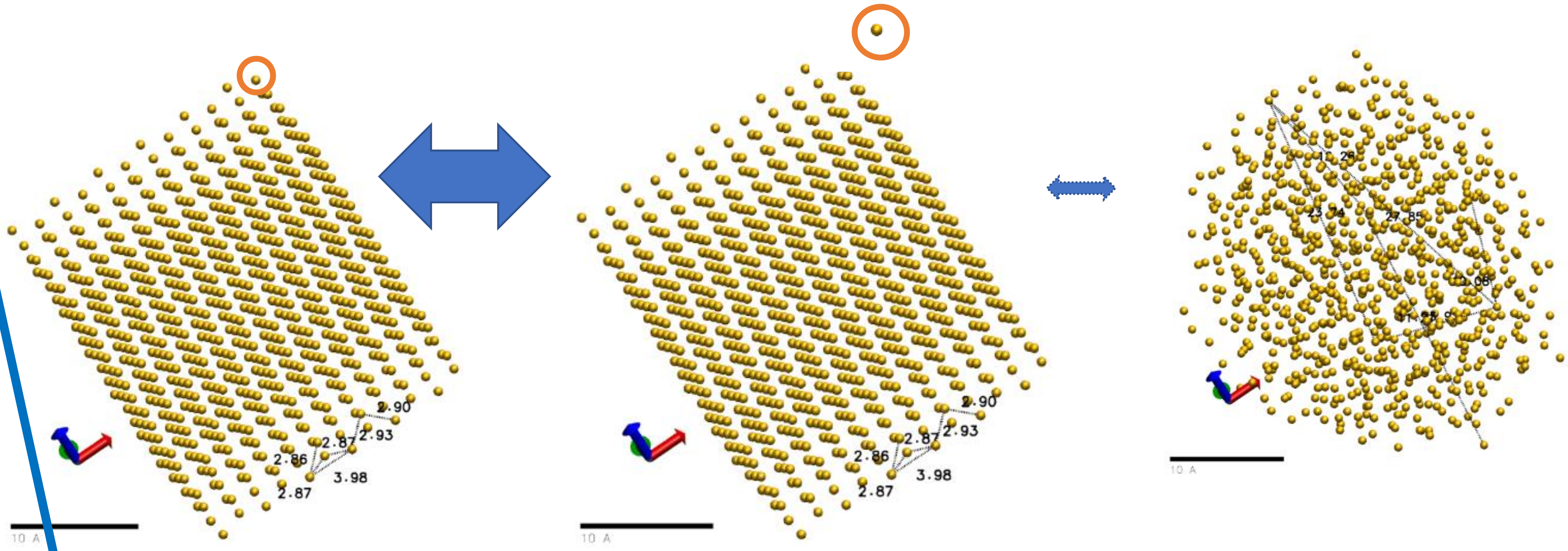

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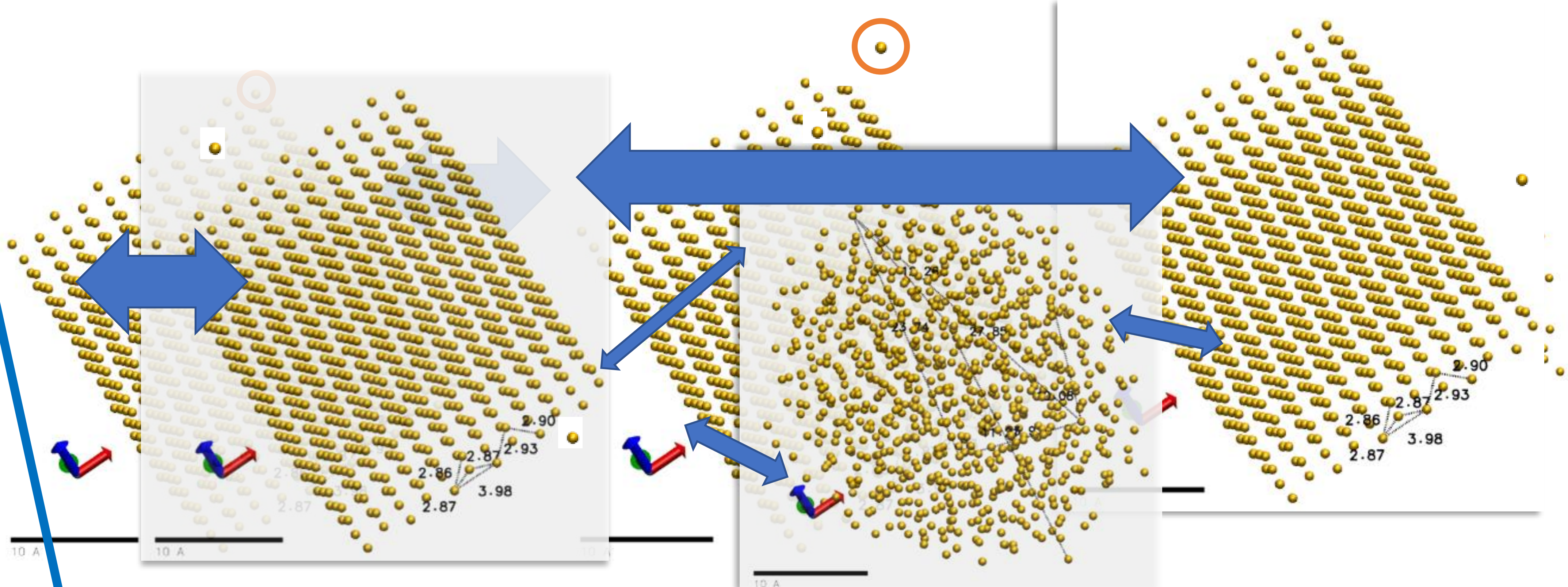

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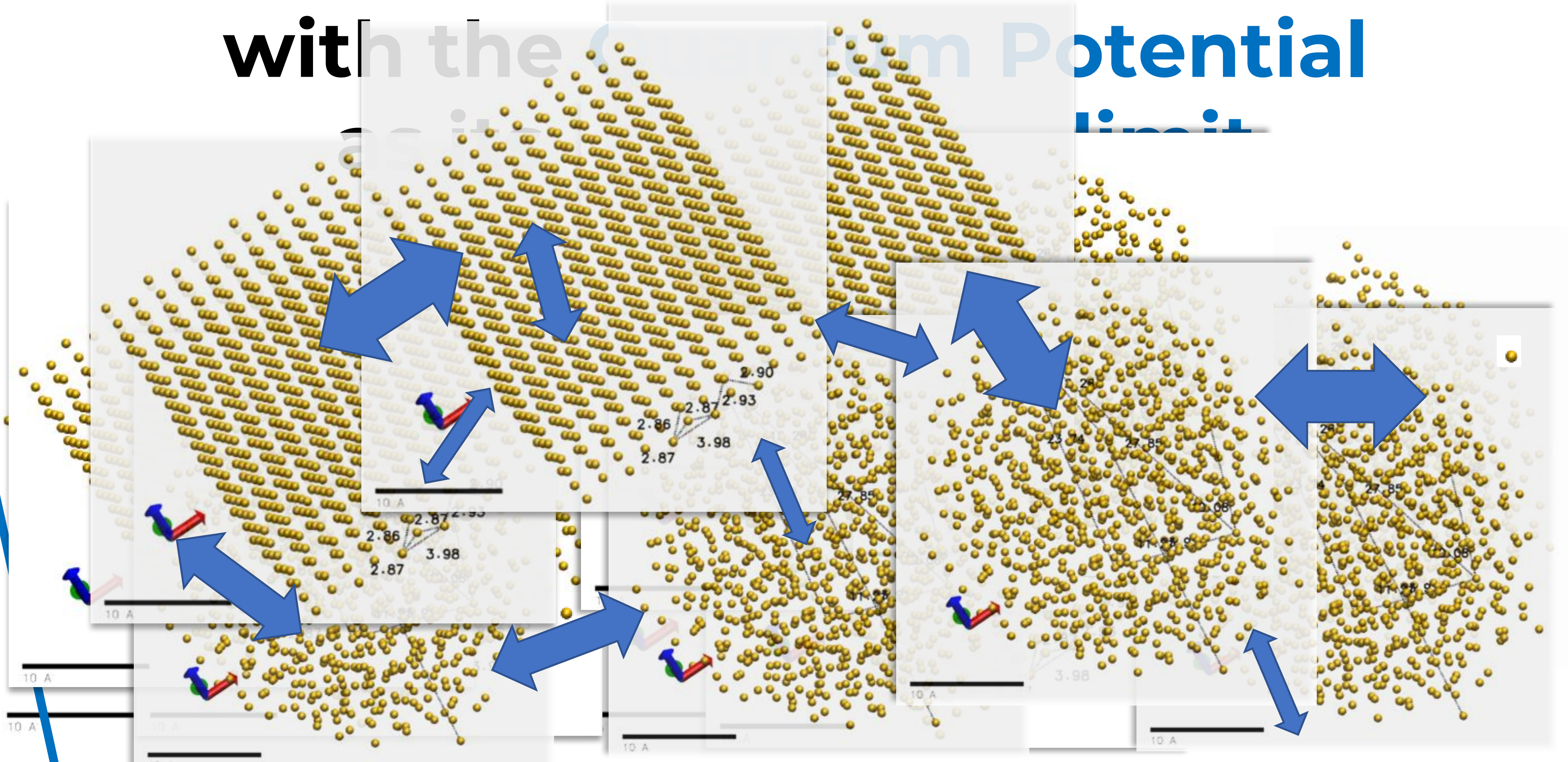

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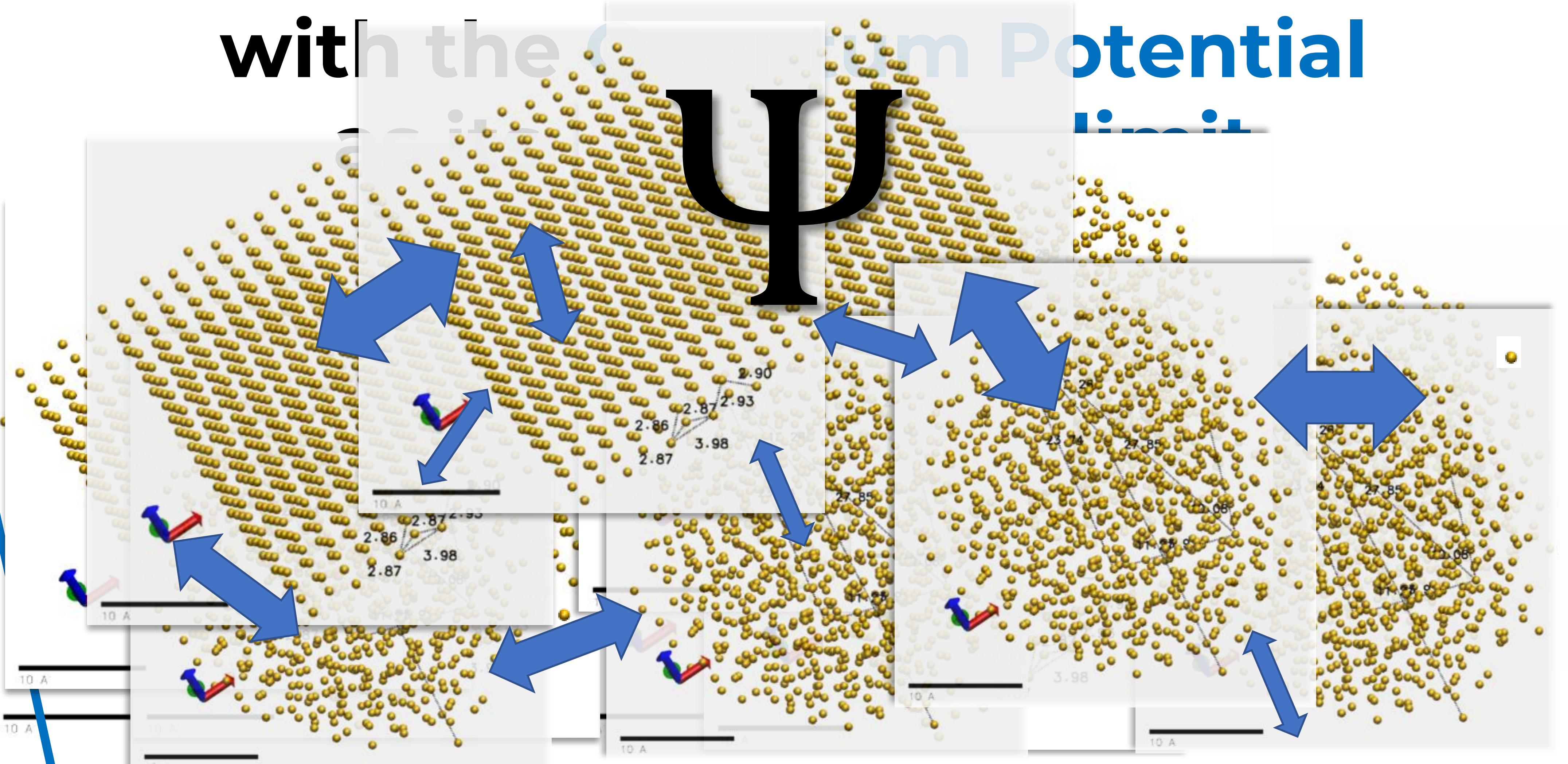

I – A Quantum Universe
=
Many Classical Universes?

I – A Quantum Universe = Many Classical Universes?

(a) A Continuum of Classical Universes

Schrödinger Equation

$$i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} = \sum_{k=1}^{n} \frac{-\hbar^2}{2m_k} \frac{\partial^2 \psi(\vec{x},t)}{\partial x_k^2} + V(\vec{x})\psi(\vec{x},t)$$

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$$\frac{\partial\rho(\vec{x},t)}{\partial t} = -\sum_{k=1}^{n}\frac{\partial}{\partial x_k}\left[\rho(\vec{x},t)v_k(\vec{x},t)\right]$$

$$-\frac{\partial S(\vec{x},t)}{\partial t} = \sum_{k=1}^{n}\frac{1}{2}m_k v_k(\vec{x},t)^2 + V(\vec{x},t) + Q(\vec{x},t)$$

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$$v_k(\vec{x},t) := \frac{1}{m_k}\frac{\partial S(\vec{x},t)}{\partial x_k}$$

Bohmian velocity

$$Q(\vec{x},t) := -\frac{\hbar^2}{4m_k}\left(\frac{1}{\rho}\sum_k\frac{\partial^2\rho}{\partial x_k^2} - \frac{1}{2\rho^2}\sum_k\left(\frac{\partial\rho}{\partial x_k}\right)^2\right)$$

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NEWTON's SECOND LAW!

$$m_k\frac{\partial^2 x_k(\vec{\xi},t)}{\partial t^2} = -\frac{\partial}{\partial x_k}\left[V(\vec{x},t)+Q(\vec{x},t)\right]\Big|_{\vec{x}=\vec{x}(\vec{\xi},t)}$$

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$$\frac{\mathrm{d}\rho(\vec{x}^{\xi}(t),t)}{\mathrm{d}t}=-\rho(\vec{x}^{\xi}(t),t)\sum_{k=1}^{n}\frac{\partial v_k(\vec{x},t)}{\partial x_k}\Big|_{\vec{x}=\vec{x}^{\xi}(t)}$$

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$$\Vert$$

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$$\vec{x}(\vec{\xi},t_0) = \vec{\xi} \in \mathbb{R}^n$$

UnCountable set of possible trajectories!

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(b) A Swarm of Classical Universes

$$\{\vec{x}^{\eta}\}_{\eta\in\sigma}$$

Countable set of possible trajectories!

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Newton's Law ~~for a Fluid~~ For M "Particles" In Configuration-space!!!

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$$W\,???$$

II – Their Proposal

Already tried in the literature:

- **Nearest Neighbour** interactions

M. J. Hall, D.-A. Deckert, and H. M. Wiseman. Physical Review X, vol. 4, no. 4, p. 041013, 2014.

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II – Their Proposal

Already tried in the literature:

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  - **Continuum limit** of **Classical Field** Theories

  - Computational **efficiency?**

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- **Moving grid approximations** of $Q(\rho(\vec{x}, t))$

  - Quantum **hydrodynamics** helpful

S. Sturniolo. Physical Review E, vol. 97, no. 5, p. 053311, 2018.

R. E. Wyatt, *Quantum dynamics with trajectories*. Springer 2005

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- **Classical Fundamental Forces** are always **Non-Local (in physical space)**

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- **Quantum Potential is non-local (in configuration** space)

- **Quantum Force** would be pretty **fundamental!**

What about looking for **a non-local force**
that is **like the classical fundamental forces?**
(but in configuration space)

$$W_{\xi,\eta}(\vec{x}^{\xi}, \vec{x}^{\eta}) = \frac{C}{||\vec{x}^{\xi} - \vec{x}^{\eta}||^{B}}$$

$$C, B > 0$$

Repulsive

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Total Inter-Universe Potential

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Inter-Universe Force

$$\vec{G}_{\xi,\eta} = \frac{A}{||\vec{x}^{\xi} - \vec{x}^{\eta}||^{K}}\hat{u}$$

$$A := C/B, \, K := B + 1$$

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III – Methods

(a) Solving the Uncountable Tangent Universes

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W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, Numerical recipies: The art of scientific computing. Cambridge university press, 2007

$$\psi(\vec{x}, t + k\Delta t) = \hat{U}^{k}_{\vec{x},\Delta t}\psi(\vec{x}, t)$$

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$$\hat{U}_{\Delta t} = \hat{U}^{-1}_{-\frac{\Delta t}{2}} \hat{U}_{\frac{\Delta t}{2}}$$

$$\hat{U}_{\vec{x},\Delta t} \simeq \left(\sum_{k=0}^{N} \frac{1}{k!} \left[\frac{i}{\hbar} \hat{H}_{\vec{x}} \frac{\Delta t}{2} \right]^{k} \right)^{-1} \sum_{k=0}^{N} \frac{1}{k!} \left[\frac{-i}{\hbar} \hat{H}_{\vec{x}} \frac{\Delta t}{2} \right]^{k}$$

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$$\hat{U}_{\vec{x},\Delta t} \simeq \left(\sum_{k=0}^{N} \frac{1}{k!}\left[\frac{i}{\hbar}\hat{H}_{\vec{x}}\frac{\Delta t}{2}\right]^k\right)^{-1} \sum_{k=0}^{N} \frac{1}{k!}\left[\frac{-i}{\hbar}\hat{H}_{\vec{x}}\frac{\Delta t}{2}\right]^k$$

$$\hat{U}_{\Delta t} = \hat{U}^{-1}_{-\frac{\Delta t}{2}}\hat{U}_{\frac{\Delta t}{2}}$$

$$\psi^{(t+\Delta t)}_{(j_1,\ldots,j_n)} - \frac{i\Delta t}{2\hbar}\left[\sum_{k=1}^{n}\frac{\hbar^2}{2m_k}\left(\frac{\psi^{(t+\Delta t)}_{(j_1,\ldots,j_k+1,\ldots,j_n)} - 2\psi^{(t+\Delta t)}_{(j_1,\ldots,j_k,\ldots,j_n)} + \psi^{(t+\Delta t)}_{(j_1,\ldots,j_k-1,\ldots,j_n)}}{(\Delta x_k)^2}\right) - V_{j_1,\ldots,j_k}\psi^{(t+\Delta t)}_{(j_1,\ldots,j_n)}\right] =$$

$$= \psi^{(t)}_{(j_1,\ldots,j_n)} + \frac{i\Delta t}{2\hbar}\left[\sum_{k=1}^{n}\frac{\hbar^2}{2m_k}\left(\frac{\psi^{(t)}_{(j_1,\ldots,j_k+1,\ldots,j_n)} - 2\psi^{(t)}_{(j_1,\ldots,j_k,\ldots,j_n)} + \psi^{(t)}_{(j_1,\ldots,j_k-1,\ldots,j_n)}}{(\Delta x_k)^2}\right) - V_{j_1,\ldots,j_k}\psi^{(t)}_{(j_1,\ldots,j_n)}\right]$$

(a) Solving the Uncountable Tangent Universes

Schrödinger Equation

W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, Numerical recipies: The art of scientific computing. Cambridge university press, 2007

$$\psi(\vec{x}, t + k\Delta t) = \hat{U}^k_{\vec{x},\Delta t}\psi(\vec{x}, t)$$

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$$\hat{U}_{\Delta t} = \hat{U}^{-1}_{-\frac{\Delta t}{2}}\hat{U}_{\frac{\Delta t}{2}}$$

$$b_{(j_1,\dots,j_n)}\psi^{(t+\Delta t)}_{(j_1,\dots,j_n)} + \sum_{k=1}^{n} a_k\left(\psi^{(t+\Delta t)}_{(j_1,..,j_k-1,..,j_n)} + \psi^{(t+\Delta t)}_{(j_1,..,j_k+1,..,j_n)}\right) =$$

$$= d_{(j_1,\dots,j_n)}\psi^{(t)}_{(j_1,\dots,j_n)} - \sum_{k=1}^{n} a_k\left(\psi^{(t)}_{(j_1,..,j_k-1,..,j_n)} + \psi^{(t)}_{(j_1,..,j_k+1,..,j_n)}\right)$$

Crank Nicolson Master Equation

(a) Solving the Uncountable Tangent Universes

$$b_{(j_1,\ldots,j_n)}\psi^{(t+\Delta t)}_{(j_1,\ldots,j_n)} + \sum_{k=1}^{n} a_k\left(\psi^{(t+\Delta t)}_{(j_1,..,j_k-1,..,j_n)} + \psi^{(t+\Delta t)}_{(j_1,..,j_k+1,..,j_n)}\right) =$$

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$$U_L\vec{\psi}^{(t+\Delta t)} = U_R\vec{\psi}^{(t)}$$

Crank Nicolson Master Equation

(a) Solving the Uncountable Tangent Universes

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Linear Equation System Resolution!

- LU decomposition

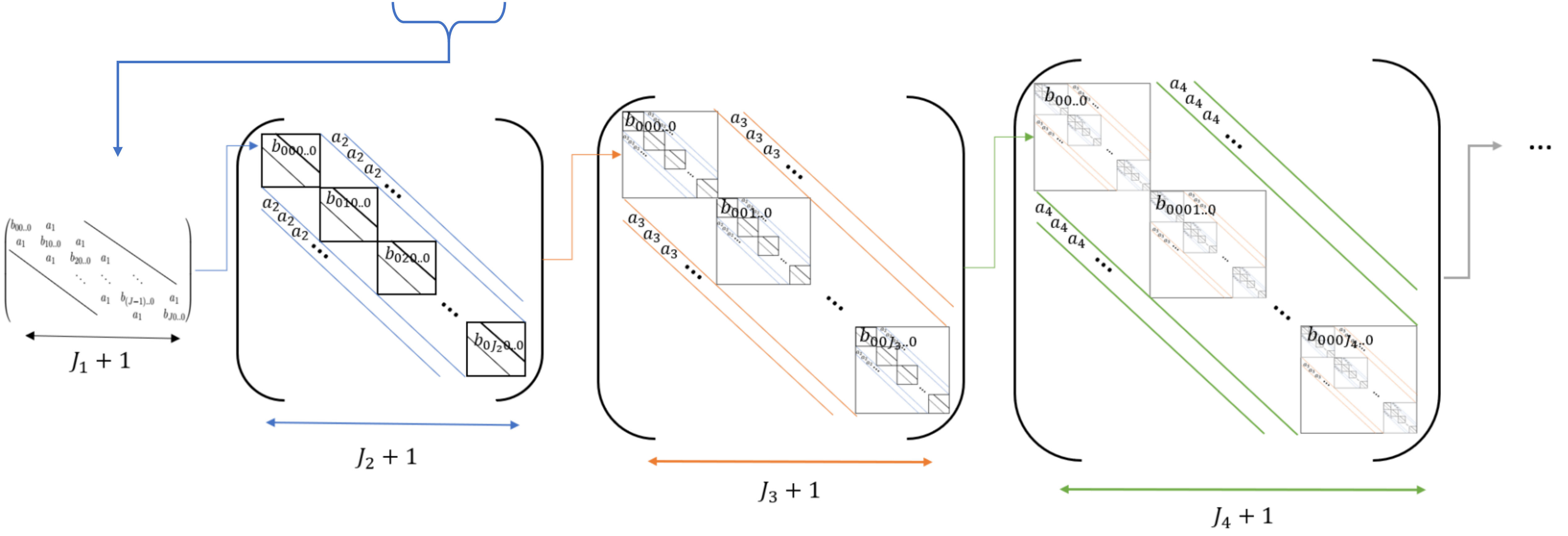
$$U_L\vec{\psi}^{(t+\Delta t)} = U_R\vec{\psi}^{(t)}$$

Crank Nicolson Master Equation

(a) Solving the Uncountable Tangent Universes

$$U_L \vec{\psi}^{(t+\Delta t)} = U_R \vec{\psi}^{(t)}$$

$$U_L = U_R^*$$



(b) Solving the Countable Tangent Universes

Verlet Algorithm

$$\vec{x}^{\xi}(t+\Delta t)+\vec{x}^{\xi}(t-\Delta t) = 2\vec{x}^{\xi}(t)+\frac{\mathrm{d}^2\vec{x}^{\xi}(t)}{\mathrm{d}t^2}\Delta t^2+O(\Delta t^4)$$

(b) Solving the Countable Tangent Universes

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"Reconstruct" Eulerian fields

$$\rho(\vec{x},t) \simeq \mathcal{N}\sum_{\vec{\xi}\in\sigma} exp\left(-\frac{||\vec{x}-\vec{x}^{\xi}(t)||^2}{2s^2}\right)$$

Gaussian kernels

(b) Solving the Countable Tangent Universes

Verlet Algorithm

$$\vec{x}^{\xi}(t+\Delta t)+\vec{x}^{\xi}(t-\Delta t) = 2\vec{x}^{\xi}(t)+\frac{\mathrm{d}^2\vec{x}^{\xi}(t)}{\mathrm{d}t^2}\Delta t^2+O(\Delta t^4)$$

"Reconstruct" Eulerian fields

$$\rho(\vec{x},t) \simeq \mathcal{N}\sum_{\vec{\xi}\in\sigma} exp\left(-\frac{||\vec{x}-\vec{x}^{\xi}(t)||^2}{2s^2}\right)$$

Gaussian kernels

$$\vec{v}(\vec{x},t) \simeq \frac{\sum_{\vec{\xi}\in\sigma_{\vec{x}}}\frac{1}{||\vec{x}-\vec{x}^{\xi}(t)||}\vec{v}^{\xi}(t)}{\sum_{\vec{\xi}\in\sigma_{\vec{x}}}\frac{1}{||\vec{x}-\vec{x}^{\xi}(t)||}}$$

K-Nearest Neighbours

IV – The Implementation

IV – The Implementation

Followed Steps:

(a) Implement SE and MIW in Jupyter Notebooks:
sparse matrix calculations, plotting…

Python 3

- *Numpy*
- *Scipy*
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Grid of different **K,A** for inter-Univ **potential**

Python 3

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(d) Coordinator script of **CPU parallel** process **pool:**
Grid of different **K,A** for inter-Univ **potential**

(e) Meta-coordinator of **CPU parallel** processes**:**
Queue of different **initial conditions**
and classical potentials to try

Python 3

- *Numpy*
- *Scipy*
- *Matplotlib*

- *Cupy*

- *importlib*
- *Multiprocessing*
- *Sys*
- *os*

Oiangu9 / Countable_vs_Uncountable_Tangent_Universes Public

main 1 branch 0 tags Go to file Code

Oiangu9 Minor typos corrected 5a75bd0 3 hours ago 36 commits

PROJECT_I	Repository completely reorganized for greater usability. Only documen...	3 days ago
SANDBOX	Repository completely reorganized for greater usability. Only documen...	3 days ago
.gitignore	Writing README	last week
LICENSE.md	License uploaded	last week
PROJECT_REPORT.pdf	Minor typos corrected	3 hours ago
README.md	Repository completely reorganized for greater usability. Only documen...	3 days ago

README.md

Countable or Uncountable Tangent Universes?

Contents

(1.) Repository Structure and Contents

About

No description, website, or topics provided.

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0 forks
Report repository

Releases

No releases published

Packages

No packages published

Languages

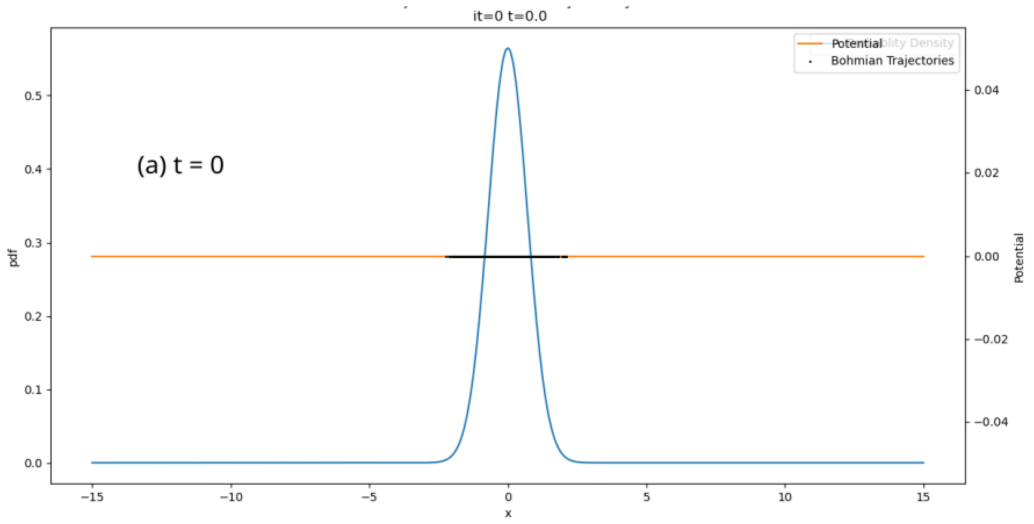
Jupyter Notebook 86.2% Python 13.8%

V – Results

V – Results

(a) Qualitatively this is Quantum Mechanics!

Broadening/Dispersion



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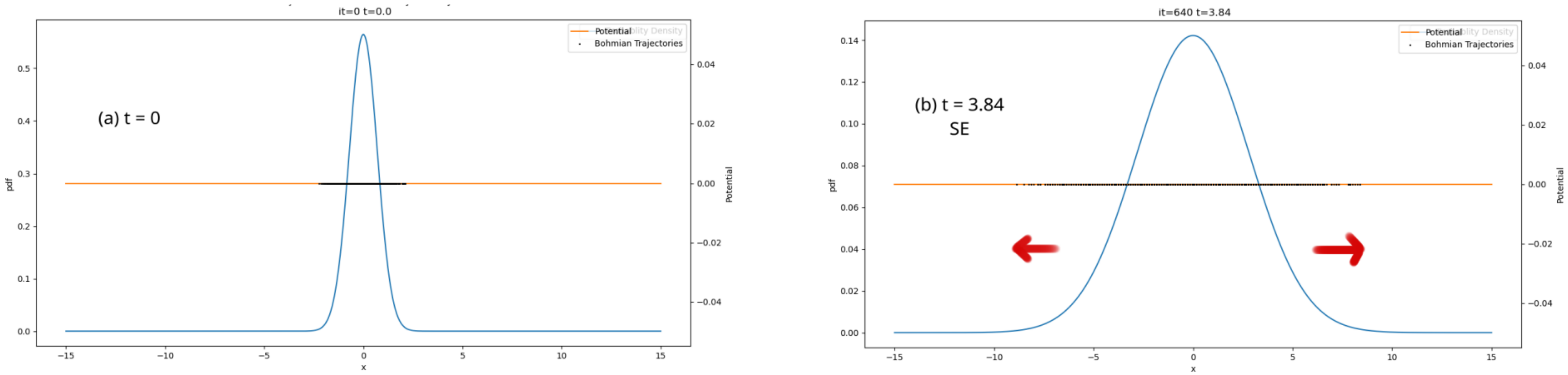

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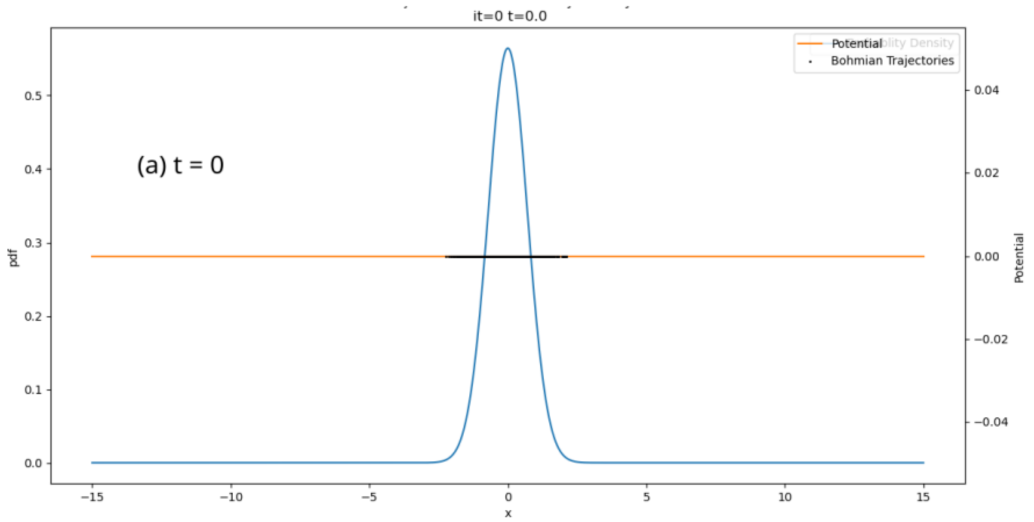

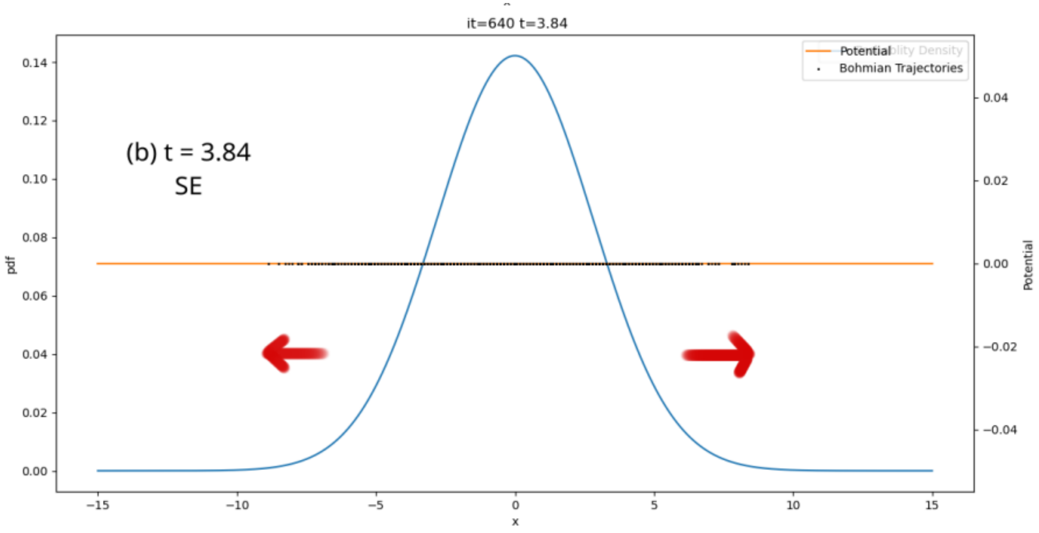

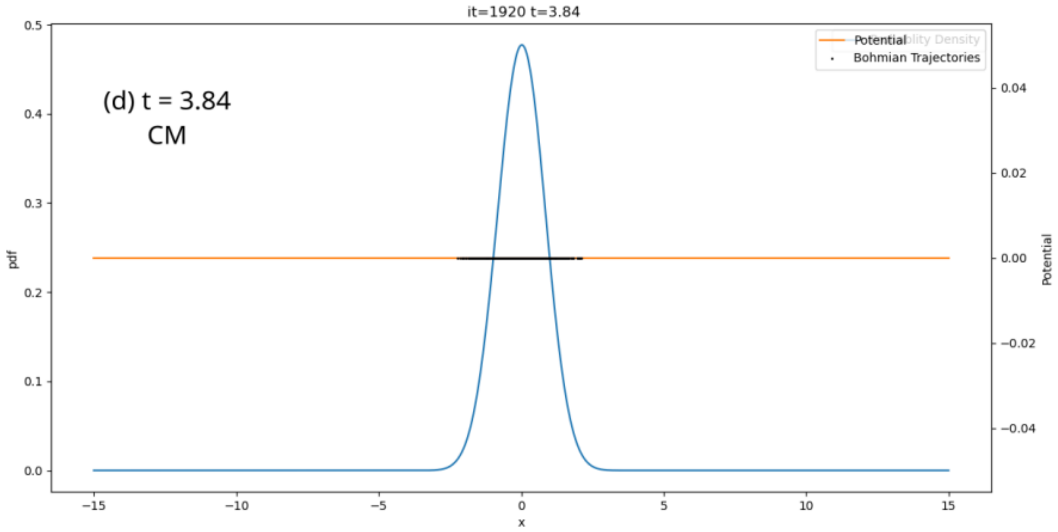

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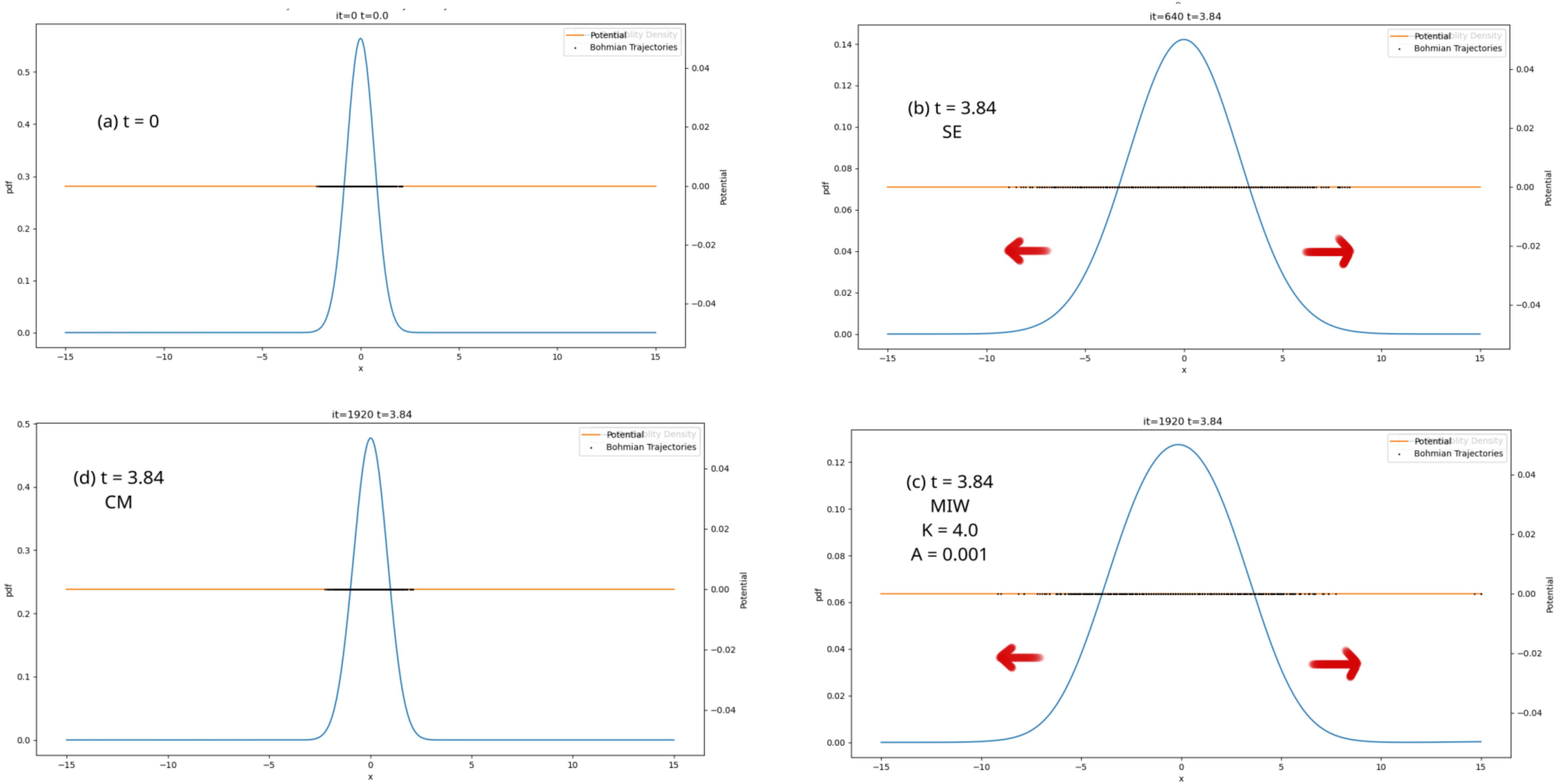

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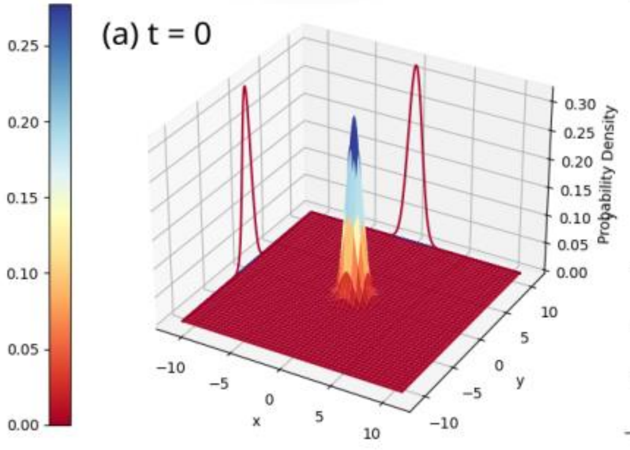

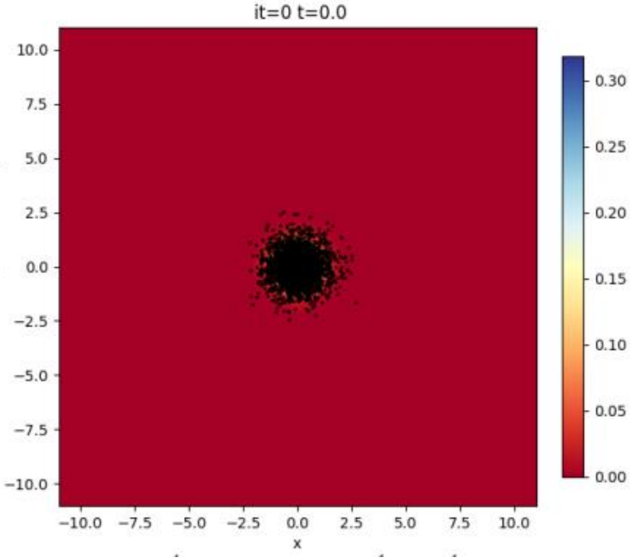

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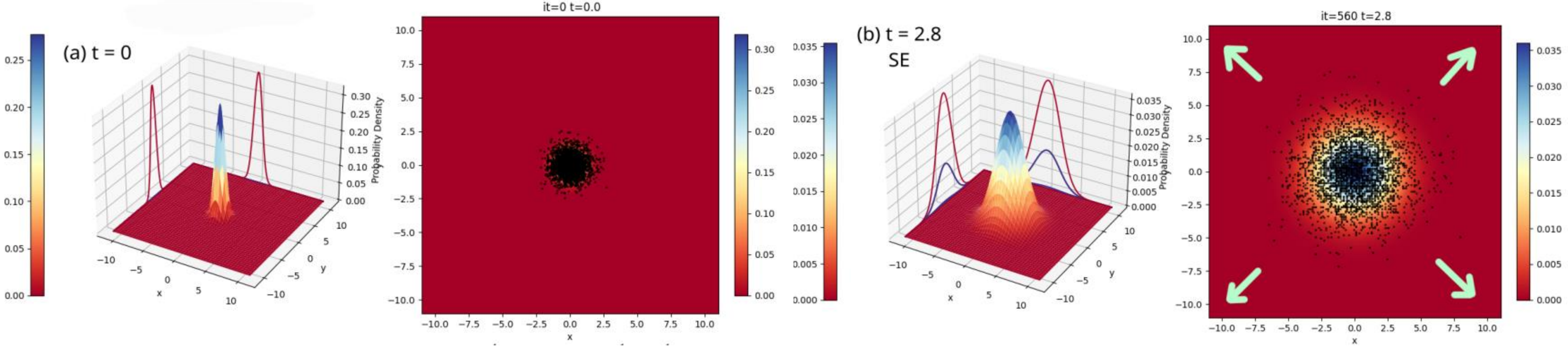

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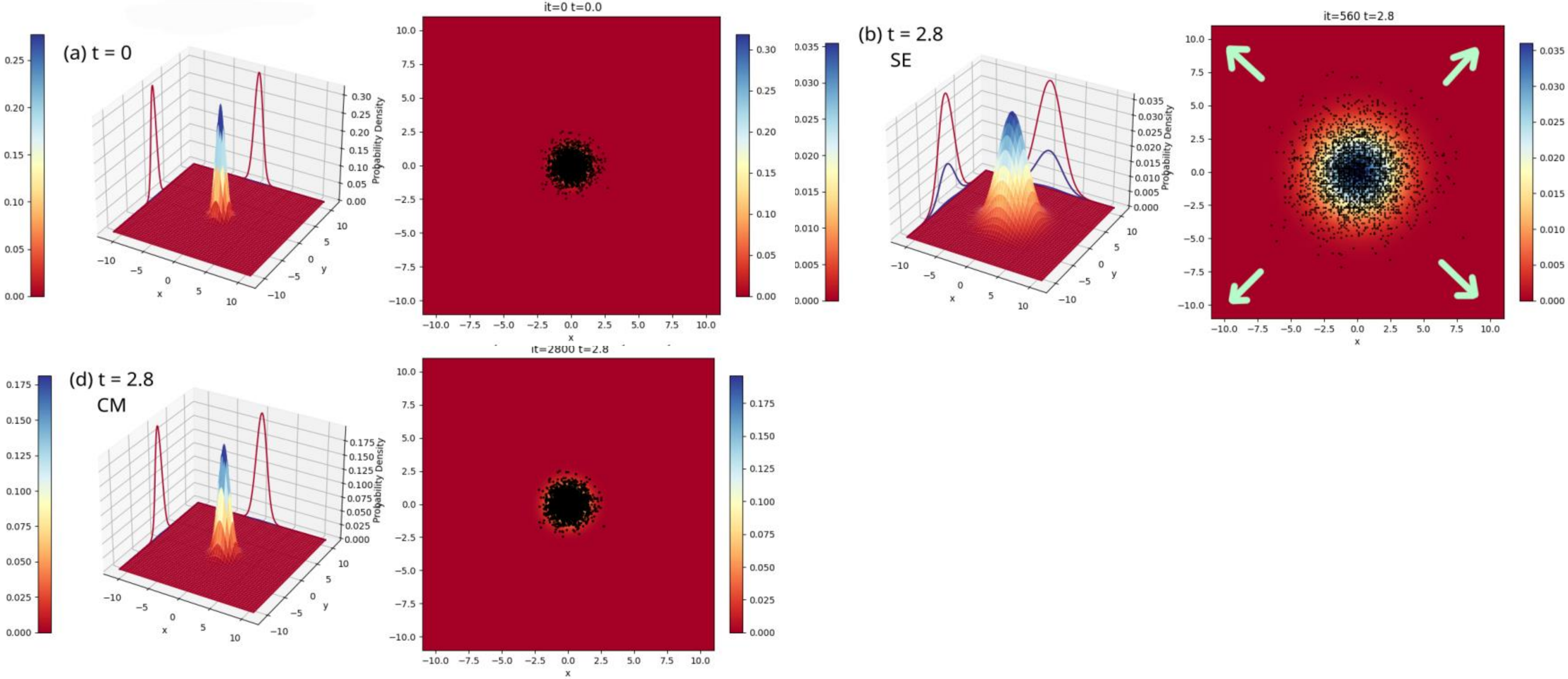

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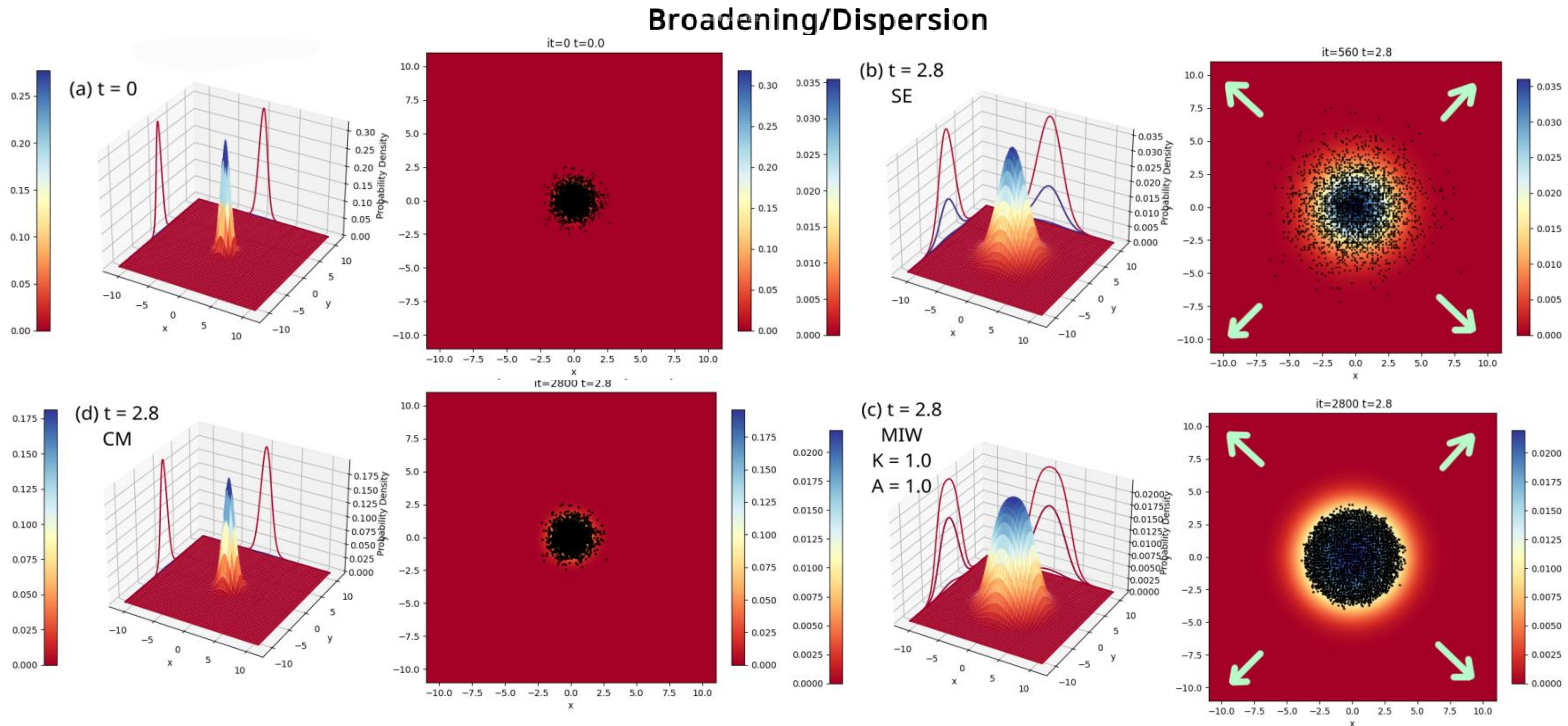

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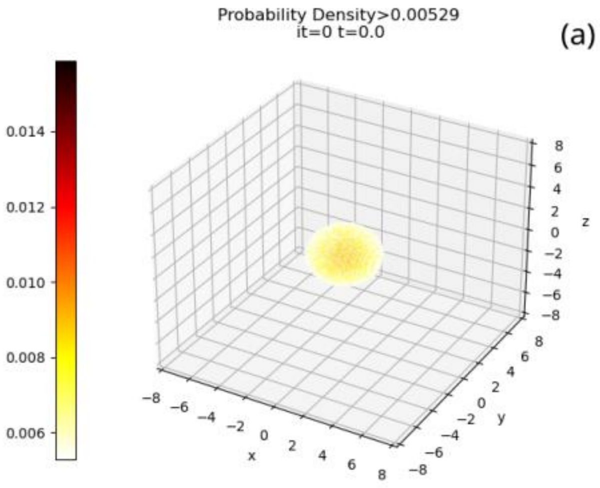

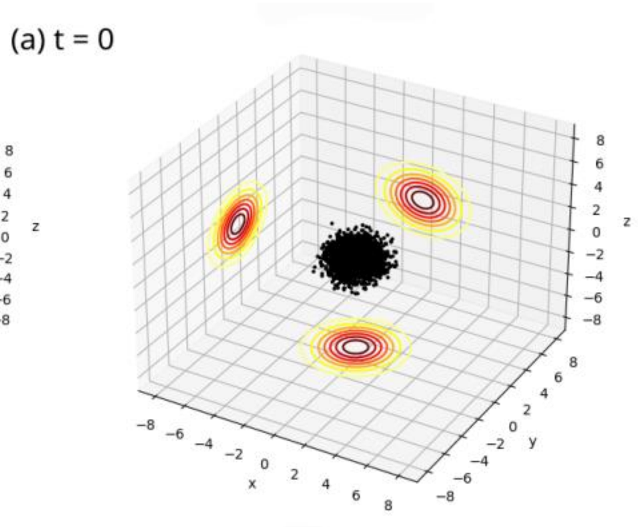

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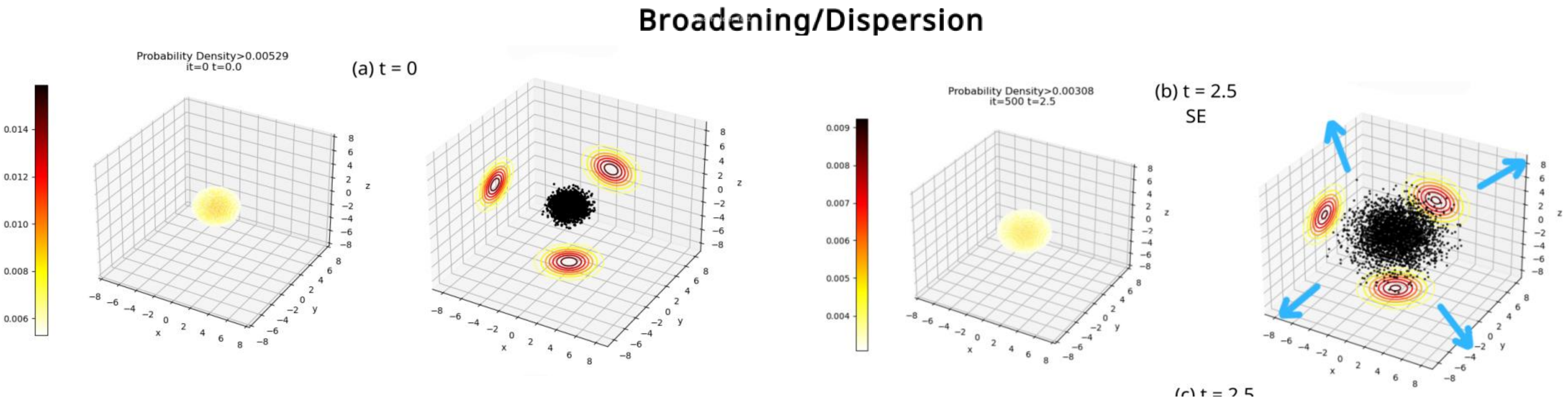

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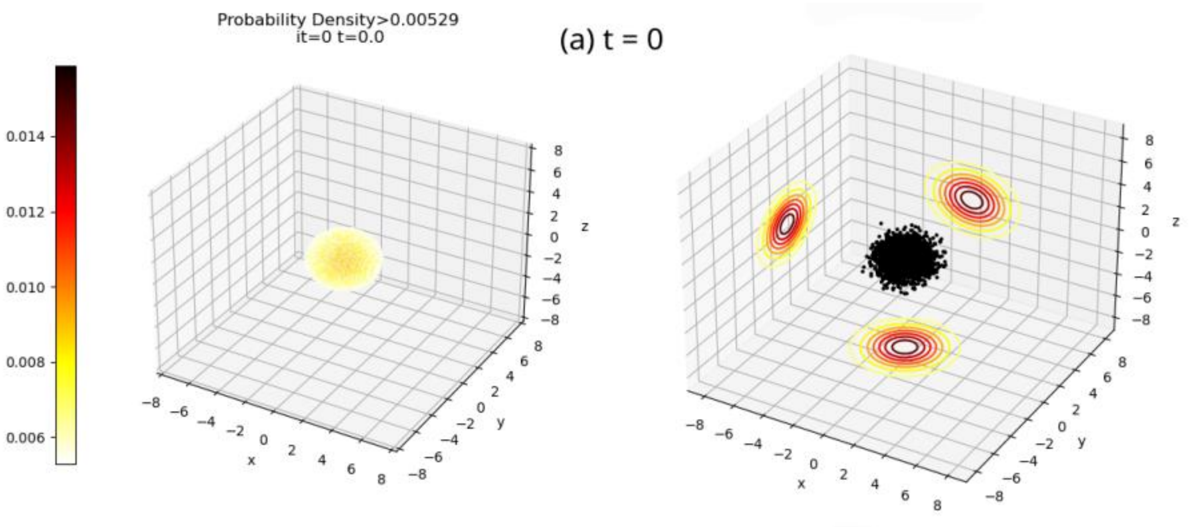

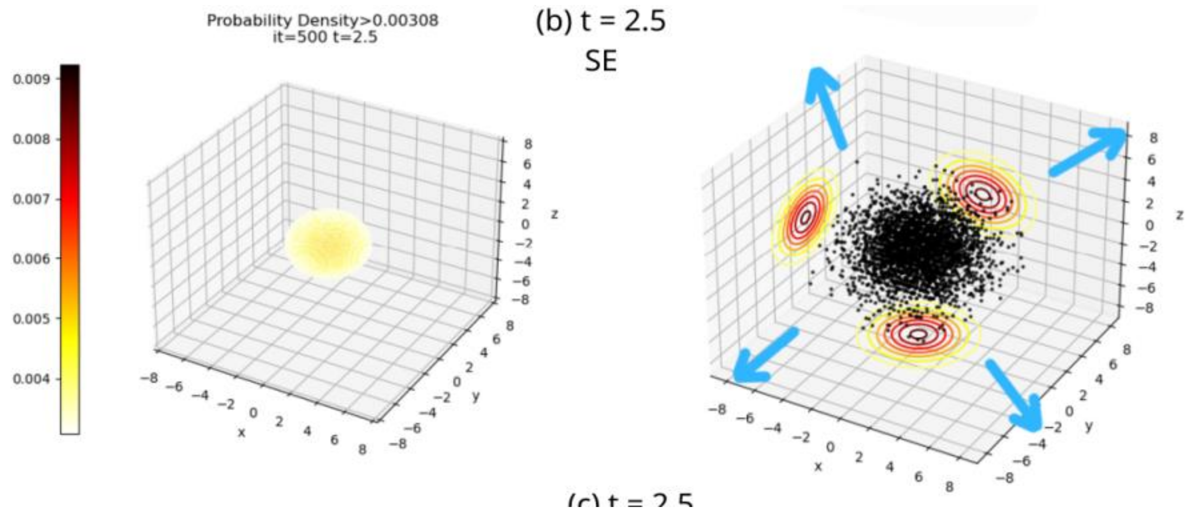

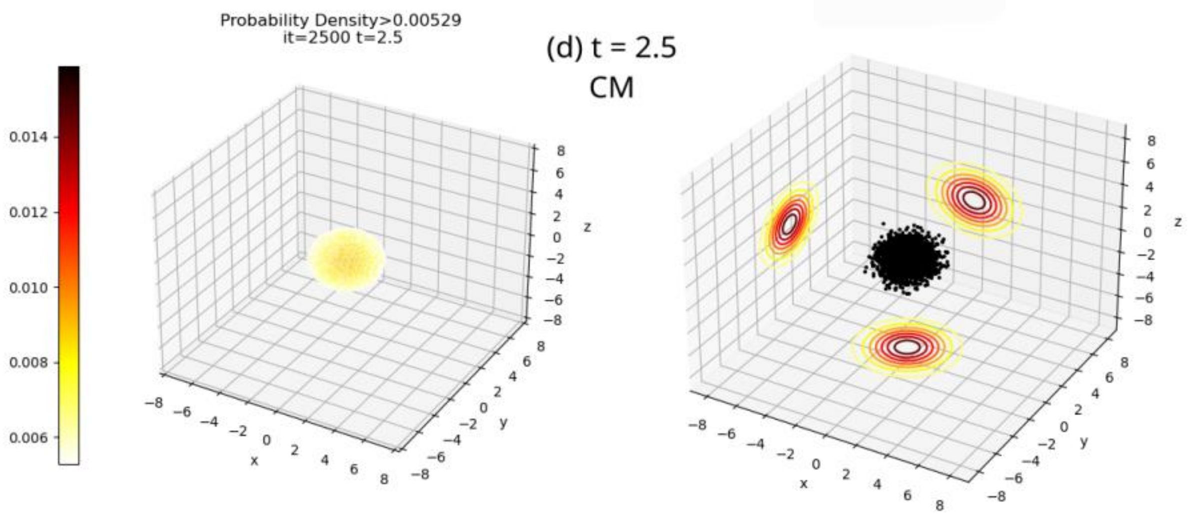

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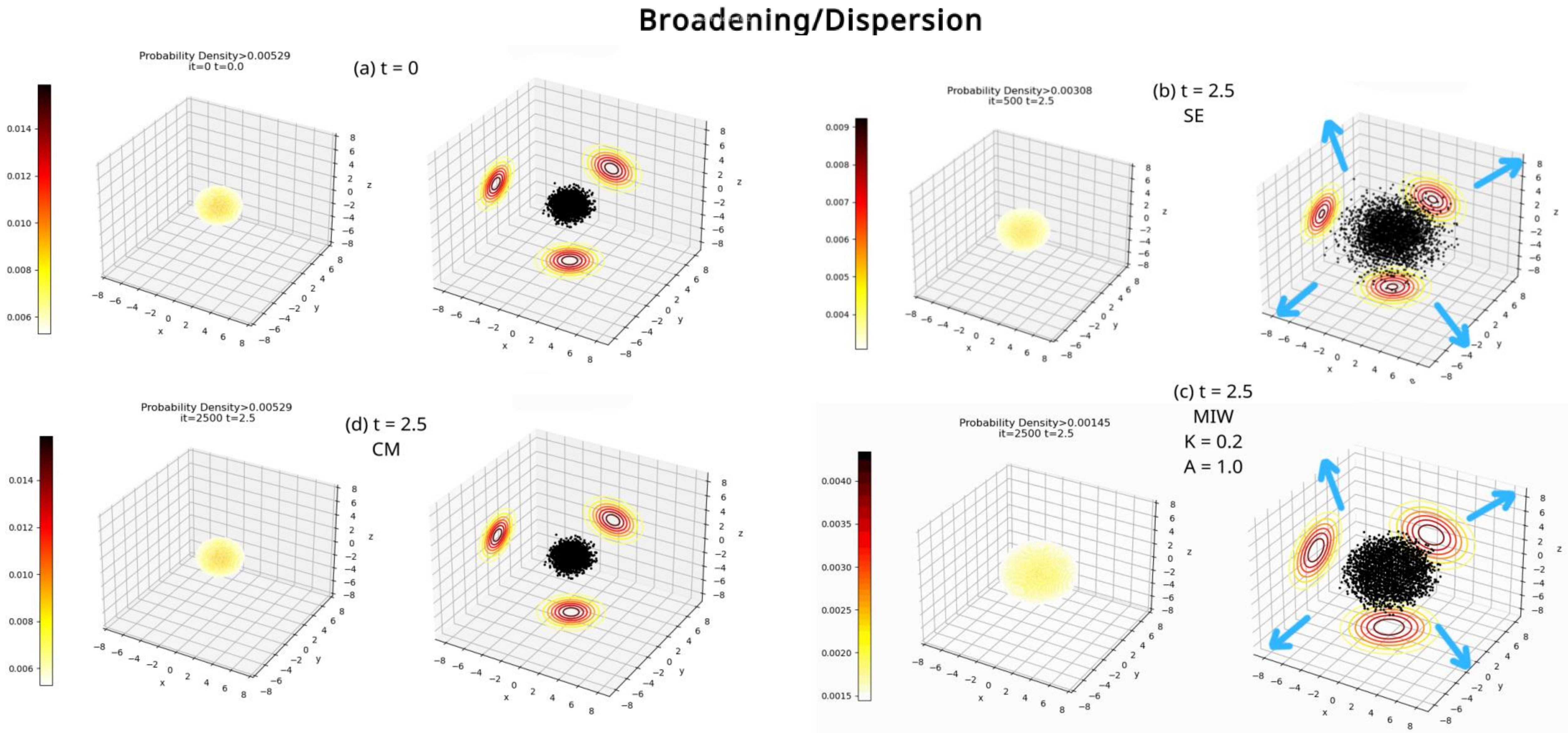

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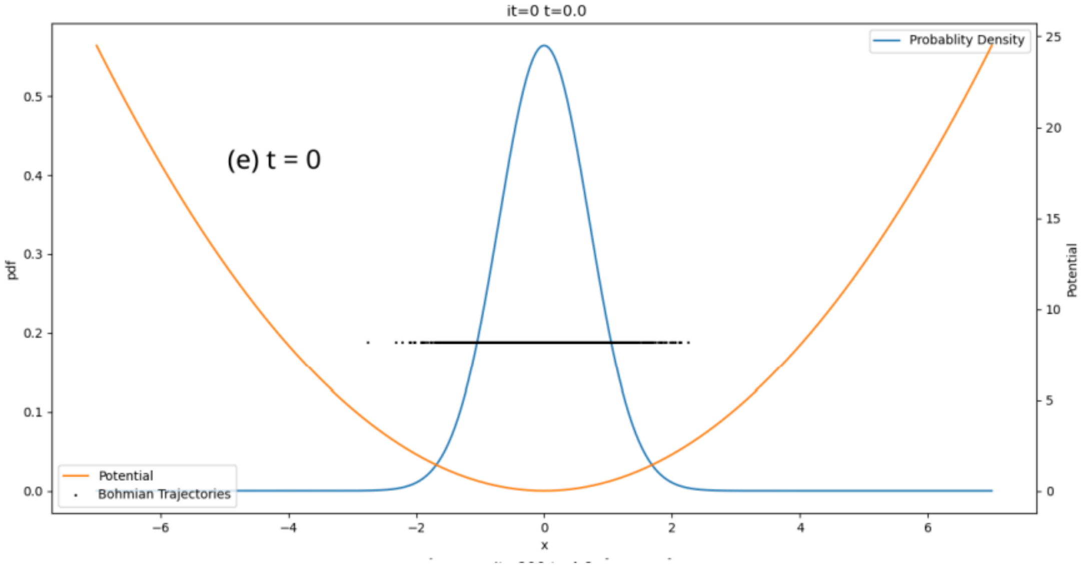
Stationary States



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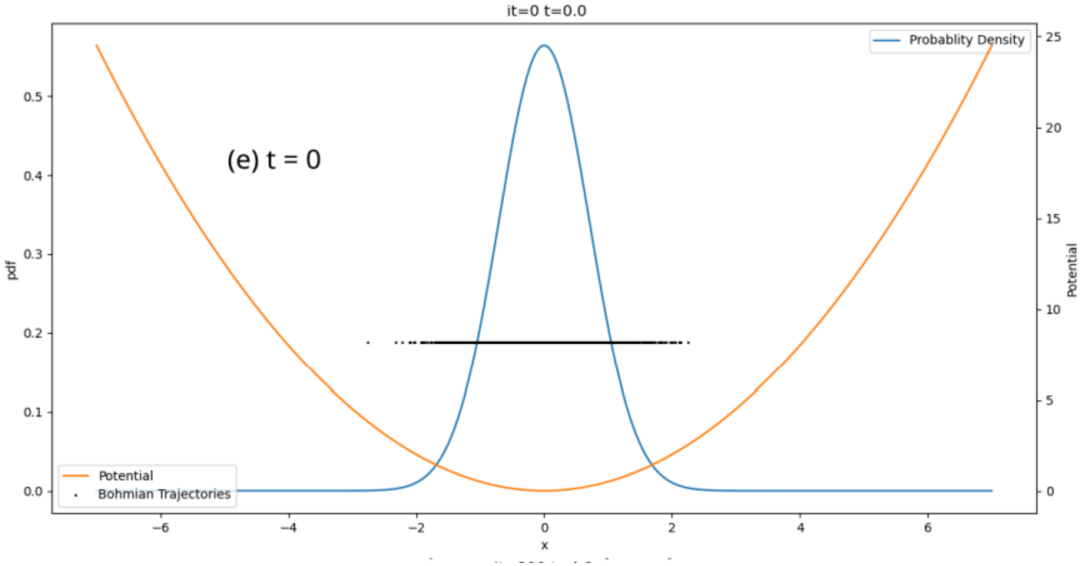

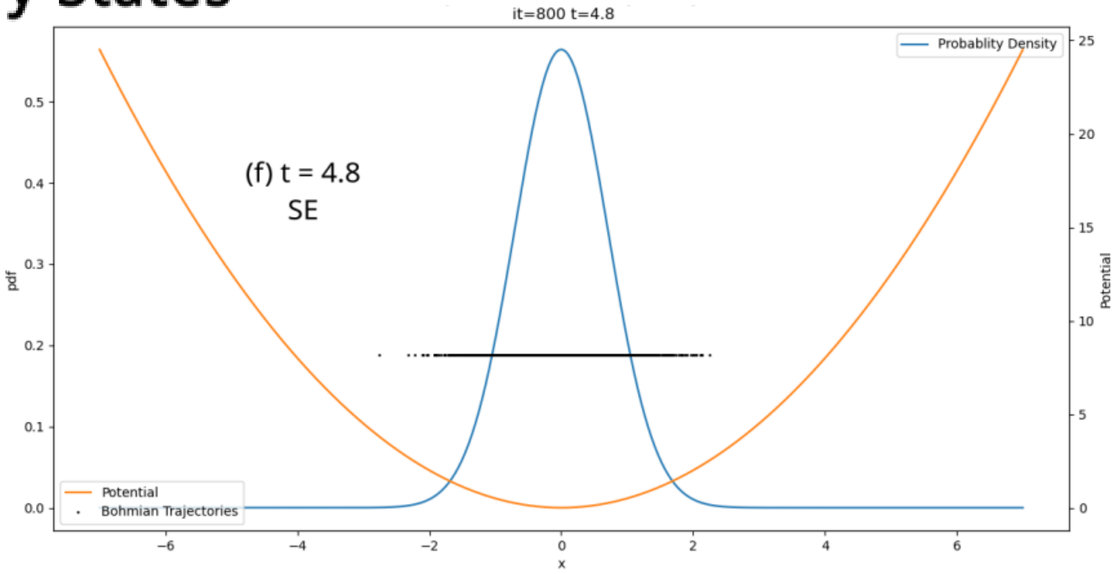

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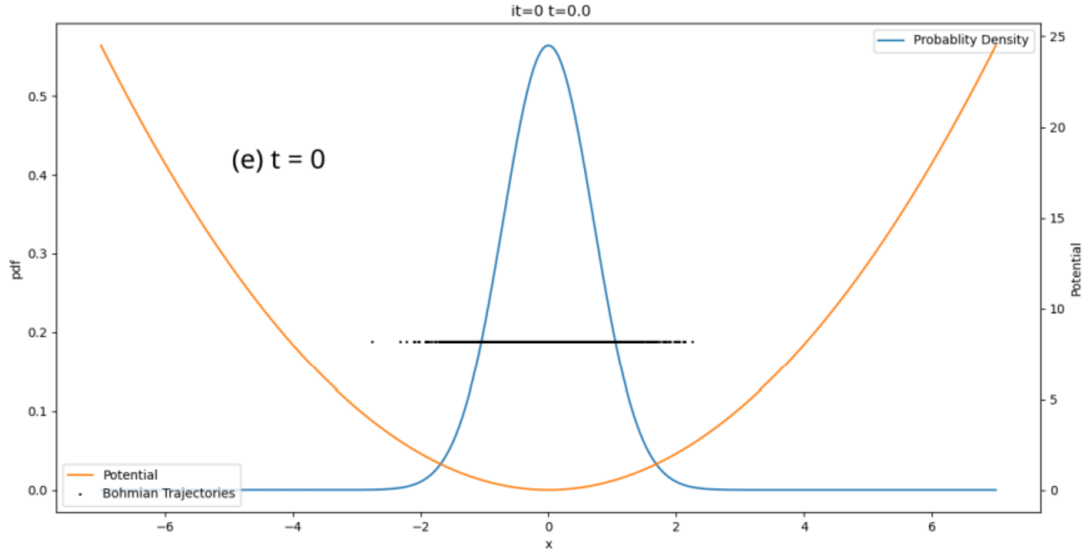

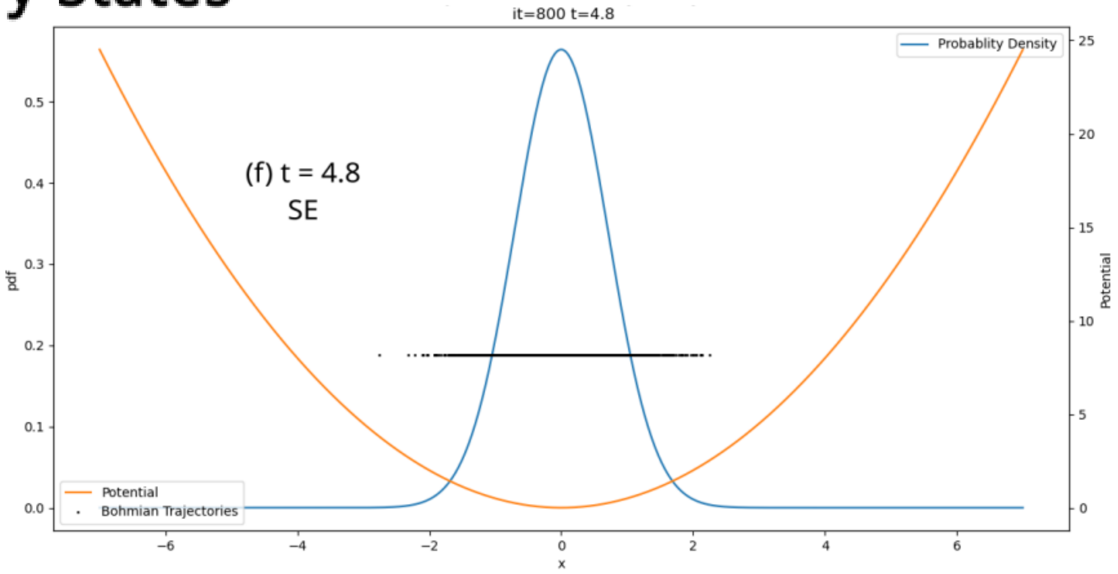

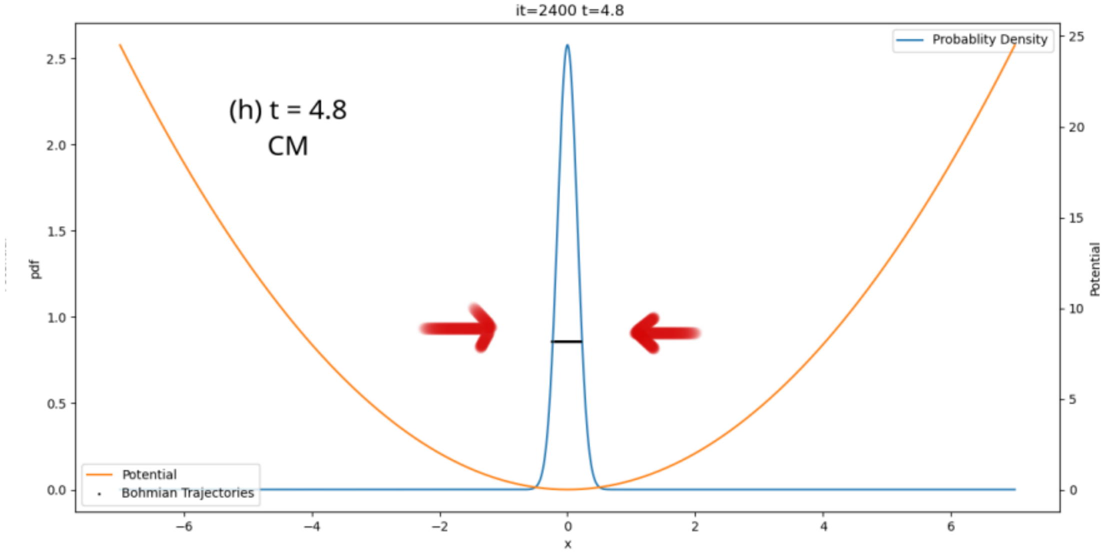

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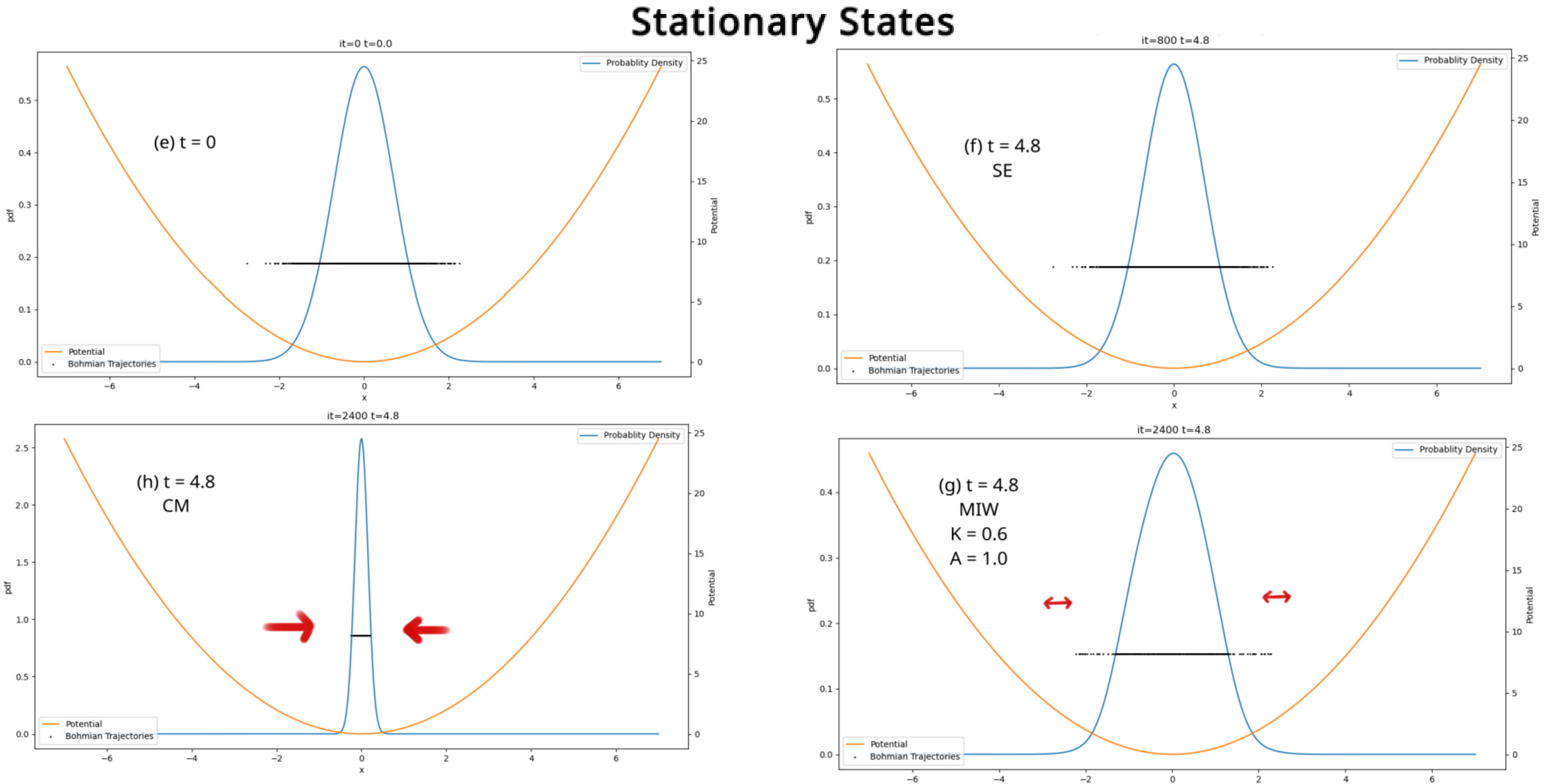

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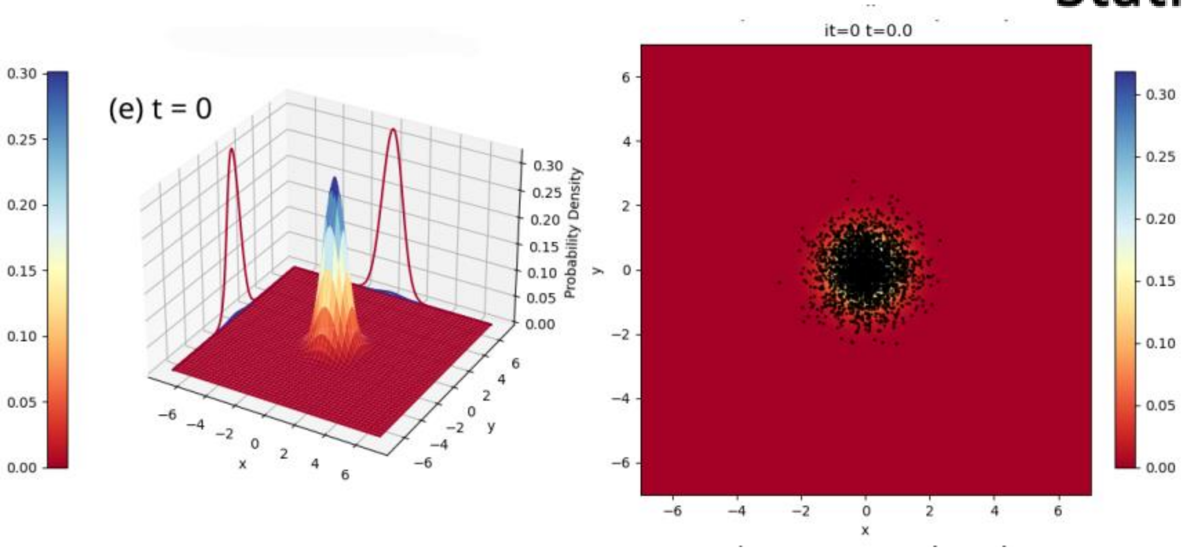

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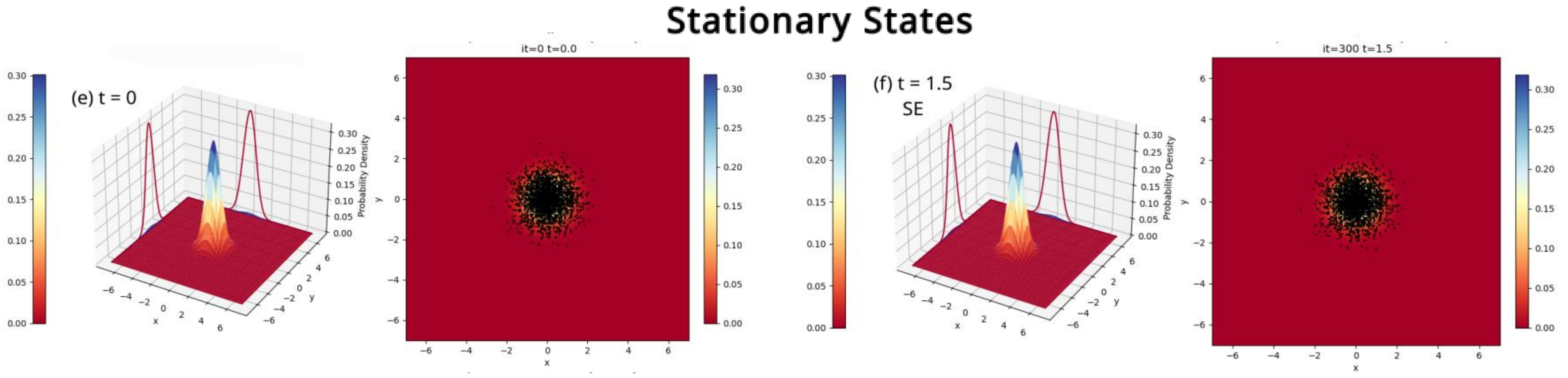

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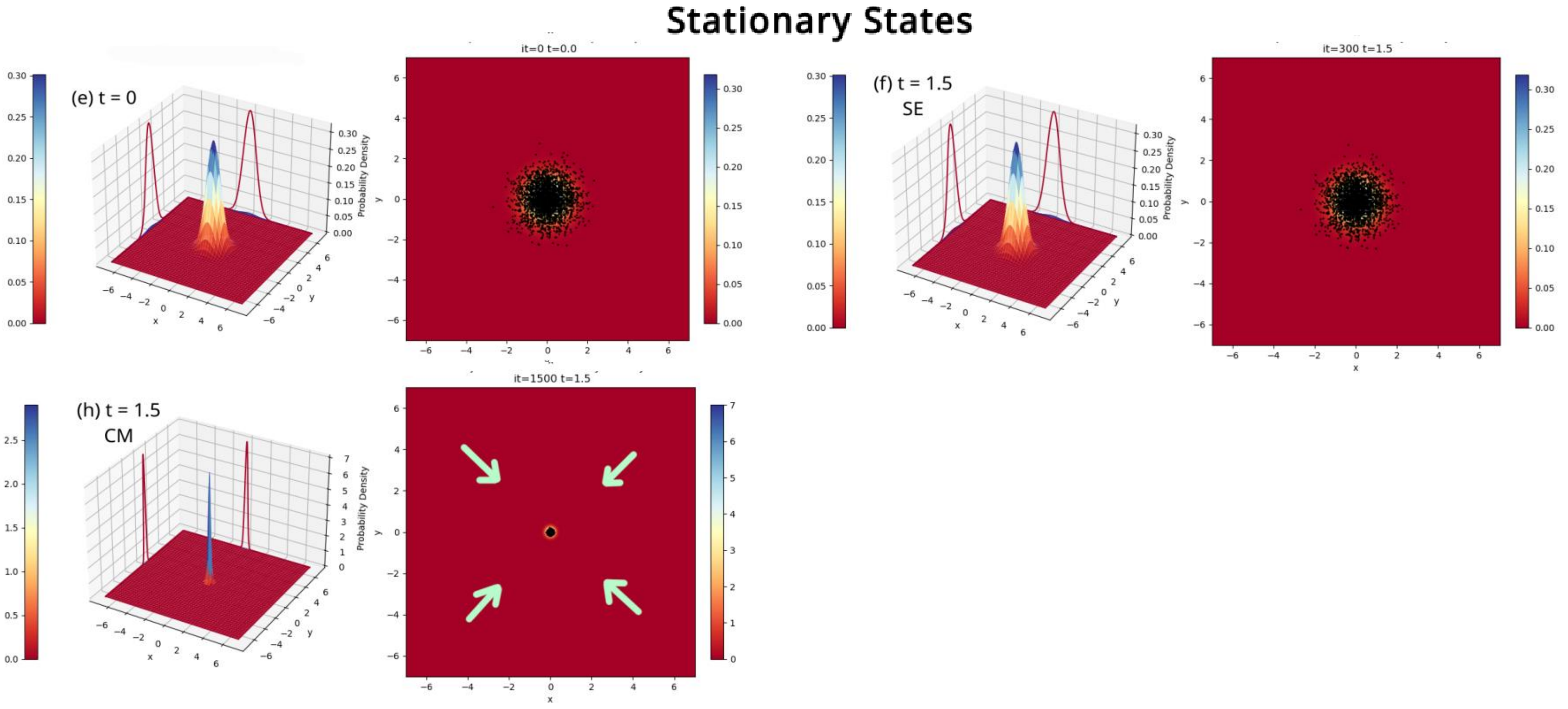

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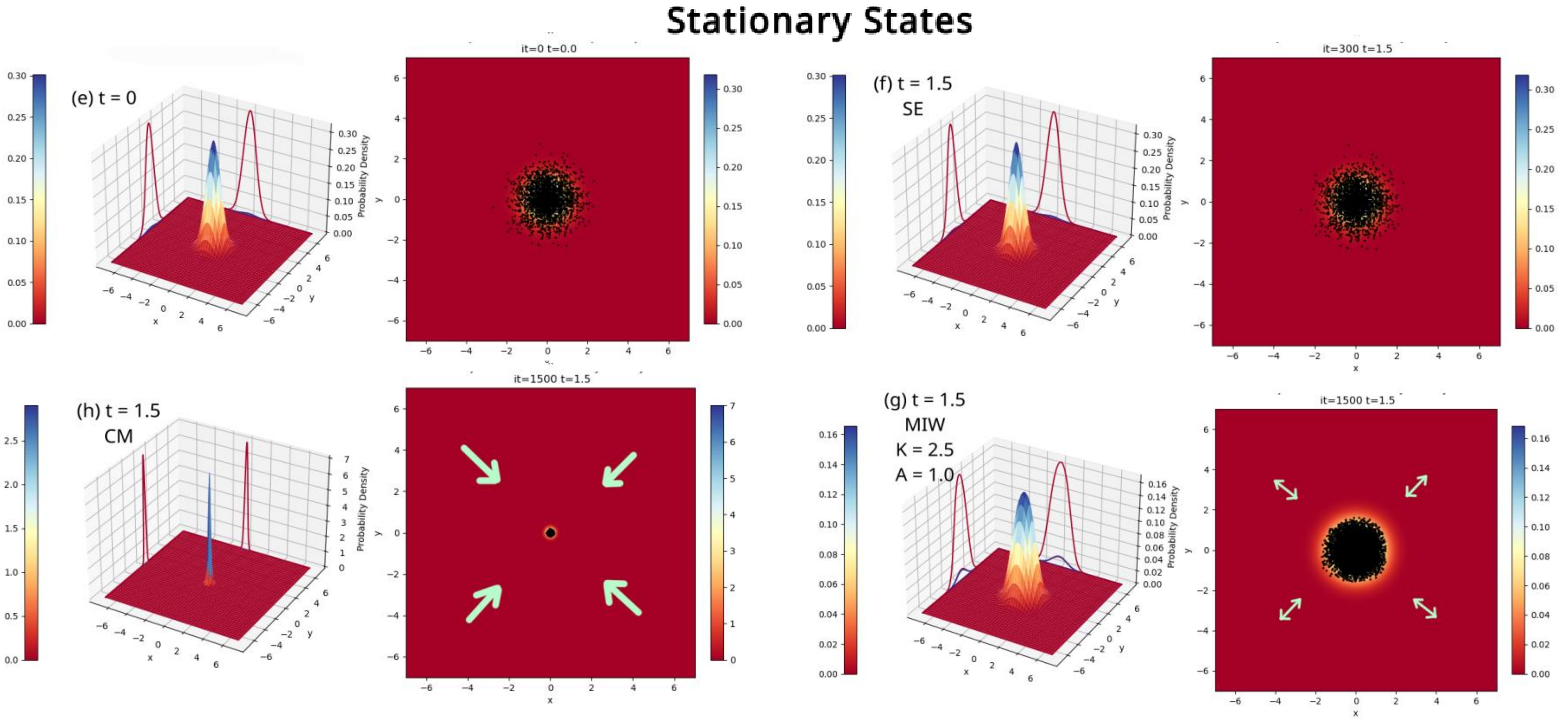

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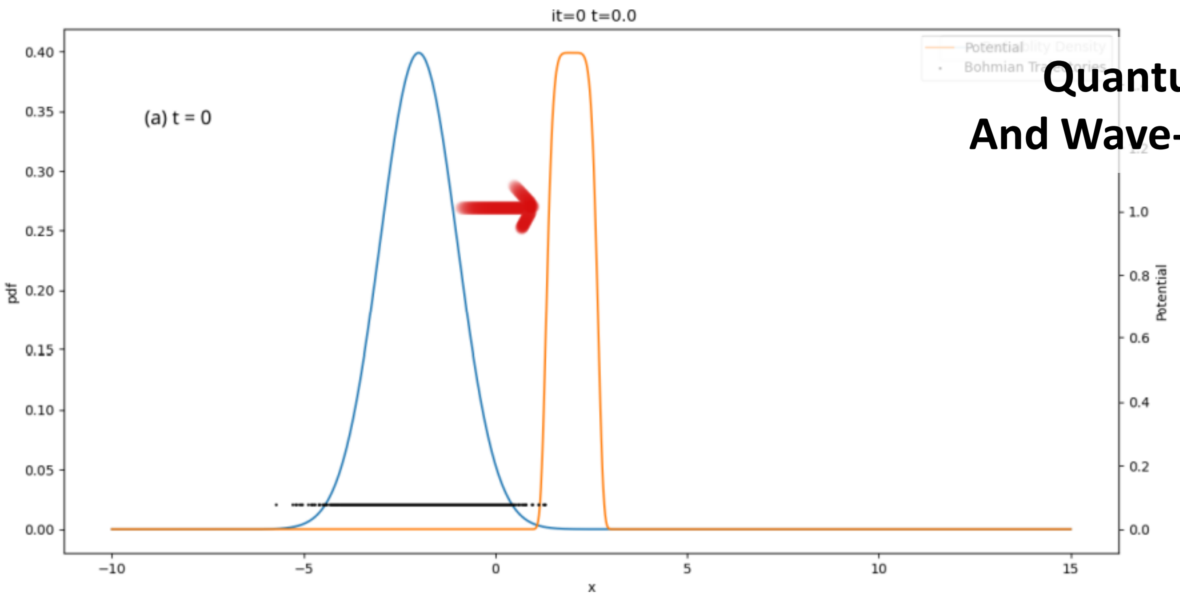

Quantum Tunneling
And Wave-like Interference

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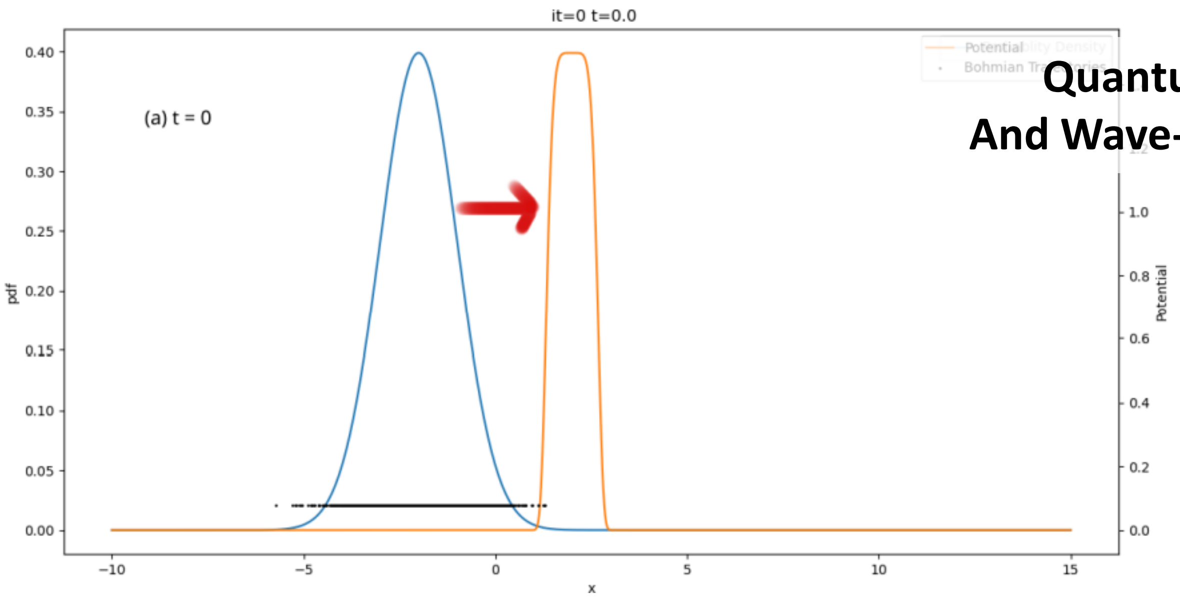

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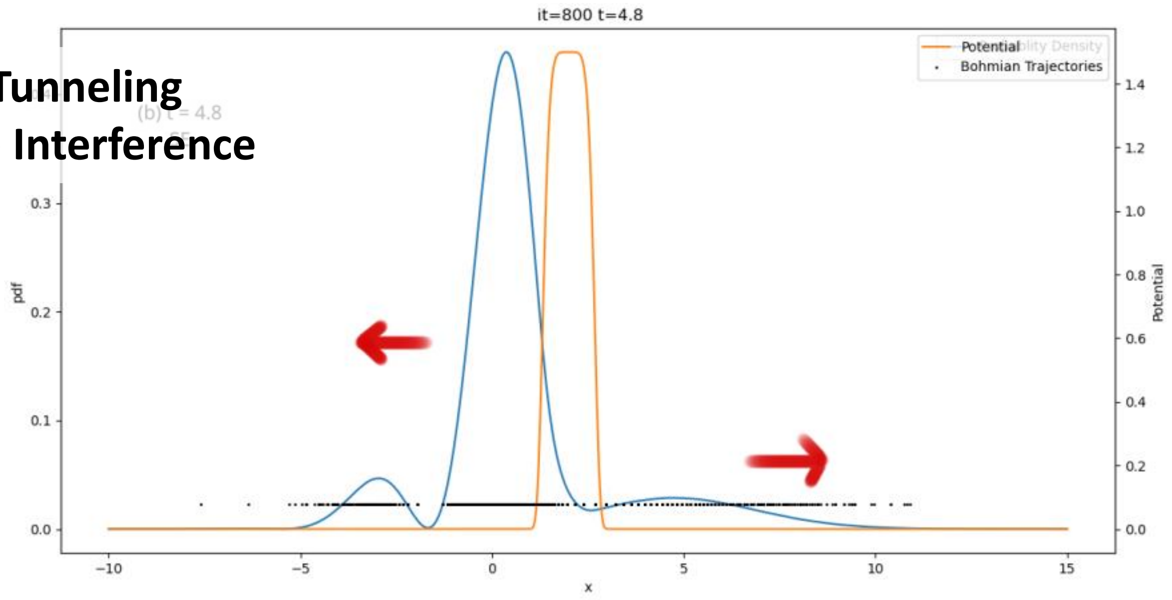

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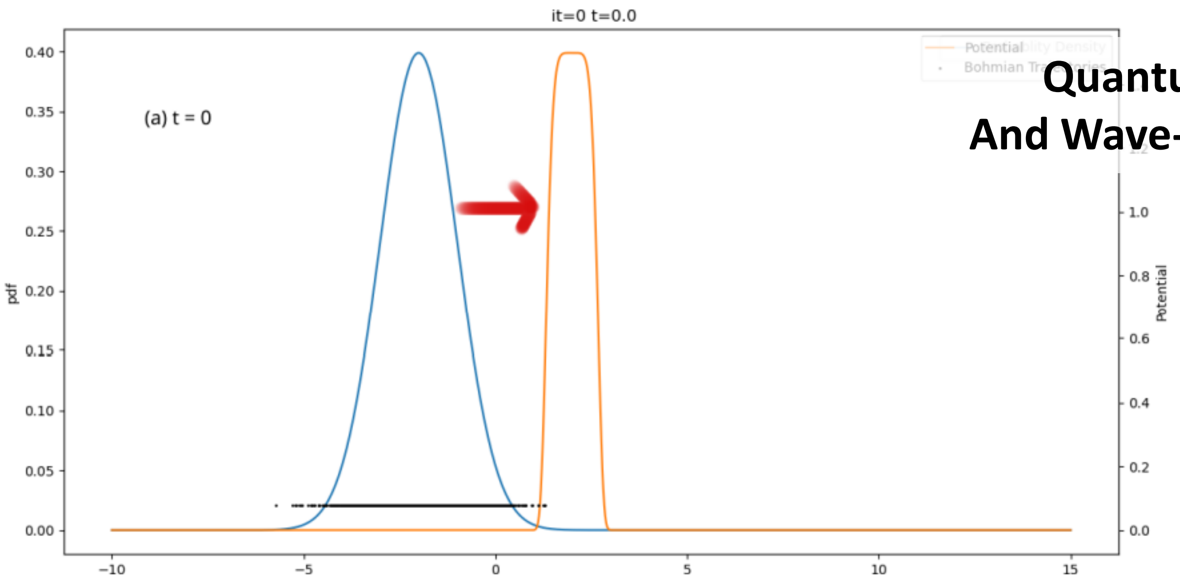

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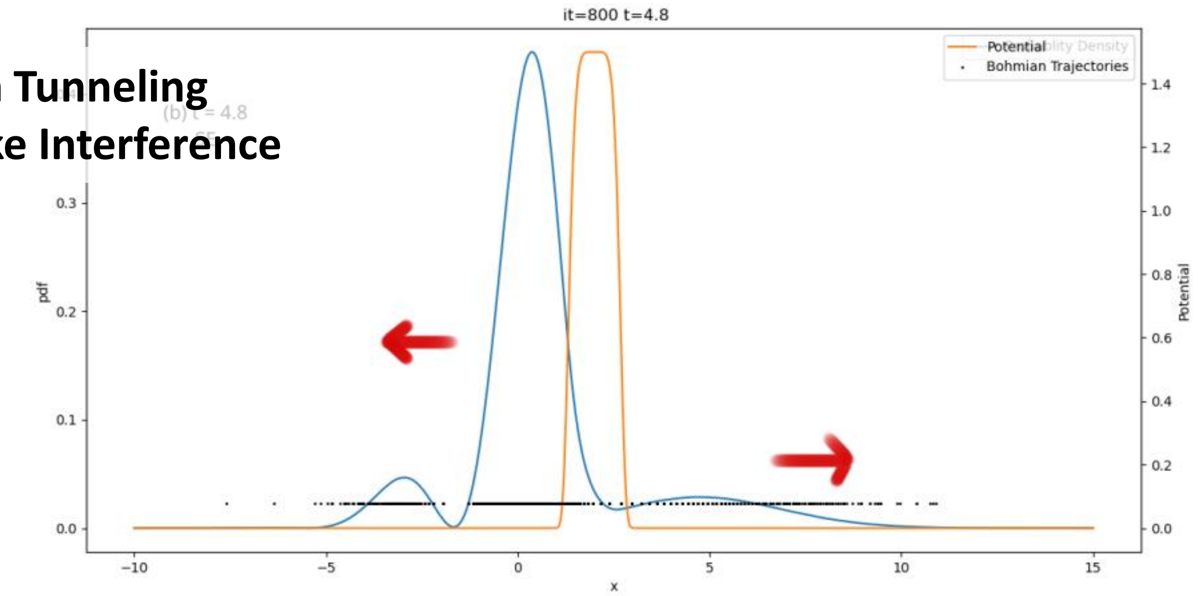

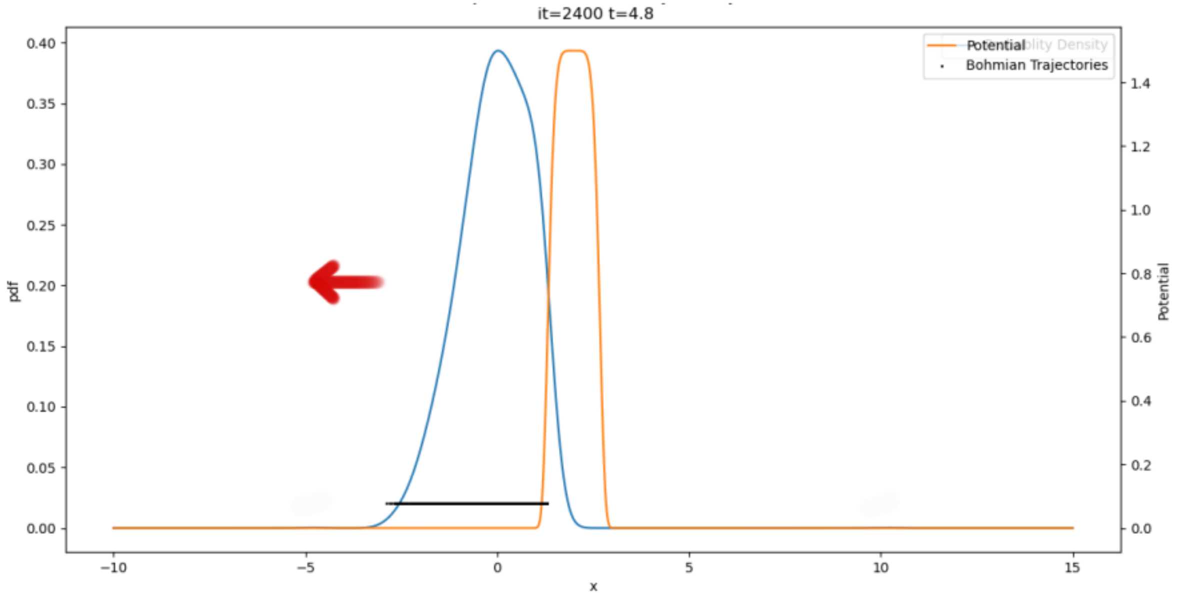

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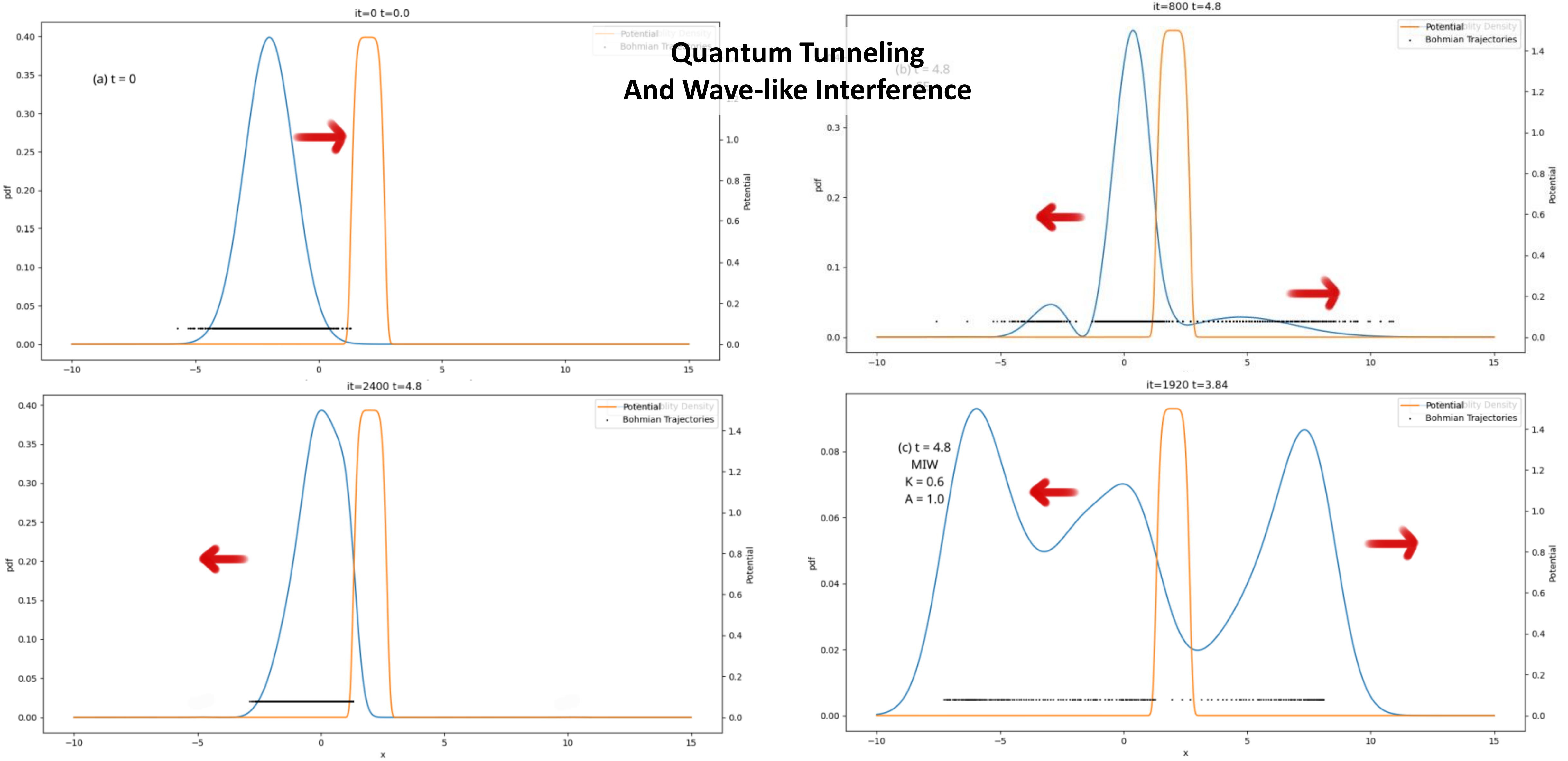

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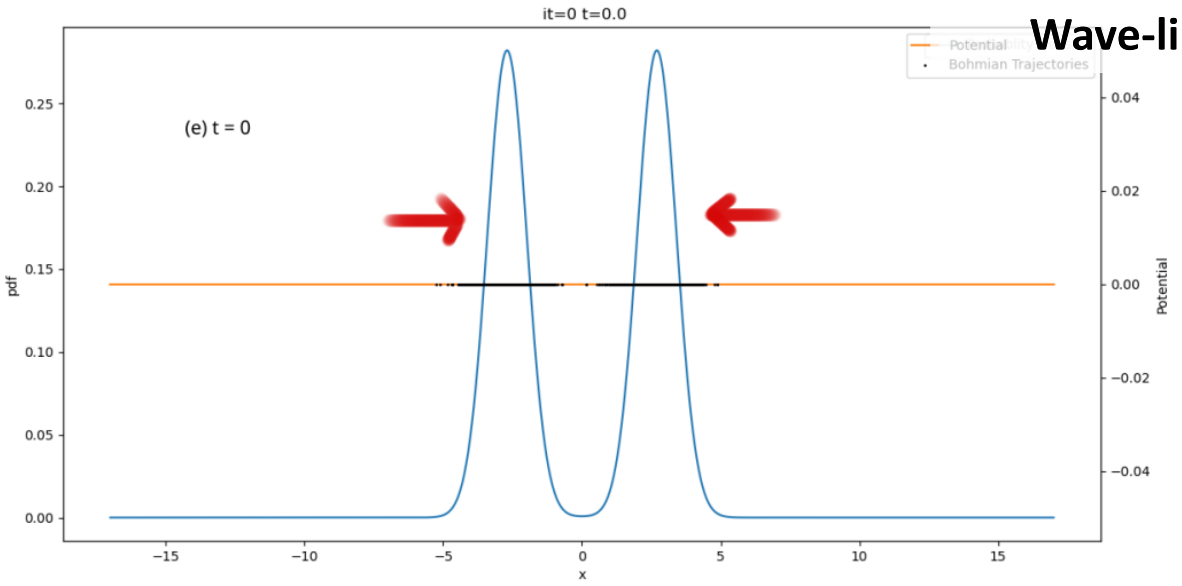

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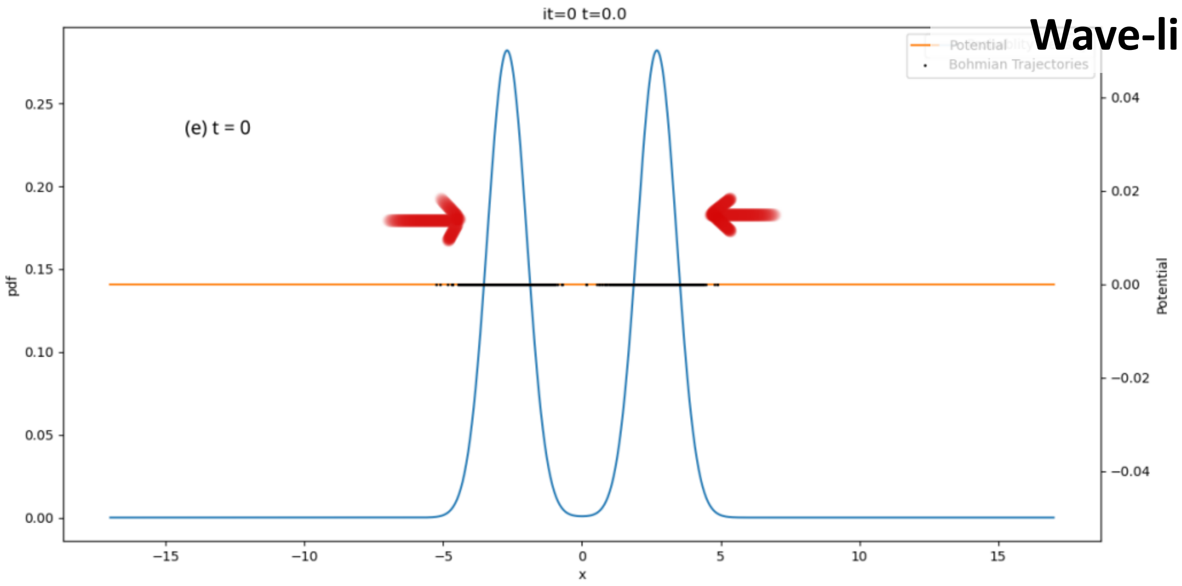

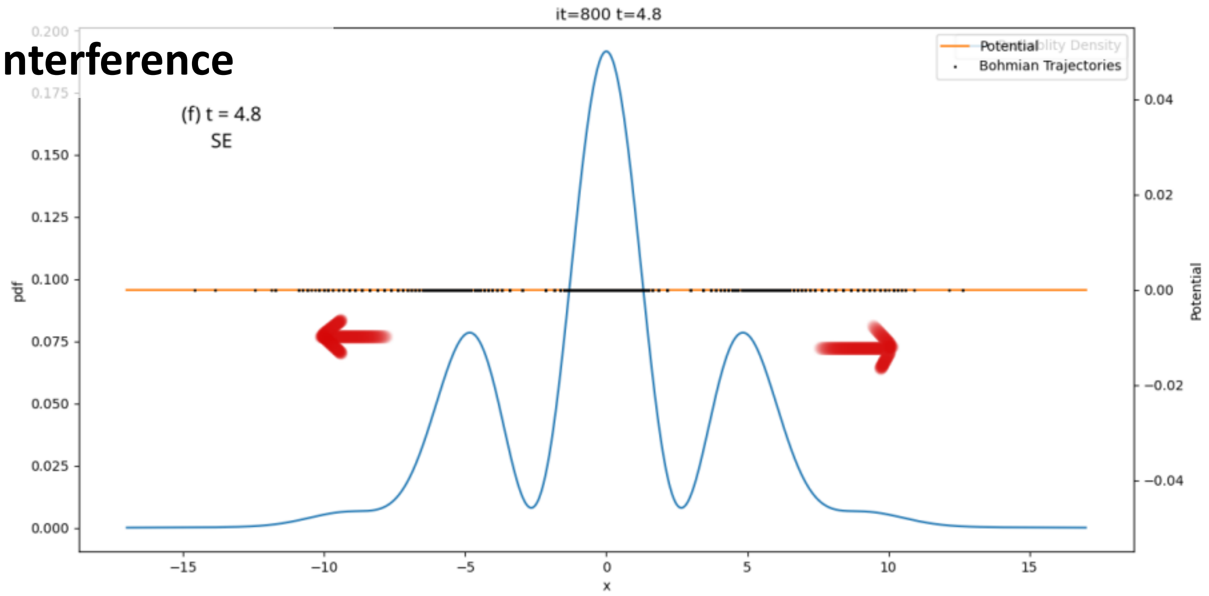

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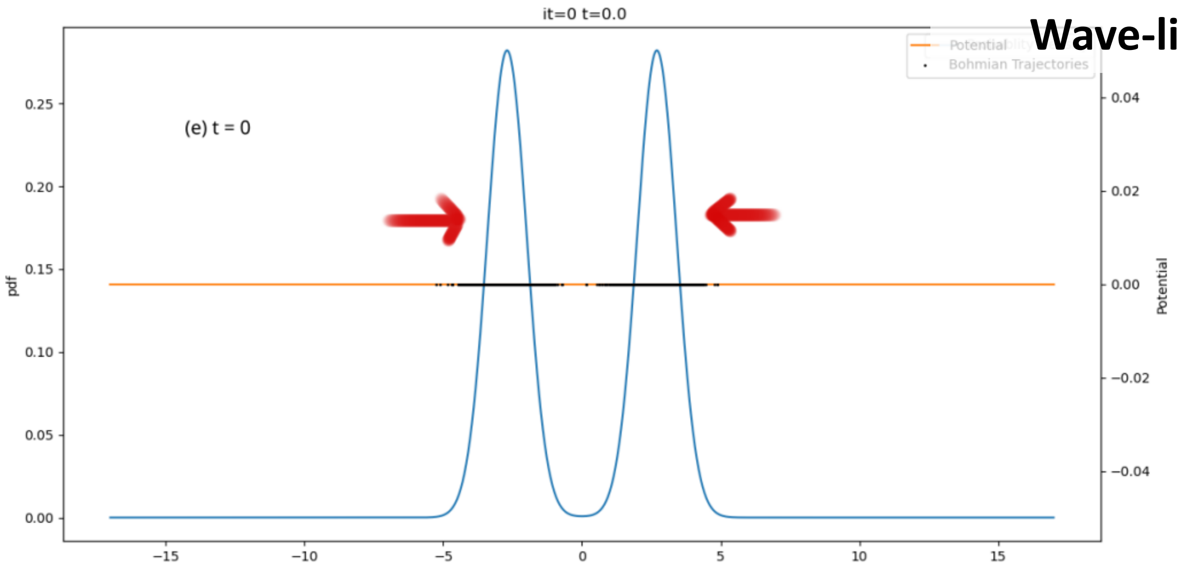
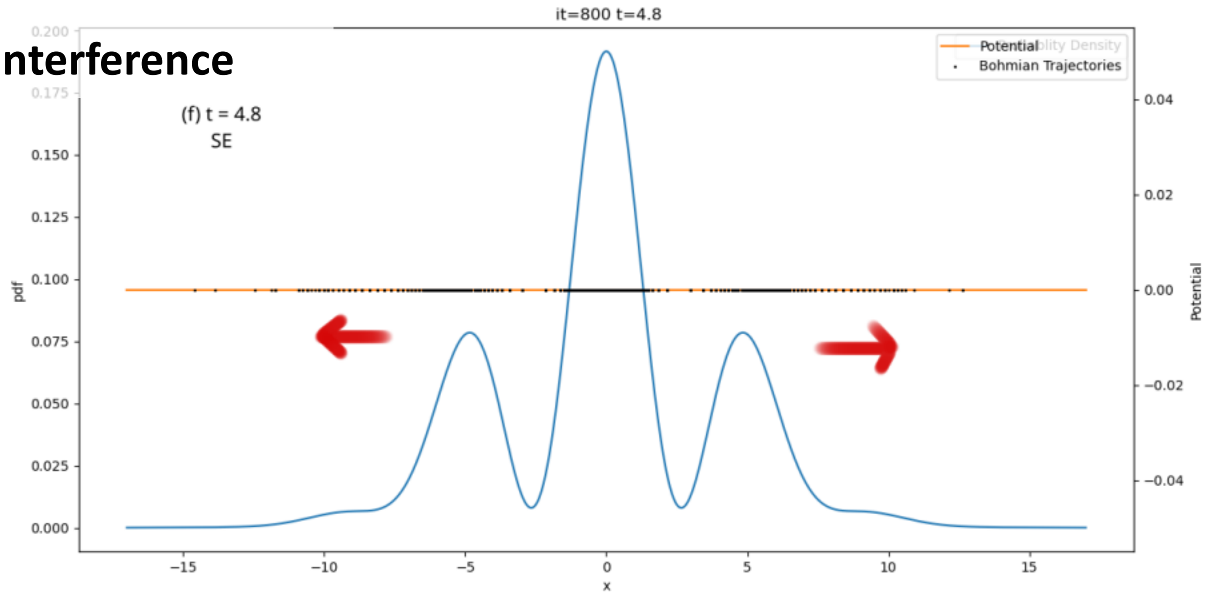
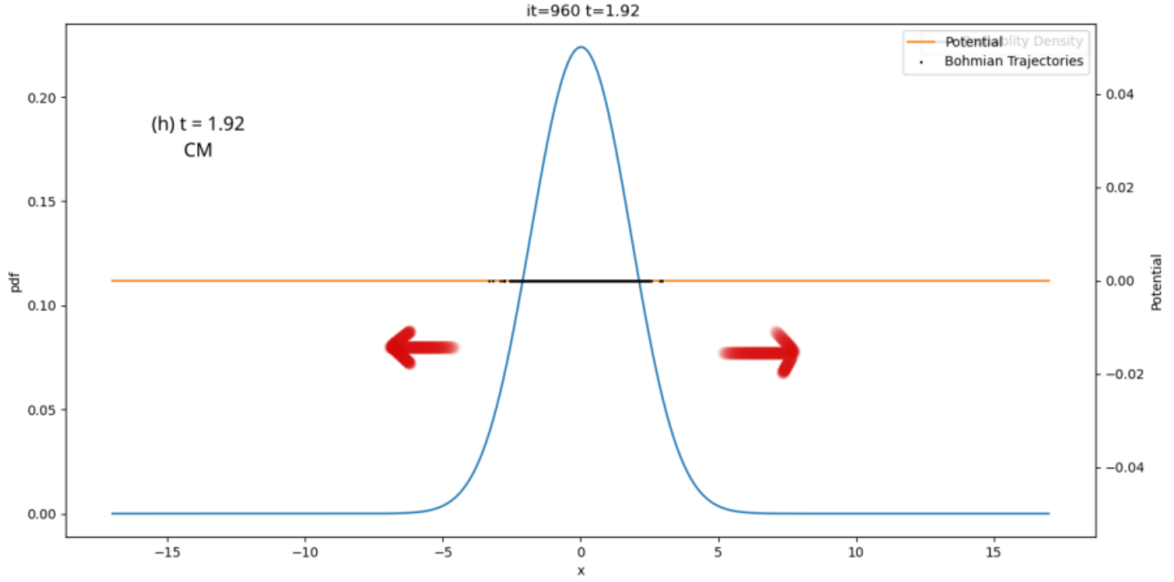
Wave-like Interference

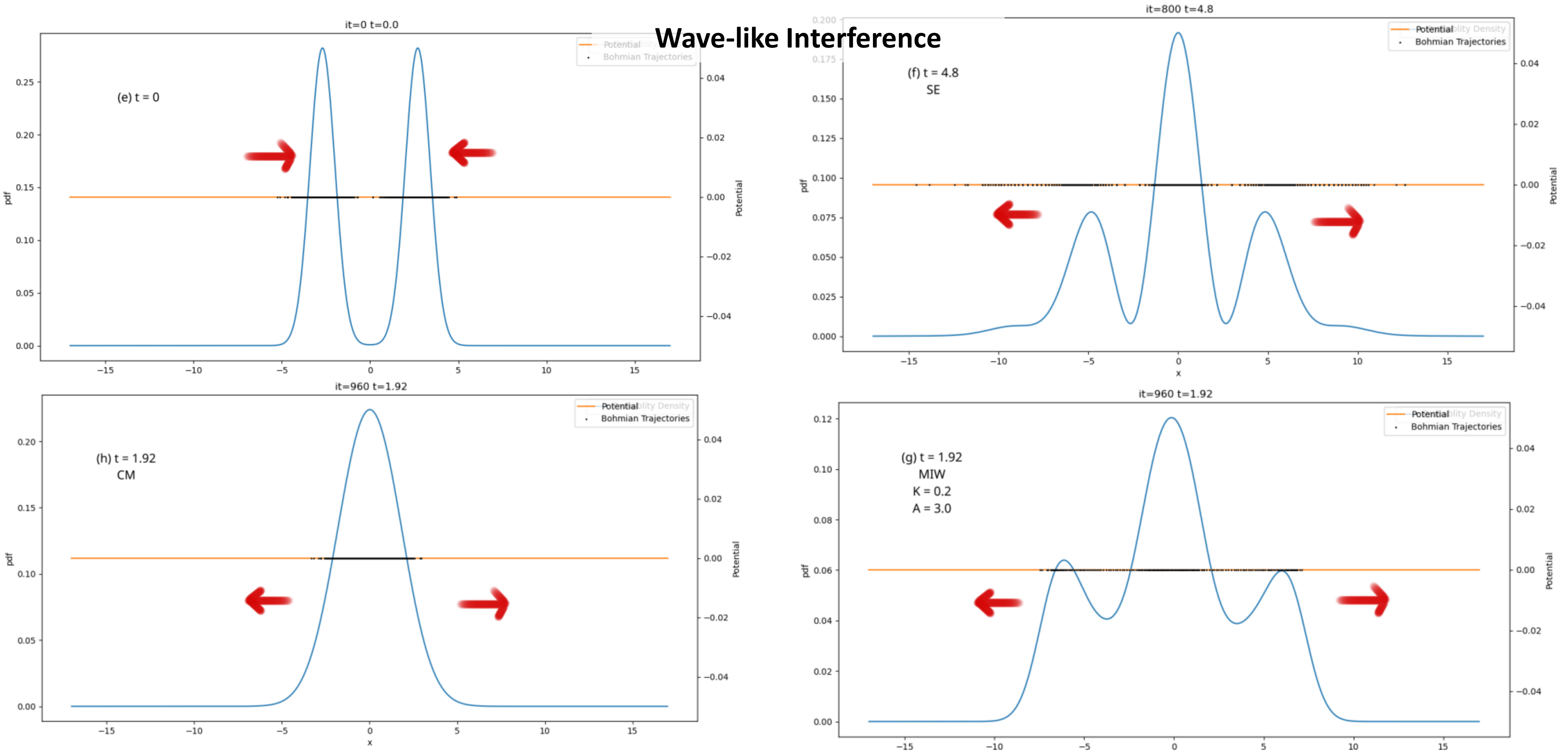






V – Results

(a) Qualitatively this is Quantum Mechanics!



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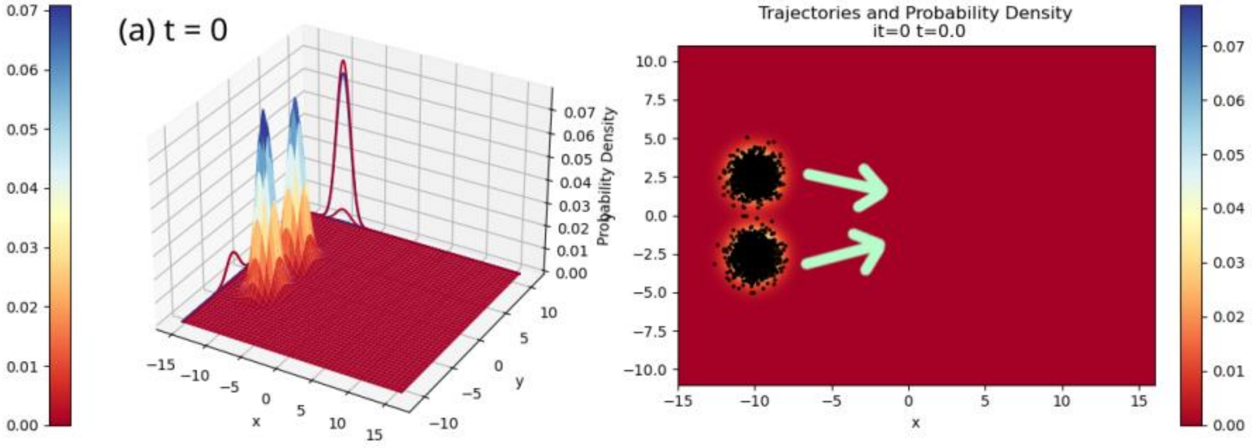

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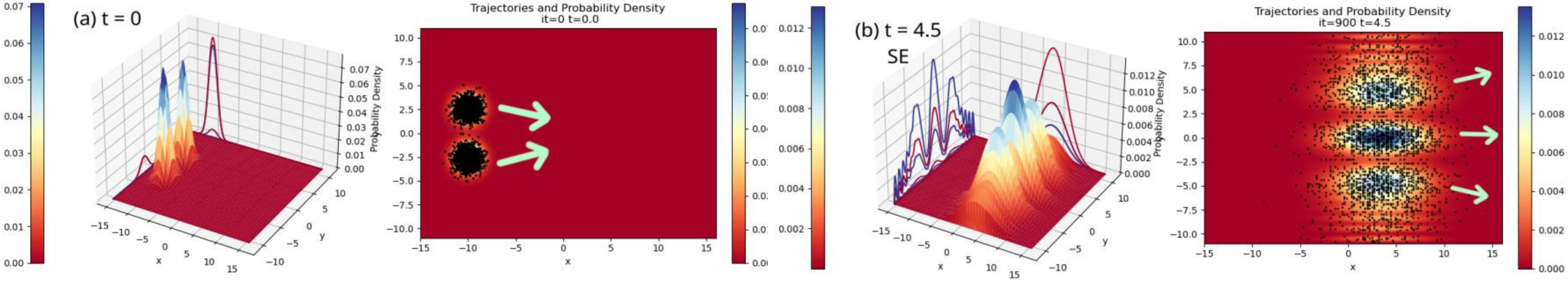

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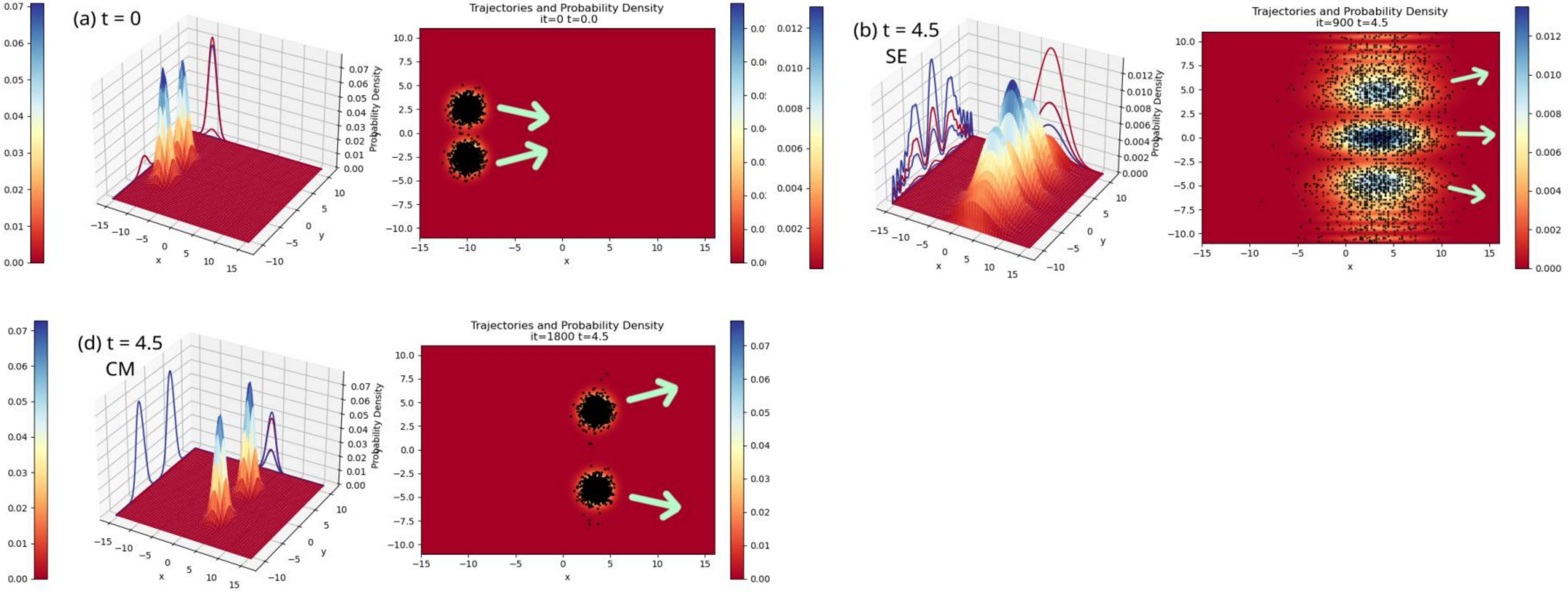

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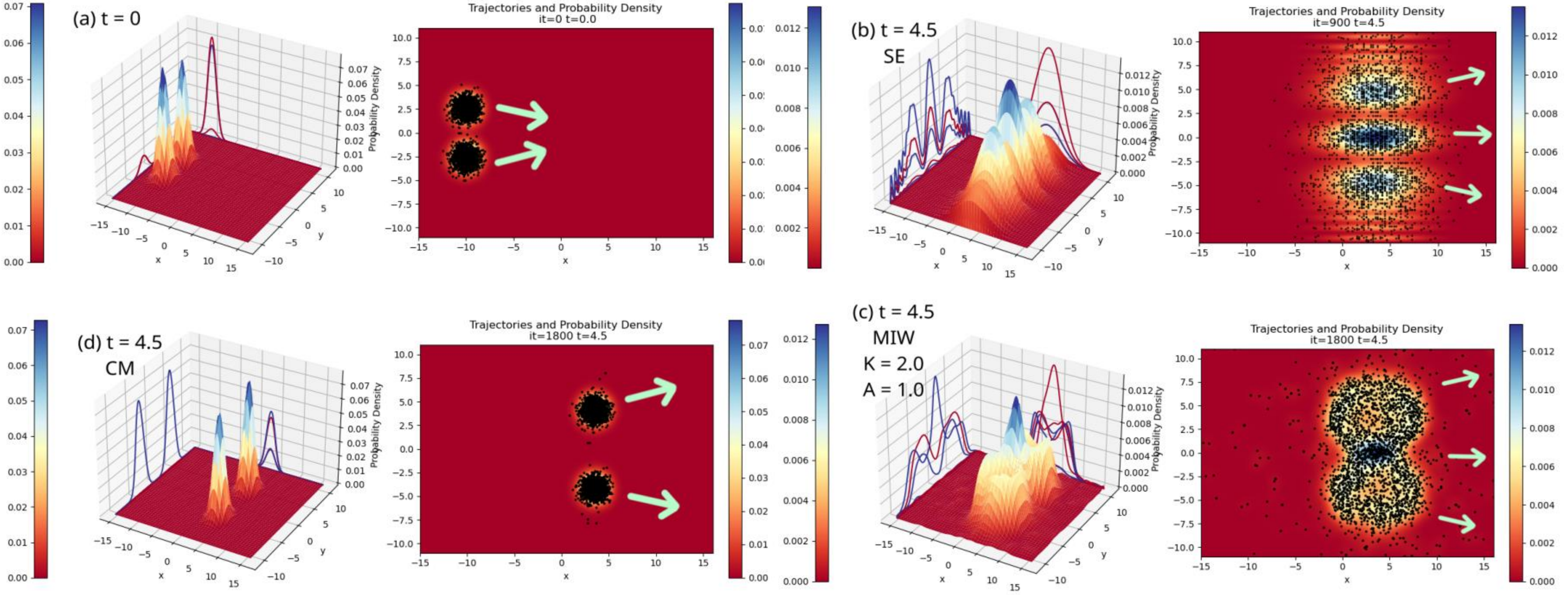

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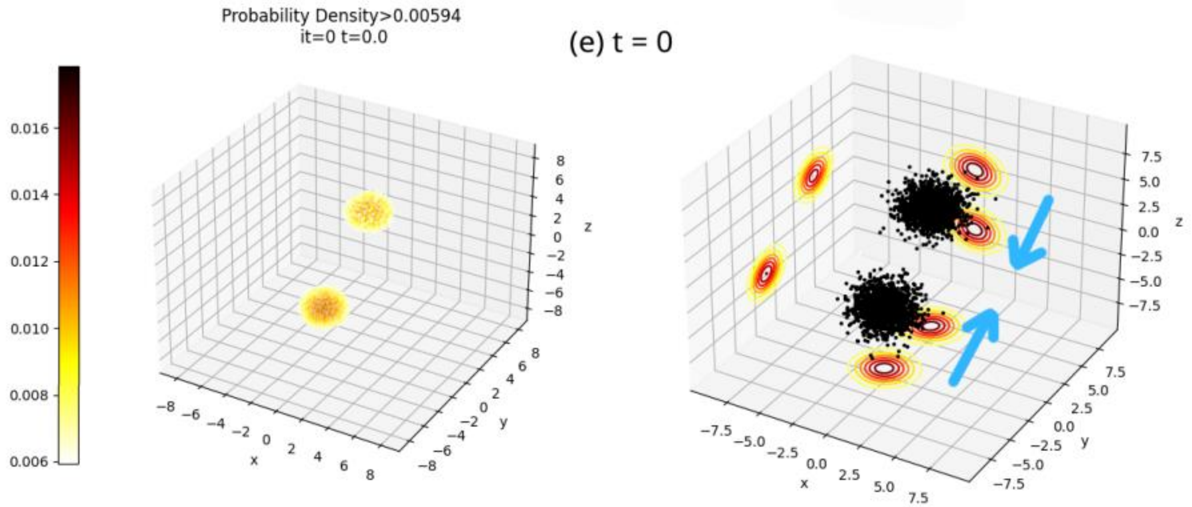

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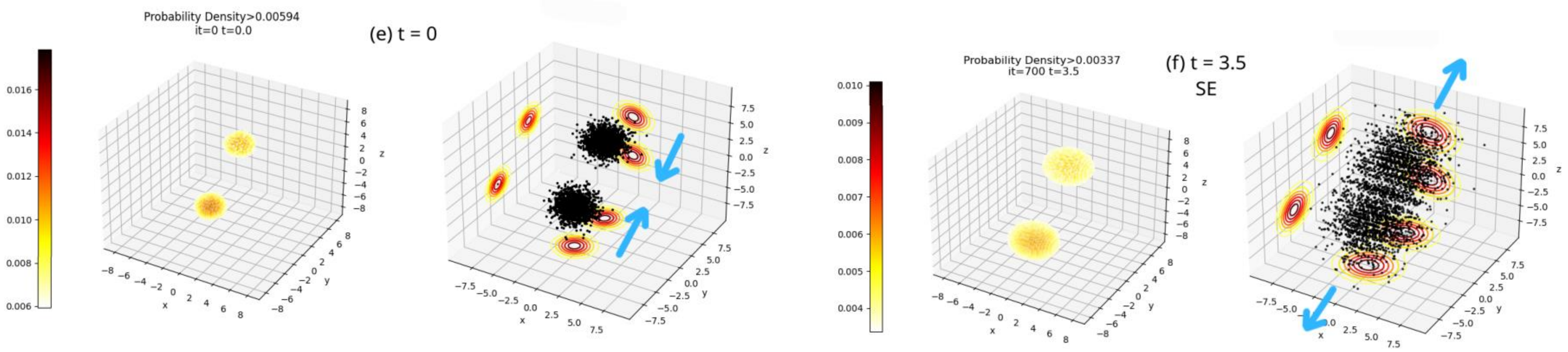

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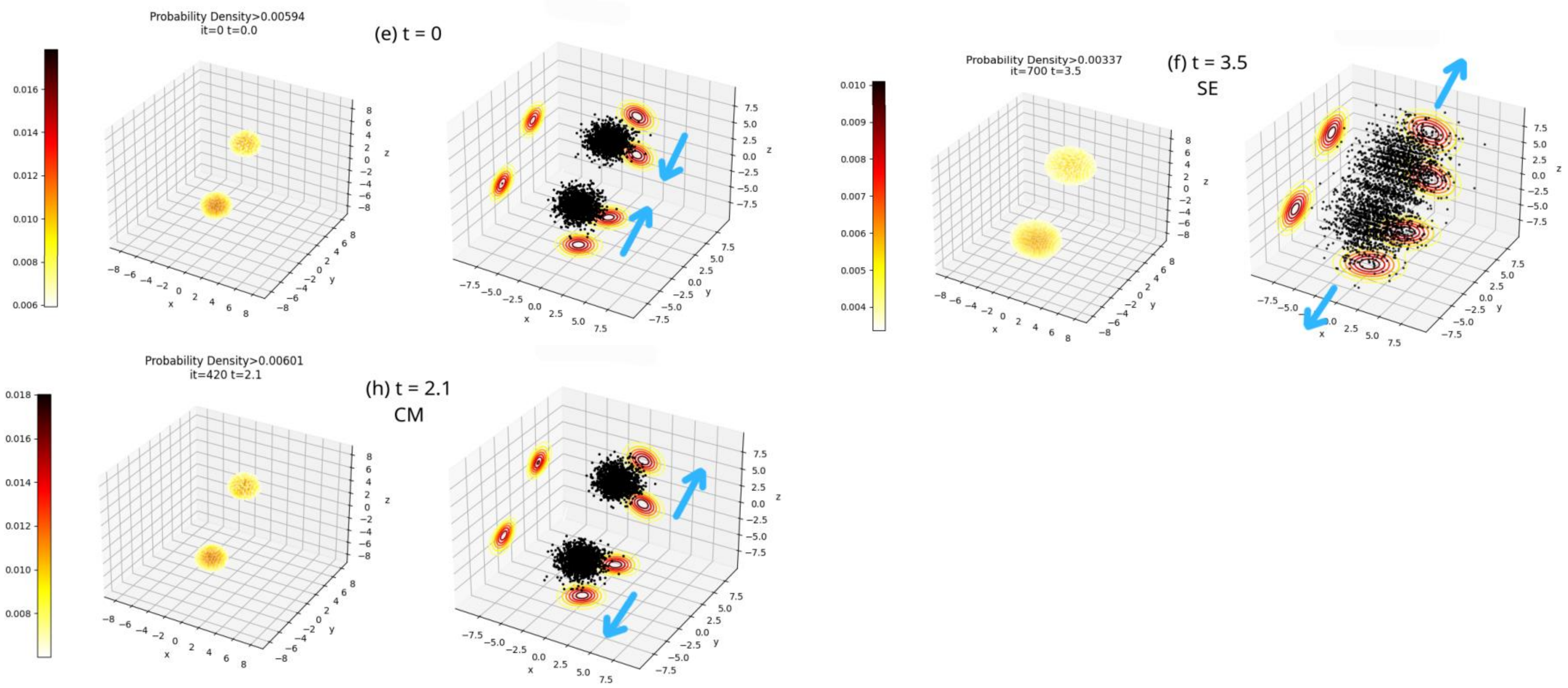

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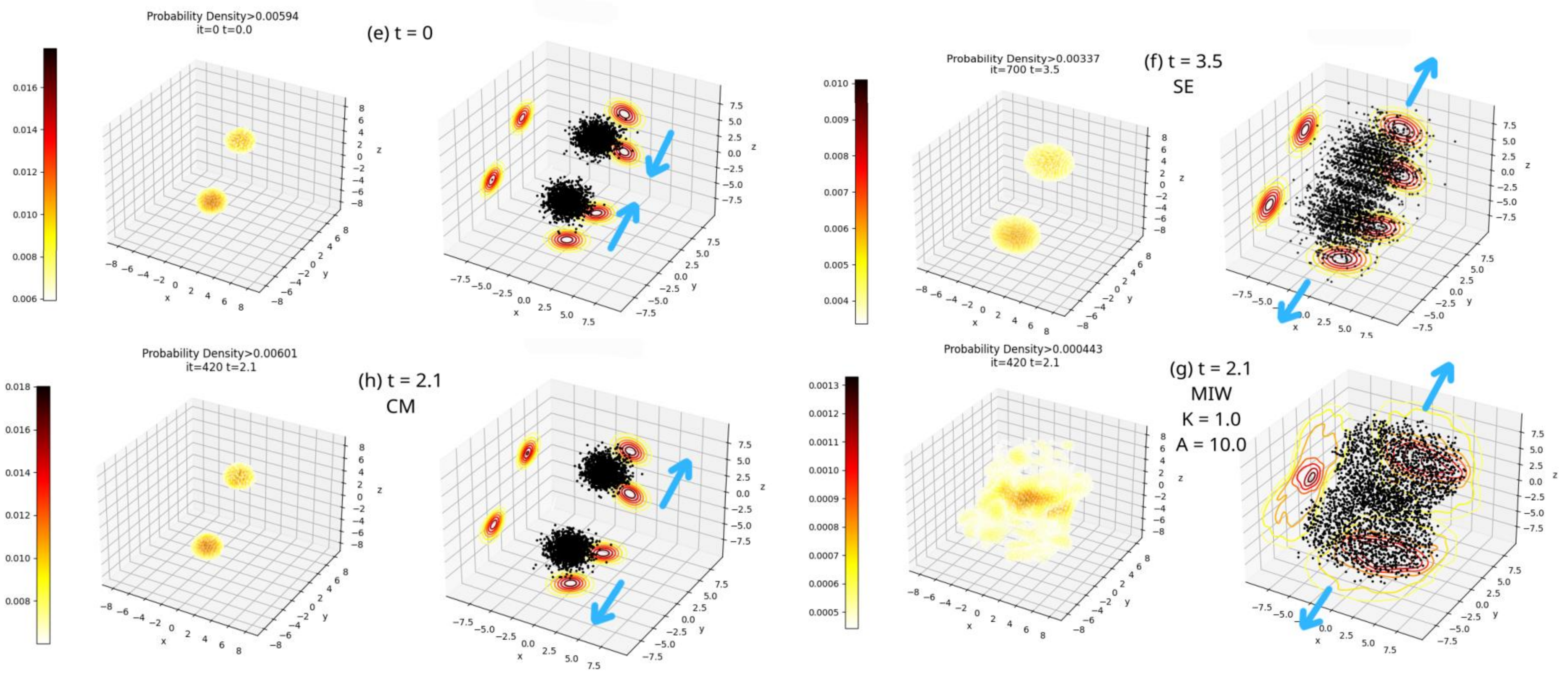

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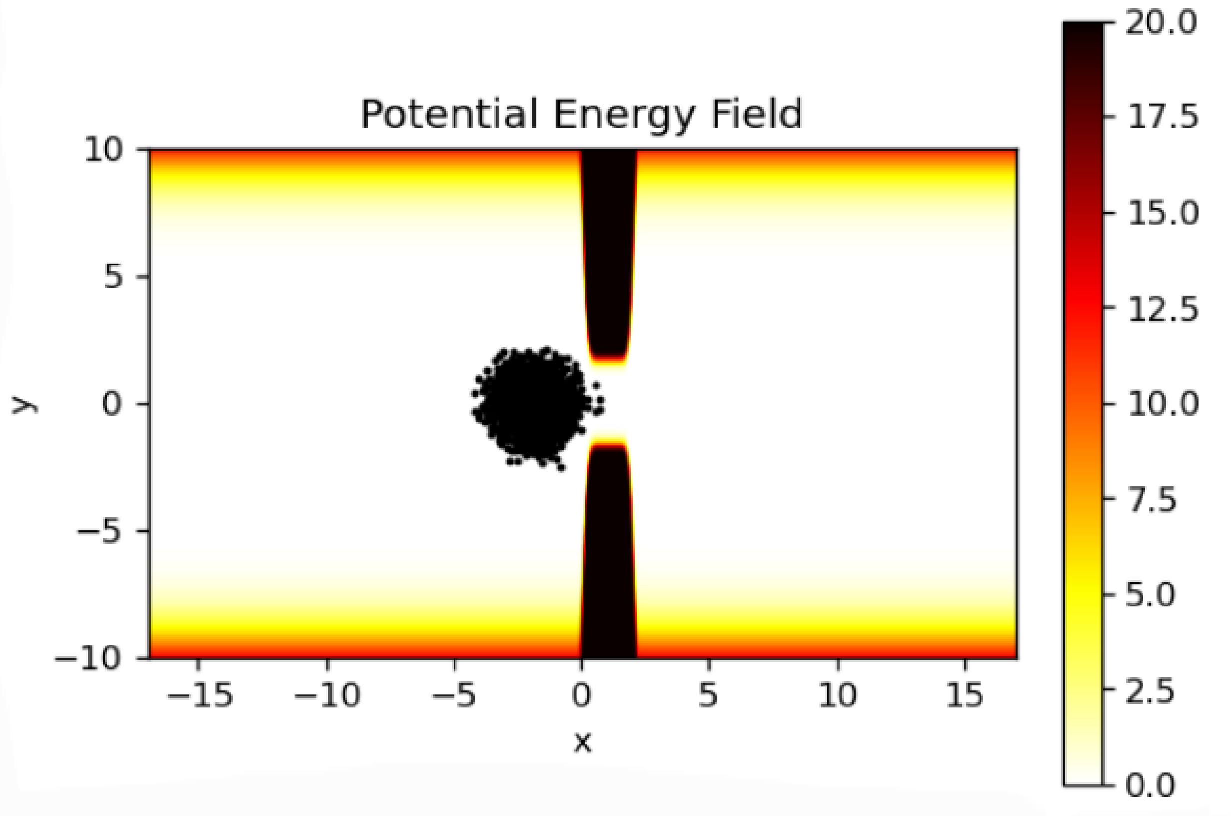
What about Entanglement?

Can we test it?

D. Pandey, X. Oriols, and G. Albareda, Materials, vol. 13, no. 13, p. 3033, 2020



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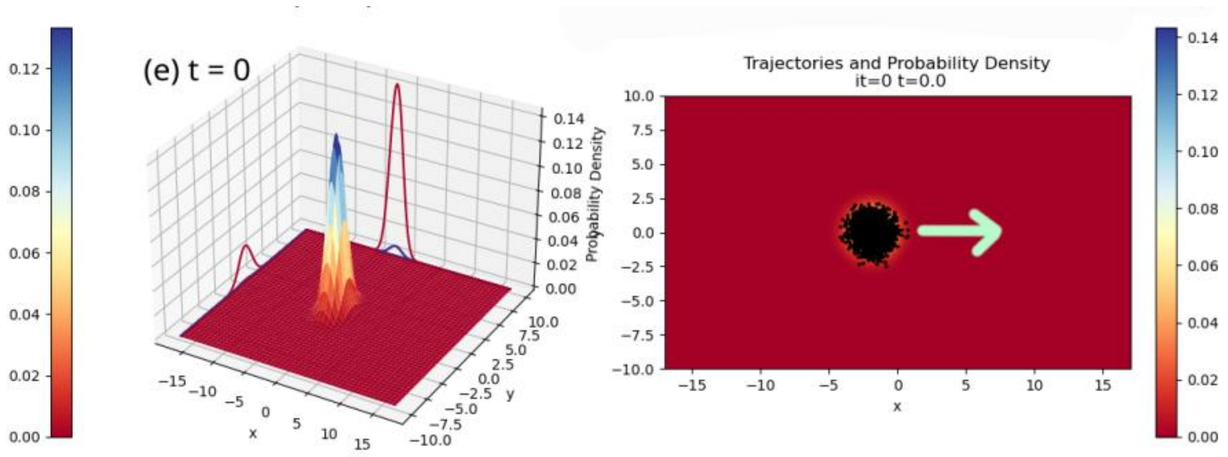
Entanglement and Tunneling



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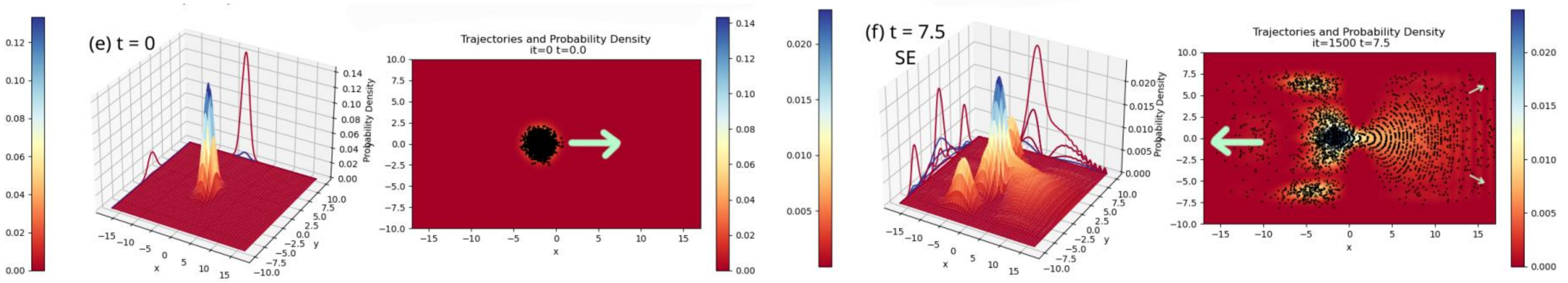

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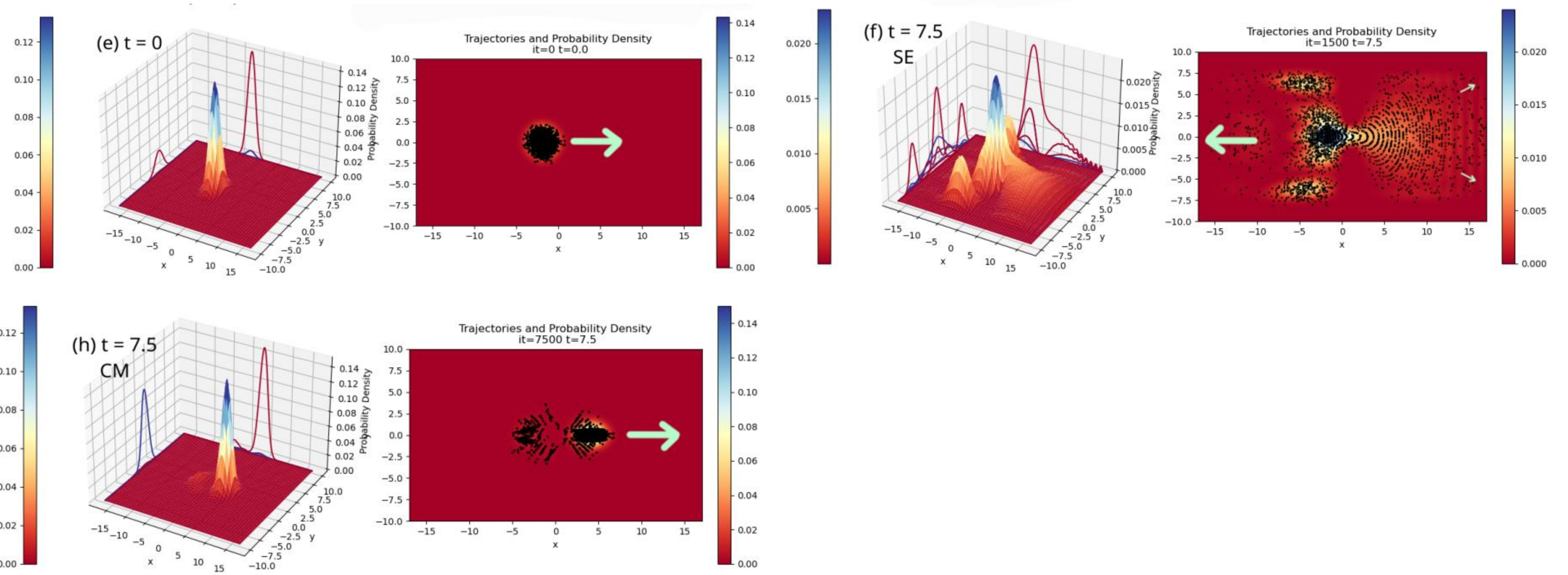

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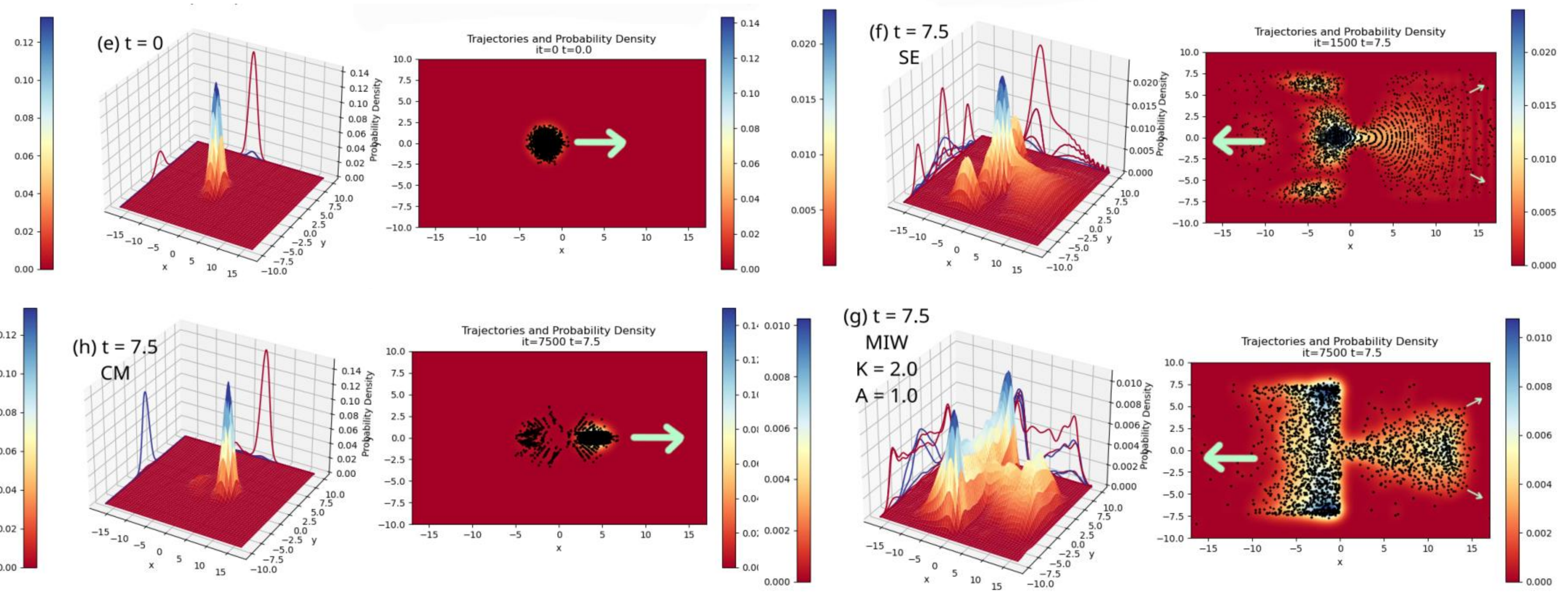
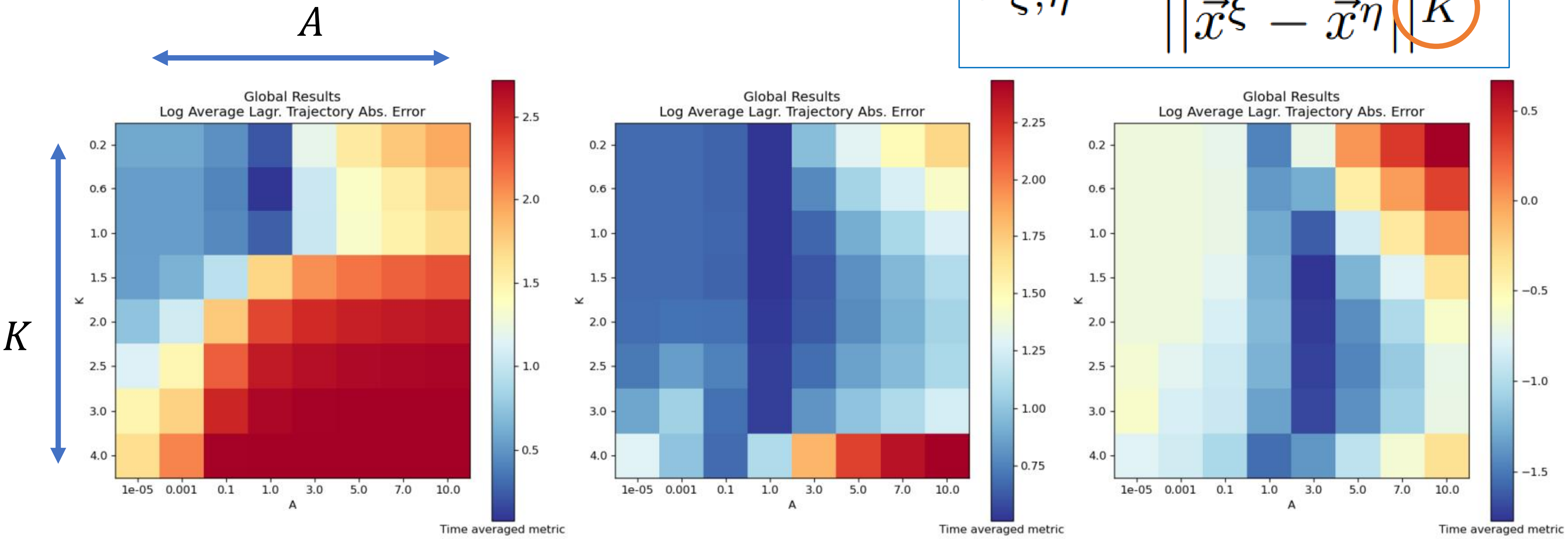


(b) Towards Quantitativeness

$$\vec{G}_{\xi,\eta} = \frac{A}{||\vec{x}^{\xi} - \vec{x}^{\eta}||^{K}}\hat{u}$$



(a) $n = 1$ (b) $n = 2$ (c) $n = 3$

Figure 1: The colormaps show the logarithm of metric (35), defiend to compare the SE simulations to our MIW simulations. It measures the divergence between the MIW and Bohmian trajectories. The plotted numbers are the averages per K, A over all the explored scenarios, which can be found in [14]. An average of 7 different potential energy profiles are included per n. Abscissa shows A, while ordinate shows K. All in atomic units.

VI – Conclusions

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- Signs that it does not depend on the classical forces besides it
- Signs that power law depends on dimensionality of configuration-space
- Open source framework that allows the next steps is ready!

Thank you
for your attention!

Questions?