October 16, 2024

Virtual International Seminar on Theoretical Advancements (VISTA)

SUNY Buffalo

Quantum Mechanics Without Wavefunctions

Bill Poirier[*] and
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[*]University of Vermont

[#]St. Mary's University

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aka *"Many Interacting Worlds"*

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Quantum Mechanics Without Wavefunctions

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Quantum Mechanics Without Wavefunctions aka *"Many Interacting Worlds"*

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Bohmian mechanics without pilot waves

Bill Poirier

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ABSTRACT

In David Bohm's causal/trajectory interpretation of quantum mechanics, a physical system is regarded as consisting of *both* a particle *and* a wavefunction, where the latter "pilots" the trajectory evolution of the former. In this paper, we show that it is possible to discard the pilot wave concept altogether, thus developing a complete mathematical formulation of time-dependent quantum mechanics directly in terms of real-valued trajectories alone. Moreover, by introducing a kinematic definition of the quantum potential,

Chem. Phys. **370**, 4-14 (2010).

(one of most read CP articles in 2014)

damental than Eq. (11). Basically, this implies that no quantum effects can be attributed to the behavior of a single trajectory alone. Rather, all quantum behavior in nature is due to an interaction amongst the different trajectories within a given ensemble, with

We conclude with a brief discussion of some of the potential *interpretive* ramifications of the new formulation. In Bohmian mechanics, there is only one system trajectory, whereas the present approach offers an entire ensemble of trajectories. If one presumes objective existence for a single trajectory only, then the remaining trajectories in the ensemble must be regarded as "virtual," in some sense. On the other hand, one might prefer to regard *all* trajectories in the quantum ensemble as equally valid and real. It is hard to imagine how this could be achieved, without positing that each trajectory inhabits a separate world. It must be emphasized, however, that this version of the many worlds interpretation would be very different from the standard form [19–21]. In a nutshell, the latter associates

Communication: Quantum mechanics without wavefunctions

Jeremy Schiff[1,a)] and Bill Poirier[2,b)]

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J. Chem. Phys. **136**, 031102 (2012); http://dx.doi.org/10.1063/1.3680558

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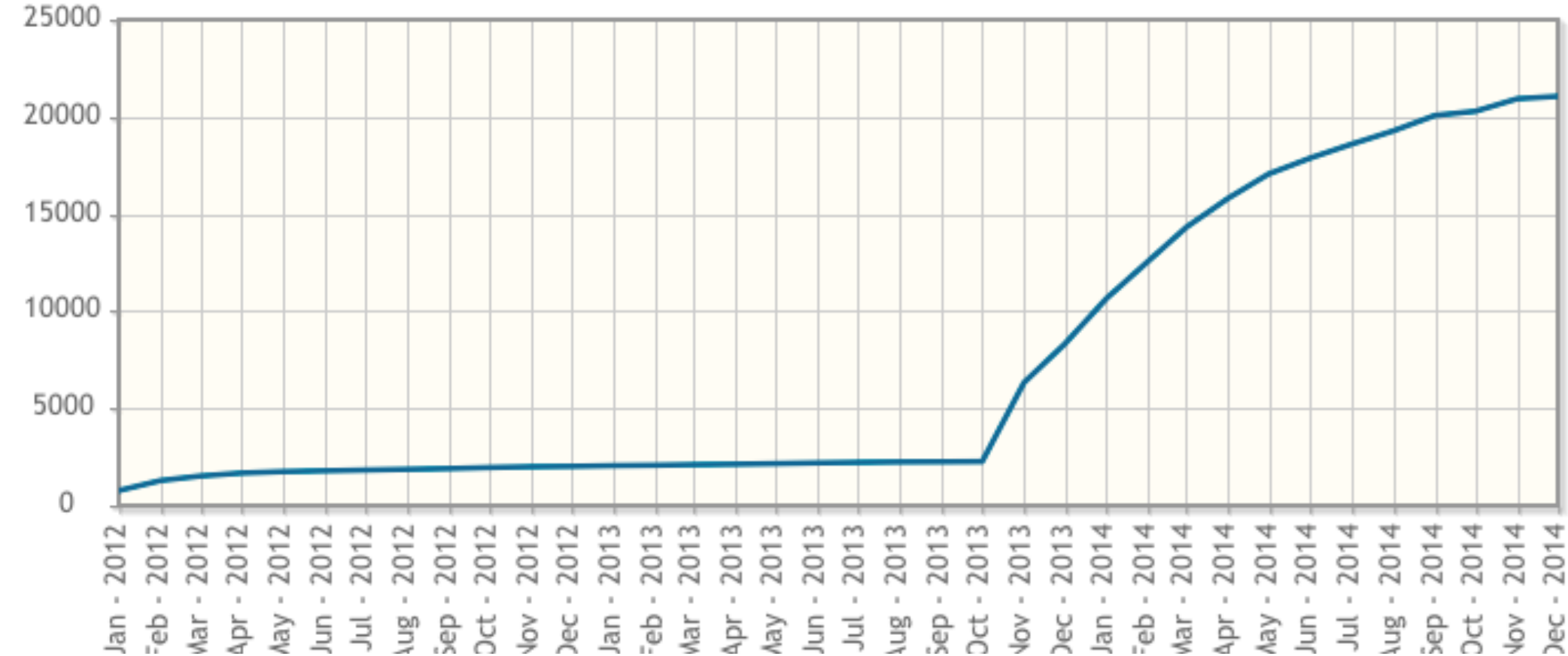


Editorial: Does Research on Foundations of Quantum Mechanics Fit into PRX's Scope?

And we have invited a Commentary by Bill Poirier from Texas Tech University that we hope will enhance your understanding of the paper and of our decision to publish it.

The Editors

The Many Interacting Worlds Approach to Quantum Mechanics

Bill Poirier*, Department of Chemistry and Biochemistry, and Department of Physics, Texas Tech University, Box 41061, Lubbock, Texas 79409-1061

A Commentary on:
Quantum Phenomena Modeled by Interactions between Many Classical Worlds
Michael J. W. Hall, Dirk-André Deckert, and Howard M. Wiseman
Phys. Rev. X, 4, 041013 (2014)

About the Commentary author:

Bill Poirier is Chancellor's Council Distinguished Research Professor and also Barnie E. Rushing Jr. Distinguished Faculty Member at Texas Tech University, in the Department of Chemistry and Biochemistry and also the Department of Physics. He received his Ph.D. in theoretical physics from the University of California, Berkeley, followed by a chemistry research associateship at the University of Chicago. His research interest is in understanding and solving the Schrödinger equation, from both foundational and practical perspectives.

INTERNATIONAL BUSINESS TIMES

Parallel and interacting worlds could explain weirdness of quantum mechanics, says a new theory. But these are parallel worlds at atomic scale, not the kind we saw in Interstellar.(Warner Bros)

Quantum mechanics, that explains the world of atoms and quarks, confers certain weirdness on the world by referring to objects in terms of the wave function. This only gives a probability of finding an object at a certain position and time.

Hence, the world is not well-defined.

Texas Tech University chemical physicist Bill Poirier's theory does away with the wave and gives a classical world status to quantum reality.

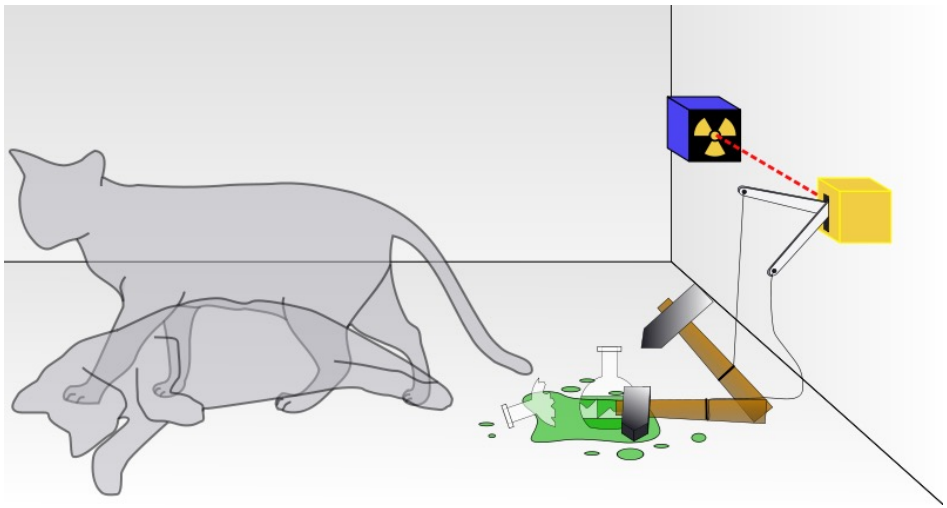
Brief Outline for Remainder of Talk

1. Brief description of what this approach is.
2. First principles derivation: 1D time-independent case
3. Noether's theorem / symplectic structure / numerics
4. Time dependent case / multi-dimensional case
5. Relativistic generalization

Getting Rid of Ψ Altogether:

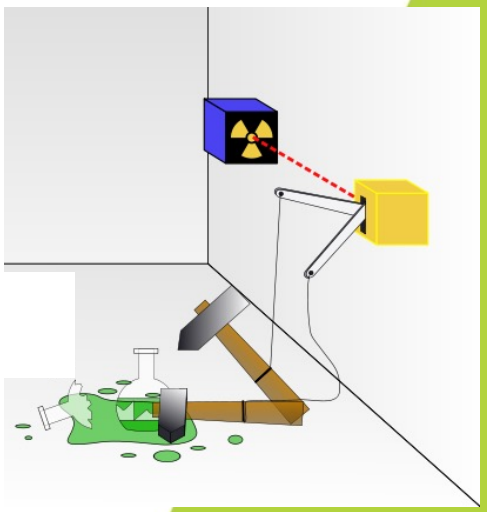
How can that even be possible?

Not , **But**



Ψ

$\not{h}$



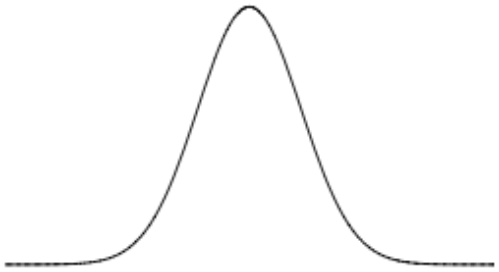
Is Ψ Alive or Dead ?

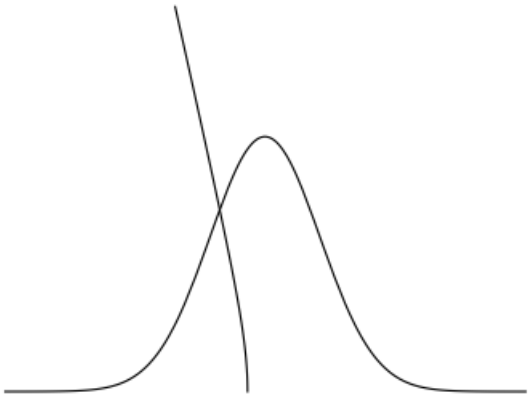
But if not Ψ, then what?

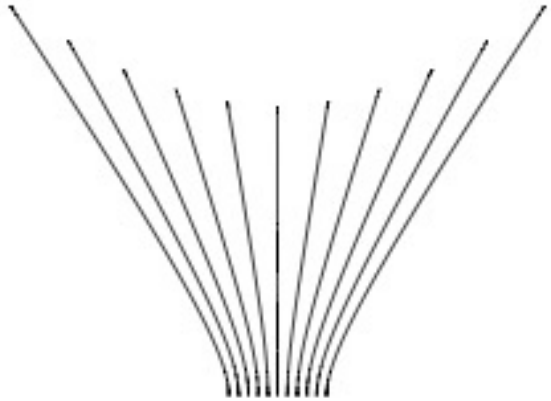
Answer: Trajectories only

- The wavefunction $\Psi(x,t)$ is replaced with an *ensemble* (family) of trajectories, $x(C,t)$.
  - parameter C labels individual trajectories within the ensemble.
  - resembles classical statistical mechanics/trajectory simulations.
- The individual trajectories turn out to be the quantum trajectories of David Bohm. *However…*
- *This is* **NOT** *Bohmian Mechanics!*
  - Bohm uses a *single* trajectory, $x(t)$.
  - Bohm *also* uses the wavefunction, $\Psi(x,t)$.

Copenhagen quantum mechanics	Bohmian mechanics	Quantum trajectory-based formulation (non-relativistic)
Ψ represents the state of the system. TDSE drives evolution of $\Psi(x,t)$.	Ψ and $x(t)$ together represent the state of the system. Ψ leads to quantum potential Q, driving trajectory dynamics via: $$m\ddot{x}+\frac{\partial V(x)}{\partial x}+\frac{\partial Q(x,t)}{\partial x}=0$$	There is no Ψ. $x(t, C)$ (trajectory ensemble) alone represents the state of the system, and leads to Q. $x(t, C)$ satisfies its own PDE that replaces the TDSE (with $'$ denoting partial derivative w/ respect to C.) $$m\ddot{x}+\frac{\partial V(x)}{\partial x}+\frac{\hbar^2}{4m}\left(\frac{x''''}{x'^4}-8\frac{x'''x''}{x'^5}+10\frac{x''^3}{x'^6}\right)=0$$







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[2] P. Holland, Ann. Phys. 315, 505 (2005).
[3] B. Poirier, Chem. Phys. 370, 4 (2010).
[4] J. Schiff and B. Poirier, J. Chem. Phys. 136, 031102 (2012).
[5] B. Poirier, arXiv:1208.6260 [quant-ph], (2012).

Copenhagen quantum mechanics	Bohmian mechanics	Quantum trajectory-based formulation (non-relativistic)
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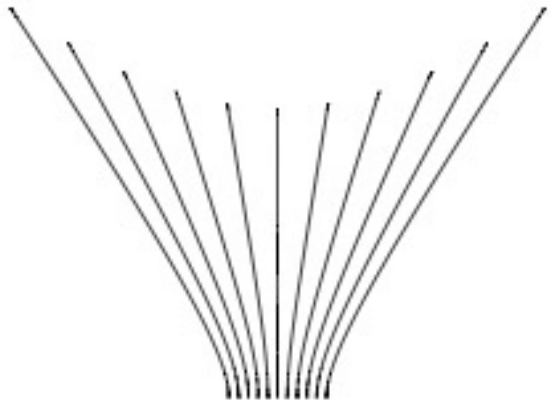
Key Mathematical Features:

1. x was an *independent* variable, but is now the *dependent* field quantity.
2. PDE 4th order in "space" (C), 2nd order in time (t). C and t not treated on equal footing; *are x and t ?*
3. "Spatial" derivatives = interworld interaction = quantum "weirdness."
4. ***Trajectory PDE shows no explicit dependence on C and t (and x if V = const) unlike in Bohm.***
5. Ensemble of quantum trajectories foliate spacetime (no crossing trajectories).



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Theoretical/Mathematical Ramifications

First Principles Derivation

- Start "from scratch"; assume almost no knowledge of:
  - classical mechanics (Newton's Laws)
  - quantum mechanics (TISE).
- "Trial" trajectory $x(t)$ completely unconstrained
  - i.e. $x(t)$ is a *path*, not yet a trajectory.
- Posit existence of two "functional forms" of $x(t)$.
  - $f[x]$ (depends on x; essentially potential energy)
  - $g[\dot{x}]$ (depends on $\dot{x}$; essentially kinetic energy)
  - *NO* assumptions are made about form of $f[x]$ and $g[\dot{x}]$!
  - Space x assumed to be homogeneous (for simplicity).

Physical Constraint #1: Action Extremization

- For all possible smooth paths $x(t)$ that connect:
  - initial point (x_0,t_0) with final point (x_f,t_f)
  - dynamical solution trajectory = $x(t)$ path that extremizes action, S.
- Definition of action: $$S = \int_{t_0}^{t_f} L[x(t), \dot{x}(t)]dt = \int_{t_0}^{t_f} \left(g[\dot{x}] - f[x]\right)dt$$
- Solution $x(t)$ satisfies Euler-Lagrange equation:

$$\left[\frac{\partial f}{\partial x}\right] + \frac{d}{dt}\left[\frac{\partial g}{\partial \dot{x}}\right] = 0$$

- Note: $f[x]$ and $g[\dot{x}]$ are still completely unspecified!
  - e.g., $g[\dot{x}] = C\dot{x}^4$ would be permissible.
  - however, for any specific choice of f and g, the solution $x(t)$ is now completely determined.

Physical Constraint #2:
Hamiltonian Energy Conservation

- For all possible smooth paths $x(t)$ with initial conditions:

  $x(t_0)=x_0$ and $\dot{x}(t_0)=\dot{x}_0$

  dynamical solution trajectory = $x(t)$ path that conserves Hamiltonian, H.

- Form of Hamiltonian:

$$H[x(t),\dot{x}(t)] = g[\dot{x}(t)] + f[x(t)]$$

- Solution $x(t)$ satisfies Hamiltonian energy conservation:

$$H[x(t),\dot{x}(t)] = H(t) = \text{constant}$$

- Note: $f[x]$ and $g[\dot{x}]$ are still completely unspecified!
  - however, for any specific choice of f and g, the solution $x(t)$ is now completely determined.

Combining Both Constraints

- Either physical constraint by itself leads to a unique set of solution trajectories
  - In general, i.e. for arbitrary choice of $f[x]$ and $g[\dot{x}]$,

    Action extremizing trajectories are not the same as Hamiltonian conserving trajectories
- Satisfying *both* conditions simultaneously is very special:
  - Noether's theorem: explicit t invariance of L implies existence of a conserved energy quantity, denoted E.
  - Our condition: that Noether E be equal to the Hamiltonian H.
  - imposes *severe* restrictions on allowed forms for $f[x]$ and $g[\dot{x}]$.

Combining Both Constraints

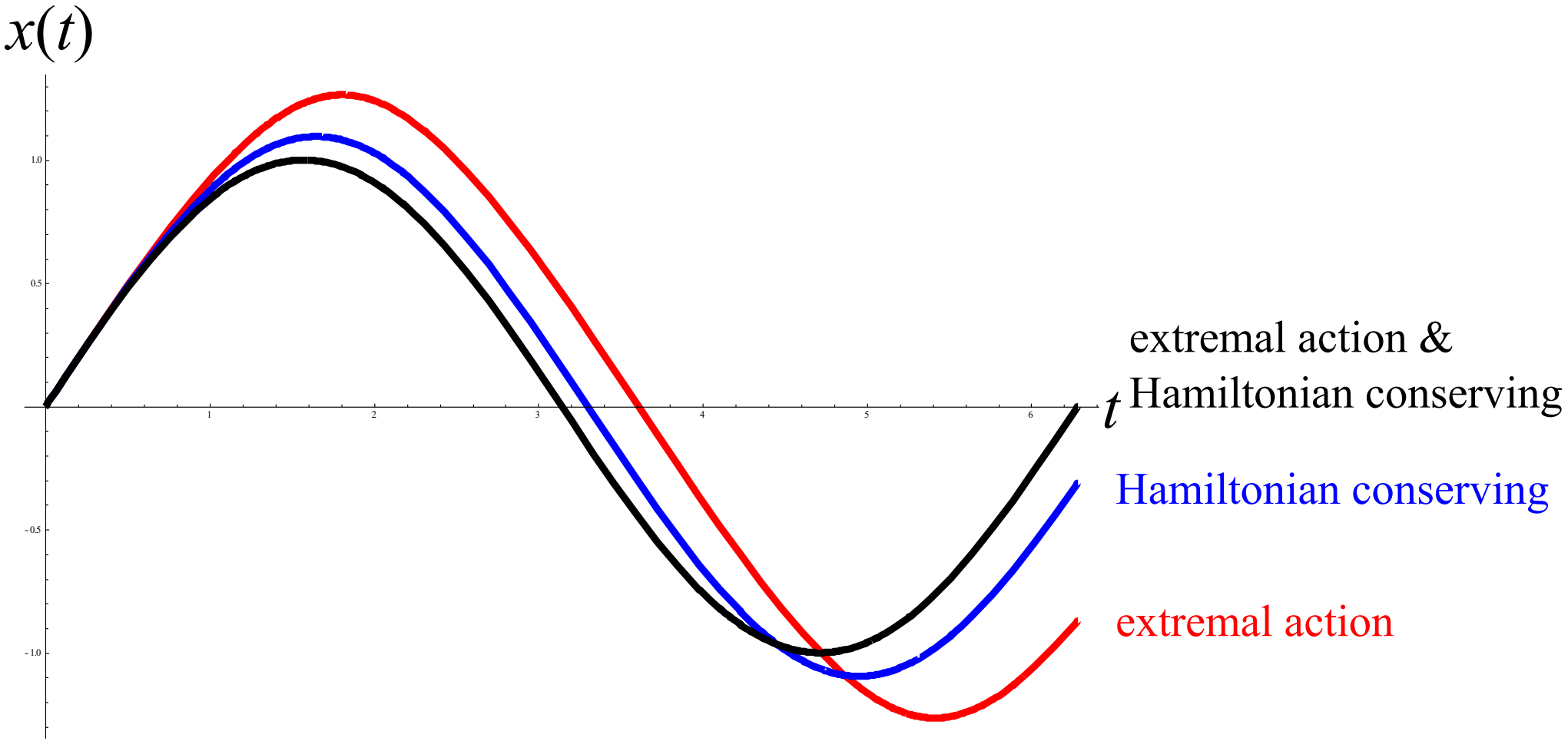
- What are the most general possible forms consistent with both action extremization and Hamiltonian conservation?

  $f[x]$ = completely unconstrained = $V[x]$

  $g[\dot{x}] = A\dot{x}^2 = (m/2)\dot{x}^2 = T[\dot{x}]$

- These are *precisely* the most general possible forms that are considered in *classical mechanics*.
  - thus, classical mechanics satisfies both of the two physical constraints, that we have imposed (already known).
  - but *no* other choices for $f[x]$ and $g[\dot{x}]$ (i.e., no other candidate dynamical laws) can do so.

Harmonic Potential Trajectories



$f[x] = V[x] = (1/2)\, x^2$

$g[\dot{x}] = (1/2)\dot{x}^2$ (black curves)

$g[\dot{x}] = (1/2)\dot{x}^2 + .1\dot{x}^4$ (red and blue curves)

Quantum Trajectories Derivation

1D Stationary Scattering States

- Requires modification of the $L[x, \dot{x}]$ and $H[x, \dot{x}]$ forms.
- Requires higher-order time derivatives.
  - consider contact/point transformation from coordinate x to y.
  - transformed functionals now mix y and $\dot{y}$, however...
  - no new physics added, i.e. result still classical mechanics.
- Posit existence of higher-order functional forms:

$$L = L[x, \dot{x}, \ddot{x}, \ldots]$$

$$H = H[x, \dot{x}, \ddot{x}, \ldots]$$

Quantum Contribution to *L* and *H* Functional Forms

- Space x assumed to be homogeneous (for simplicity).
- Posit existence of higher-order quantum correction, Q:

$$L[x, \dot{x}, \ddot{x}, \ldots] = T[\dot{x}] - V[x] - Q[\dot{x}, \ddot{x}, \ldots]$$

$$H[x, \dot{x}, \ddot{x}, \ldots] = T[\dot{x}] + V[x] + Q[\dot{x}, \ddot{x}, \ldots]$$

- Q resembles a *potential* energy:
  - connects to "quantum potential" of Bohm theory.
  - adds to H but subtracts from L, like a potential energy.
- Q resembles a *kinetic* energy:
  - kinematic quantity that cannot depend on x.
  - quantum "potential" actually comes from K.E. operator.

Functional Form of Q

- Technical Note:
  - action extremization via "generalized" Euler-Lagrange eqn:

$$\left[\frac{\partial L}{\partial x}\right]-\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}}\right]+\frac{d^2}{dt^2}\left[\frac{\partial L}{\partial \ddot{x}}\right]-\cdots=0$$

- Allowed meromorphic solutions (dynamical laws):

$V[x]$ = completely unconstrained.

$$T[\dot{x}]=(m/2)\dot{x}^2$$

$$Q[\dot{x},\ddot{x},\ldots]=\begin{cases}\Delta E=\text{constant} & \text{order 0 (classical mechanics)}\\ \text{no solutions} & \text{order 1}\\ \text{no solutions} & \text{order 2}\\ -\dfrac{B}{2m}\left(\dfrac{5}{4}\dfrac{\ddot{x}^2}{\dot{x}^4}-\dfrac{1}{2}\dfrac{\dddot{x}}{\dot{x}^3}\right) & \text{order 3 (quantum mechanics, } B=\hbar^2)\end{cases}$$

Trajectory-Based Equations

- Technical Note:
  - action extremization via "generalized" Euler-Lagrange eqn:

$$\left[\frac{\partial L}{\partial x}\right]-\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}}\right]+\frac{d^2}{dt^2}\left[\frac{\partial L}{\partial \ddot{x}}\right]-\cdots=0$$

- Final Form of Lagrangian:

$$L[x,\dot{x},\ddot{x},\dddot{x}]=\frac{m\dot{x}^2}{2}-V[x]-\frac{\hbar^2}{2m}\left(\frac{5}{4}\frac{\ddot{x}^2}{\dot{x}^4}-\frac{1}{2}\frac{\dddot{x}}{\dot{x}^3}\right)$$

- Final Euler-Lagrange ODE (4^{th}-order, real-valued)

$$m\ddot{x}+\frac{\partial V[x]}{\partial x}+\frac{\hbar^2}{4m}\left(\frac{\ddddot{x}}{\dot{x}^4}-8\frac{\dddot{x}\,\ddot{x}}{\dot{x}^5}+10\frac{\ddot{x}^3}{\dot{x}^6}\right)=0$$

Reactive Scattering Calculations: Cross Sections & Rates

Time independent

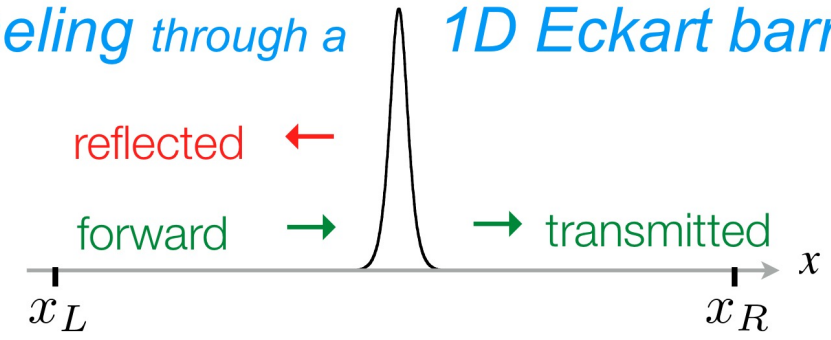
quantum trajectories (#5)

tunneling through a 1D Eckart barrier

Eckart potential:

$V(x) = V_0 \ \mathrm{sech}^2(\alpha x)$

$\alpha = 3.0\, a.u.$
$m = 2000\, a.u.$
$V_0 = 400\, cm^{-1}$



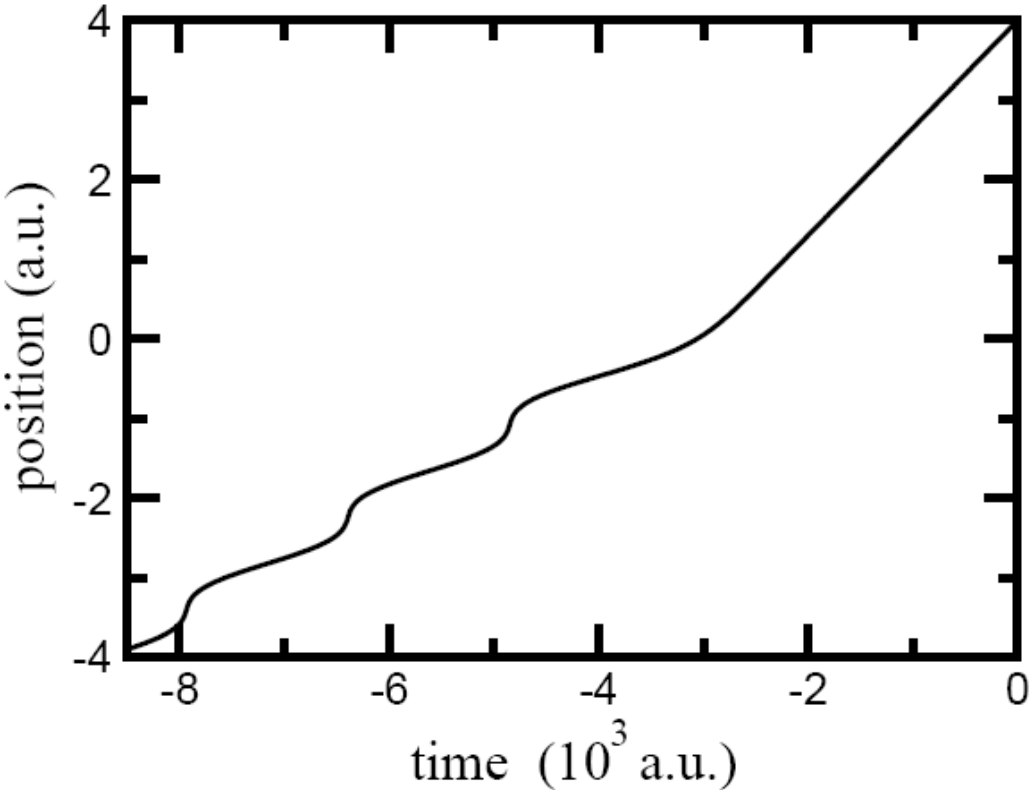
$$\Psi(x \to +\infty) = k_R^{-1/2} T \exp[ik_R x]$$

$$\Psi(x \to -\infty) = k_L^{-1/2} \left(\exp[ik_L x] + R \exp[-ik_L x]\right)$$

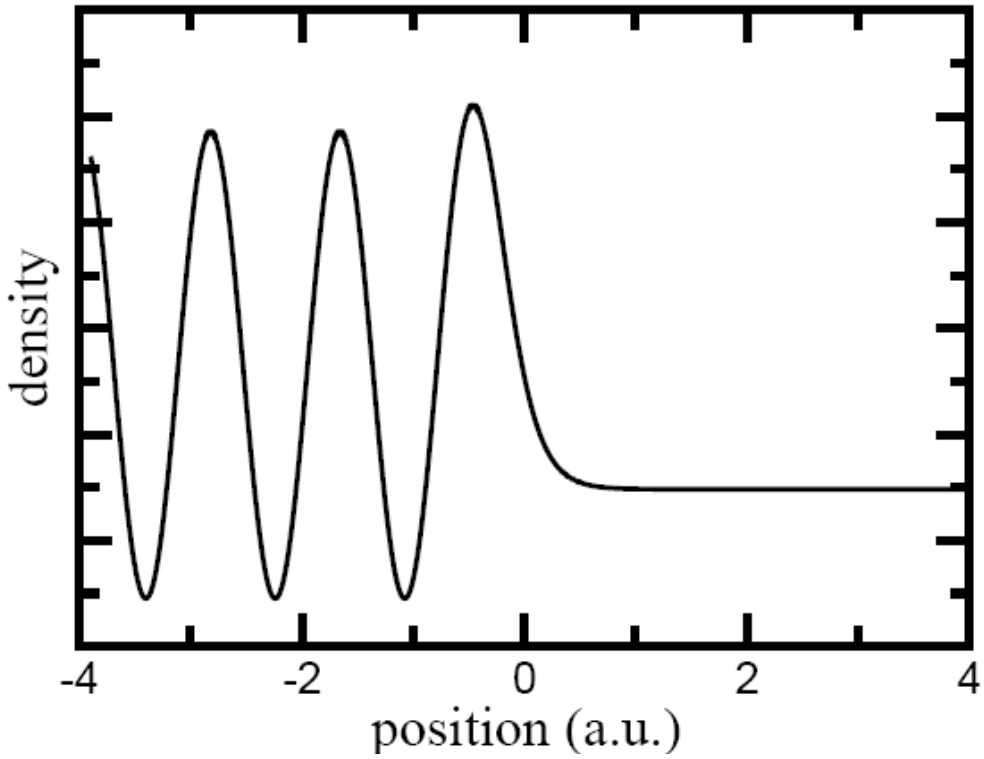
- Challenges in the continuum:
  - Two linearly independent eigenstate solutions for each energy *E*, requiring imposition of special boundary conditions.
  - Energy eigenstates extend infinitely far in both directions, necessitating use of optical potentlals to absorb outgoing flux.
  - Exact quantum dynamics calculation in the “deep” tunneling regime nearly impossible, even in 1D.

Numerical Solution of the 1D TISE:

Eckart Barrier



Trajectory, $x(t)$



Wavefunction density, $\rho(x)$

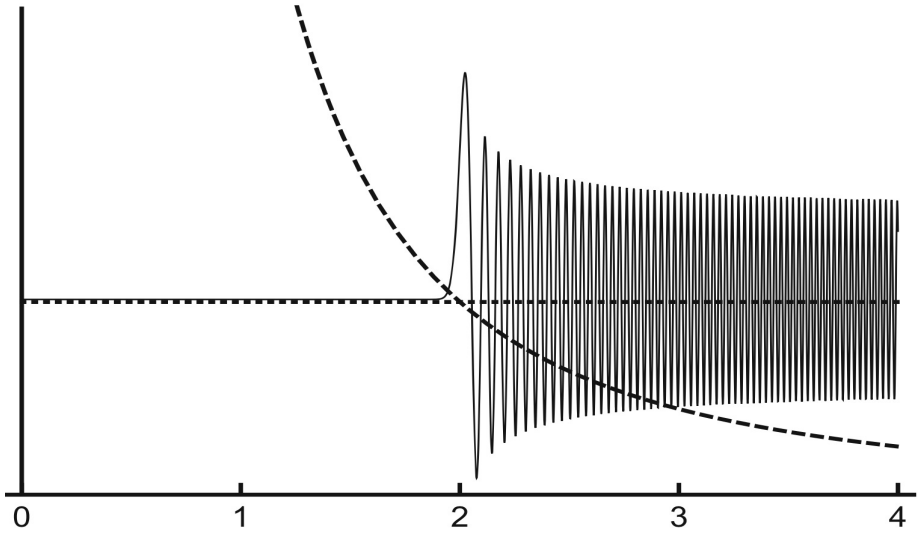
Solve 4th order real-valued ODE in t, to obtain $x(t)$.

- similar to Newton's second law, w/ extra terms.
- two initial conditions specify E and x_0.
- remaining two specify boundary conditions of solution ψ

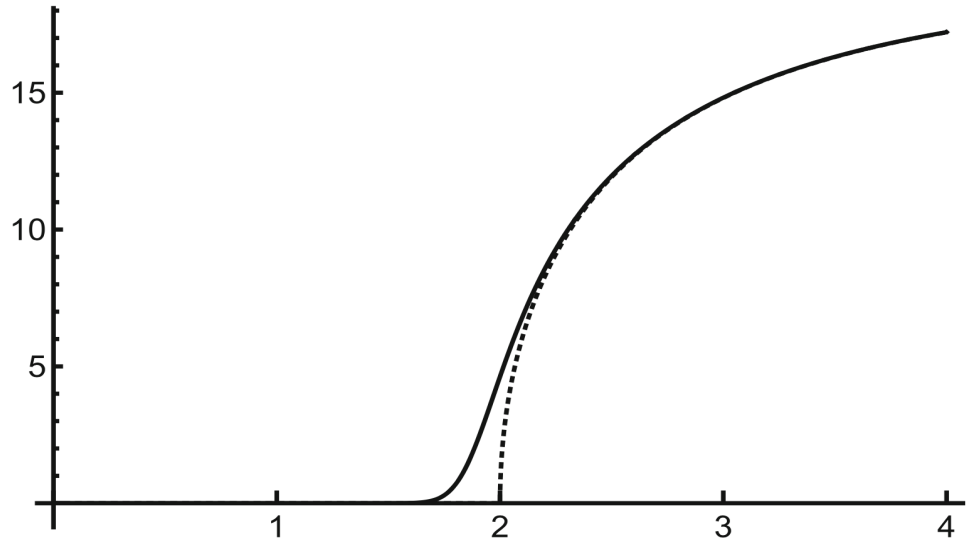
Bipolar Quantum Trajectories:
Brazilian Nuclear Physics Collaboration

- Separate Ψ into forward and backward moving parts, i.e. $\Psi = \Psi_+ + \Psi_-$.
  - contribute separate quantum trajectories for Ψ_+ and Ψ_-.
  - "bipolar" trajectories show no oscillatory interference, i.e. they are smooth and well-behaved everywhere.

M. S. Hussein and B. Poirier, "Quantum Trajectory Description of the Time-Independent (Inverse) Fermi Accelerator", *BJP* **51**, 193 (2021).



Wavefunction, $\Psi(x)$



Phase Space Trajectory, $p(x)$

Bipolar Quantum Trajectories:
Brazilian Nuclear Physics Collaboration

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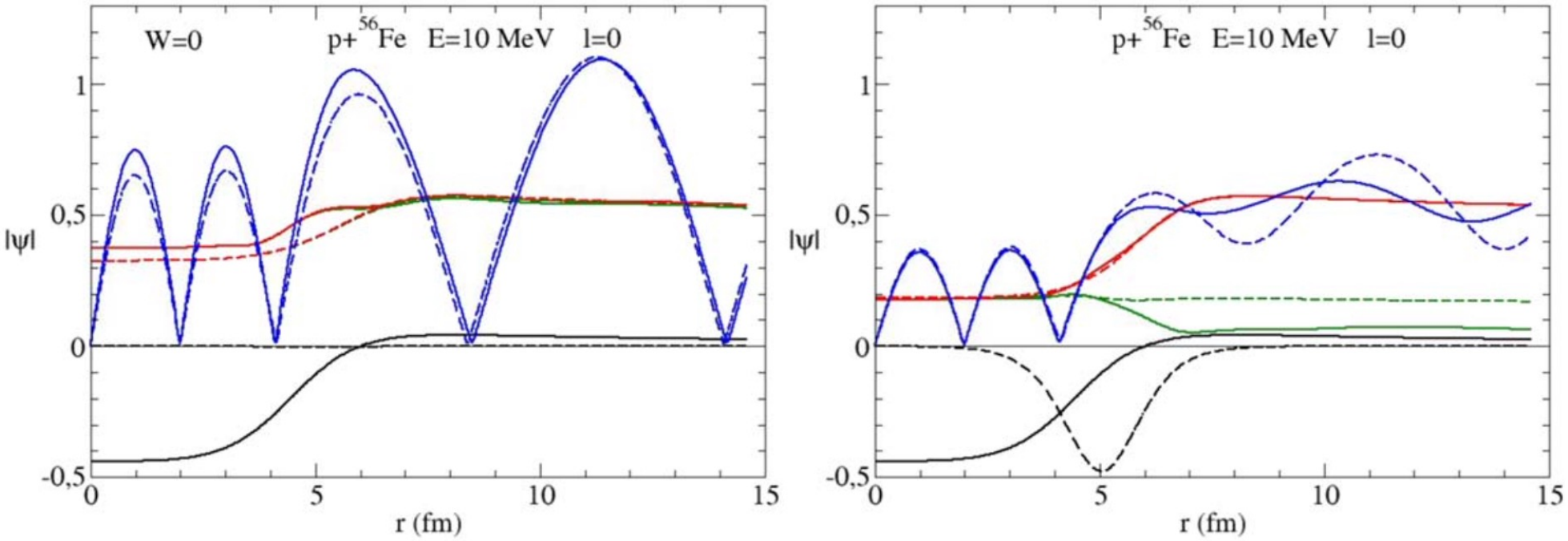
N. A. Coleta da Conceição, B. V. Carlson, and B. Poirier, "Quantum trajectories and the nuclear optical model", *Phys. Scr.* **98**, 115303 (2023).



Incoming, outgoing, and total wave functions for protons incident on ^{56}Fe at 10 MeV for partial wave $l = 0$.

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Noether's Theorem

"There is…a minority…who recognize…that the most beautiful and satisfying experiences open to humankind are not derived from the outside, but…with the development of the individual's own feeling, thinking and acting. The genuine artists, investigators and thinkers have always been persons of this kind. However inconspicuously the life of these individuals runs its course, none the less the fruits of their endeavors are the most valuable contributions which one generation can make to its successors. Within the past few days a distinguished mathematician, Professor Emmy Noether…died in her fifty-third year. In the judgment of the most competent living mathematicians, Fräulein Noether was ***the most significant creative mathematical genius thus far produced*** since the higher education of women began.

Emmy Noether Einstein's Obituary (excerpts)

"Any differentiable symmetry (invariance) of the action of a physical system has a corresponding conservation law."

scattering through a 1D Eckart barrier

- Main difference with classical trajectories on the left (reactant) asymptote:
  - $p = m\dot{x}$ is ***not*** conserved.
  - one can show that ***Noether momentum***

$$p_{Noether} = m\dot{x} + \frac{\hbar^2}{4m}\left(\frac{\dddot{x}}{\dot{x}^4} - \frac{2\ddot{x}^2}{\dot{x}^5}\right)$$

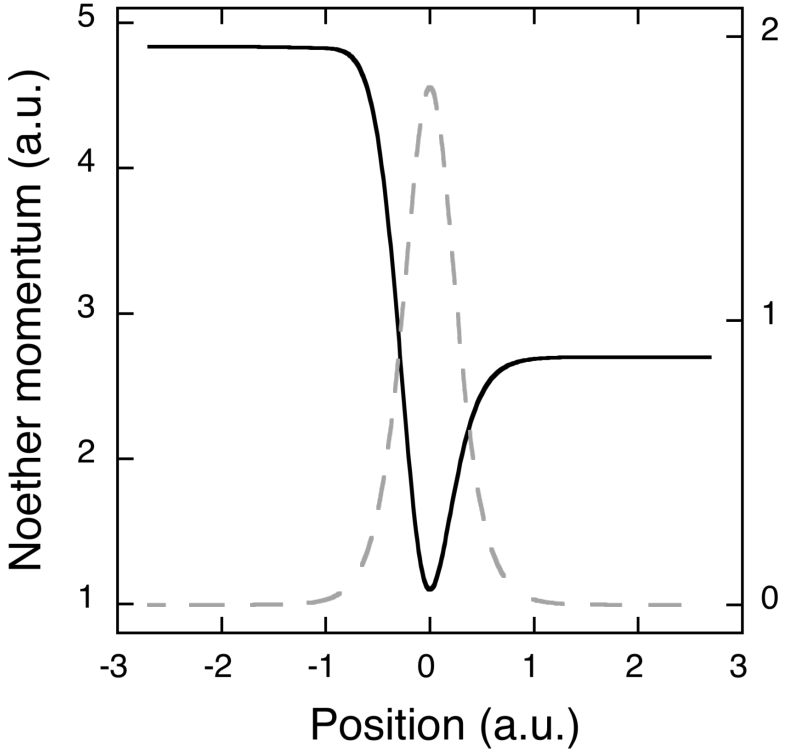
    is conserved

- Asymptotic $p_{Noether}$:

$$p_L = p_{Noether}(t \to -\infty) = \hbar k_L \left(\frac{1+|R|^2}{1-|R|^2}\right)$$

- Transmission probability:

$$P_T = \frac{2\hbar k_L}{\hbar k_L + p_L}$$



scattering through a 1D Eckart barrier

Transmission as a function of Energy

E/V_0	Exact	Present calculation	Rel. error
1.(−12)	.28508(−12)	.28522(−12)	+5.(−04)
1.(−09)	.28507873(−09)	.28507863(−09)	−4.(−07)
1.(−06)	.28507940681(−06)	.28507940697(−06)	+5.(−10)
1.(−03)	.285757547947374(−03)	.285757547947352(−03)	−8.(−14)
1.(−01)	.356449541539905(−01)	.356449541539893(−01)	−4.(−14)
0.5	.318986860221912	.318986860221873	−1.(−13)
1.0	.716641955866101	.716641955866092	−1.(−14)
1.5	.900592641583308	.900592641583281	−3.(−14)
2.0	.963615495020163	.963615495020159	−4.(−15)
10.0	.999998078464427	.999998078464407	−2.(−14)

Can propagate for 10^8 a.u. of time with energy conservation ~ 1. 10^{-12}

Classical Hamiltonian Form for the 1D TISE ODE

Turns out to be identical to Ostrogradski Approach...

- Search for a quantum Hamiltonian form to describe the 1D TISE ODE for $x(t)$.
  - Fourth-order ODE equivalent to four coupled 1st order ODEs
  - Incredibly, *these can be written as ordinary* ***classical*** *Hamilton's equations* for a two degree of freedom system!)

$$\dot{x} = \frac{\partial H}{\partial p} \; ; \; \dot{p} = -\frac{\partial H}{\partial x} \; ; \; \dot{r} = \frac{\partial H}{\partial s} \; ; \; \dot{s} = -\frac{\partial H}{\partial r}$$

$$H(x, p, r, s) = \frac{s(2p - s)}{2m} + V(x) - \frac{2r^2 s^4}{m\hbar^2}$$

- (x,p) are "classical" conjugate phase space variables, and (r,s) describe an additional "quantum" coordinate.

$$s = m\dot{x} \; ; \; r = \frac{\hbar^2 \ddot{x}}{4m^2 \dot{x}^4} \; ; \; p = m\dot{x} + \frac{\hbar^2}{4m}\left(\frac{\dddot{x}}{\dot{x}^4} - \frac{2\ddot{x}^2}{\dot{x}^5}\right)$$

$$\dot{x} = \frac{s}{m} \; ; \; \dot{p} = -\frac{\partial V(x)}{\partial x} \; ; \; \dot{s} = \frac{4rs^4}{m\hbar^2} \; ; \; \dot{r} = \frac{p - s}{m} - \frac{8r^2 s^3}{m\hbar^2}$$

Brief Outline for Remainder of Talk

1. Brief description of what this approach is.
2. First principles derivation: 1D time-independent case
3. Noether's theorem / symplectic structure / numerics
4. Time dependent case / multi-dimensional case
5. Relativistic generalization

Quantum Trajectories Derivation
1D Time-dependent Wavepackets

- Individual trajectories no longer able to represent $\psi(x,t)$.
  - the wavefunction $\psi(x,t)$ is replaced with an *ensemble* of trajectories, $x(C,t)$.
  - parameter C labels individual trajectories within the ensemble.
  - resembles classical statistical mechanics.
- Variables x and t no longer related via coordinate transformation.
  - trajectory field description provided by $x=x(C,t)$.
  - C is a parameter used to distinguish a given trajectory for *all* t.
  - e.g., $C = x_0=x(x_0,t=0)$ is the initial value of a given trajectory in the ensemble.
  - other choices of the C parameter also exist.

Quantum Trajectories Derivation

1D Time-dependent Wavepackets

- Trajectories governed by their own self-contained PDE.
  - we now have "spatial" derivatives in terms of C, (i.e., across trajectories), in addition to time derivatives.
  - allowed forms of T[], V[], and Q[] turn out to be identical to time-independent case, except with C rather than t derivatives for Q[].
  - all quantum effects/quantum forces arise from C derivatives, i.e. stem from interaction across nearby worlds.

- Goal: Derive a PDE to describe time evolution of $x(C,t)$ field.
  - depends on partial derivatives in both time *and* space (really C):

$$m\frac{\partial^2 x}{\partial t^2} + V_x(x,t) + \frac{\hbar^2}{4m}\left(\frac{x''''}{x'^4} - 8\frac{x''x'''}{x'^5} + 10\frac{x''^3}{x'^6}\right) = 0\ .$$

1D Time-dependent Wavepackets

Noether's Theorem and Conservation Laws

Energy Conservation Law (requires only that V be independent of t):

$$\partial_t \left(\frac{m}{2}\dot{x}^2 + V(x) + \frac{\hbar^2}{8m}\frac{x''^2}{x'^4} \right) + \frac{\hbar^2 \partial_C}{4m} \left(\left(\frac{x'''}{x'^4} - \frac{2x''^2}{x'^5} \right) \dot{x} - \frac{x''\dot{x}'}{x'^4} \right) = 0$$

Momentum Conservation Law (requires only that V be independent of x):

$$\partial_t \left(m\dot{x} \right) + \frac{\hbar^2}{4m}\partial_C \left(\frac{x'''}{x'^4} - \frac{2x''^2}{x'^5} \right) = 0$$

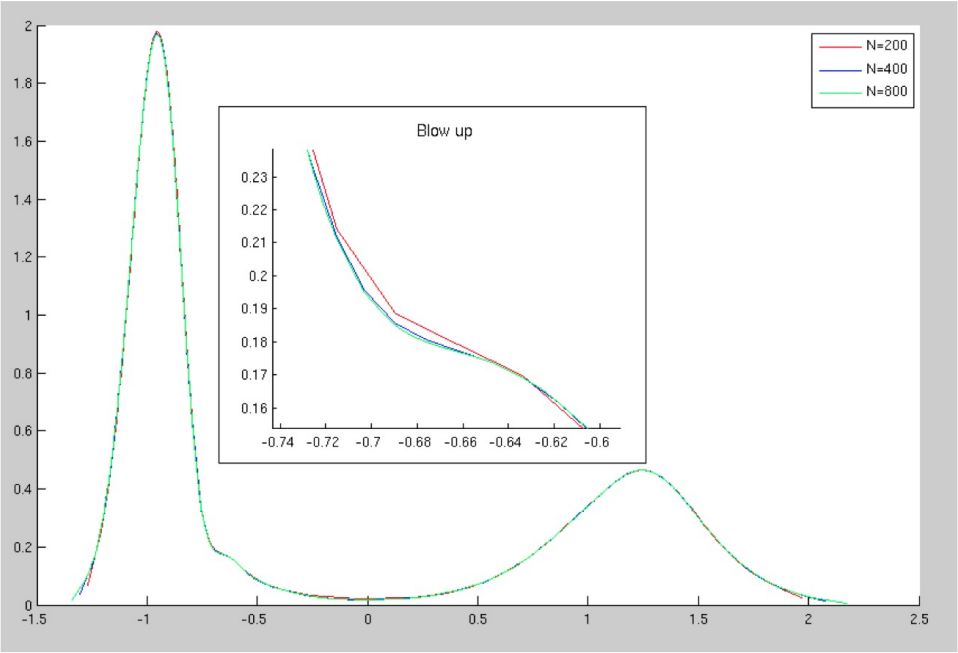
"C" Conservation Law *(always true !!):*

$$\partial_t \left(m\dot{x}x' \right) + \partial_C \left(-\frac{1}{2}m\dot{x}^2 + V(x) + \frac{\hbar^2}{8m} \left(\frac{2x'''}{x'^3} - \frac{5x''^2}{x'^4} \right) \right) = 0$$

note: $m\dot{x}x' = \left. \frac{dS}{dx}\frac{\partial x}{\partial C} \right|_t = \frac{dS}{dC}$ where $S =$ phase/action

Quantum Trajectories Derivation

1D Time-dependent Wavepackets



Density $\frac{1}{x'} = \psi^2$ against x at $t = 1$ for $p_c = 30$, using $N = 200, 400, 800$ trajectories, and a time step close to the stability limit.

Trajectories for Wavepacket Dynamics
Arbitrary Dimensionality

ManyD Case

$$\mathbf{K}^{-1} = \mathbf{J} = \text{ Jacobian matrix } (J^i_j = \partial x^i / \partial C^j)$$

$$L = \frac{m}{2}\dot{\mathbf{x}}\cdot\dot{\mathbf{x}} - V(\mathbf{x}) - Q$$

$$Q = -\frac{\hbar^2}{4m}\left(K^k_j \frac{\partial^2 K^l_j}{\partial C^k \partial C^l} + \frac{1}{2}\frac{\partial K^k_j}{\partial C^k}\frac{\partial K^l_j}{\partial C^l} \right)$$

$$m\ddot{x}^i + \frac{\partial V(\mathbf{x})}{\partial x^i} - \frac{\hbar^2}{4m}\frac{\partial}{\partial C^m}\left(K^k_i K^m_j \frac{\partial^2 K^l_j}{\partial C^k \partial C^l} \right) = 0$$

1D case

$$K^{-1} = J = \partial x / \partial C = x'$$

$$L = \frac{m}{2}\dot{x}^2 - V(x) - Q$$

$$Q = -\frac{\hbar^2}{2m}\left(\frac{1}{2}\frac{x'''}{x'^3} - \frac{5}{4}\frac{x''^2}{x'^4} \right)$$

$$= m\ddot{x} + \frac{\partial V(x)}{\partial x} + \frac{\hbar^2}{4m}\left(\frac{x''''}{x'^4} - 8\frac{x'''x''}{x'^5} + 10\frac{x''^3}{x'^6} \right)$$

- ManyD "C" Conservation Law:
  - trajectory ensemble now vector field, **x**(**C**,t)
  - symmetries, conservation laws, stress-energy tensors, etc.

Brief Outline for Remainder of Talk

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Relativistic Generalization

- Usual approach with Ψ-based Lagrangian leads to Klein-Gordon wave equation, which fails to give a meaningful single-particle interpretation.
  - The free-particle Klein-Gordon equation is:

$$\left(-\frac{\partial^2}{\partial(ct)^2}+\nabla^2+\left(\frac{mc}{\hbar}\right)^2\right)\Phi(t,x)=0$$

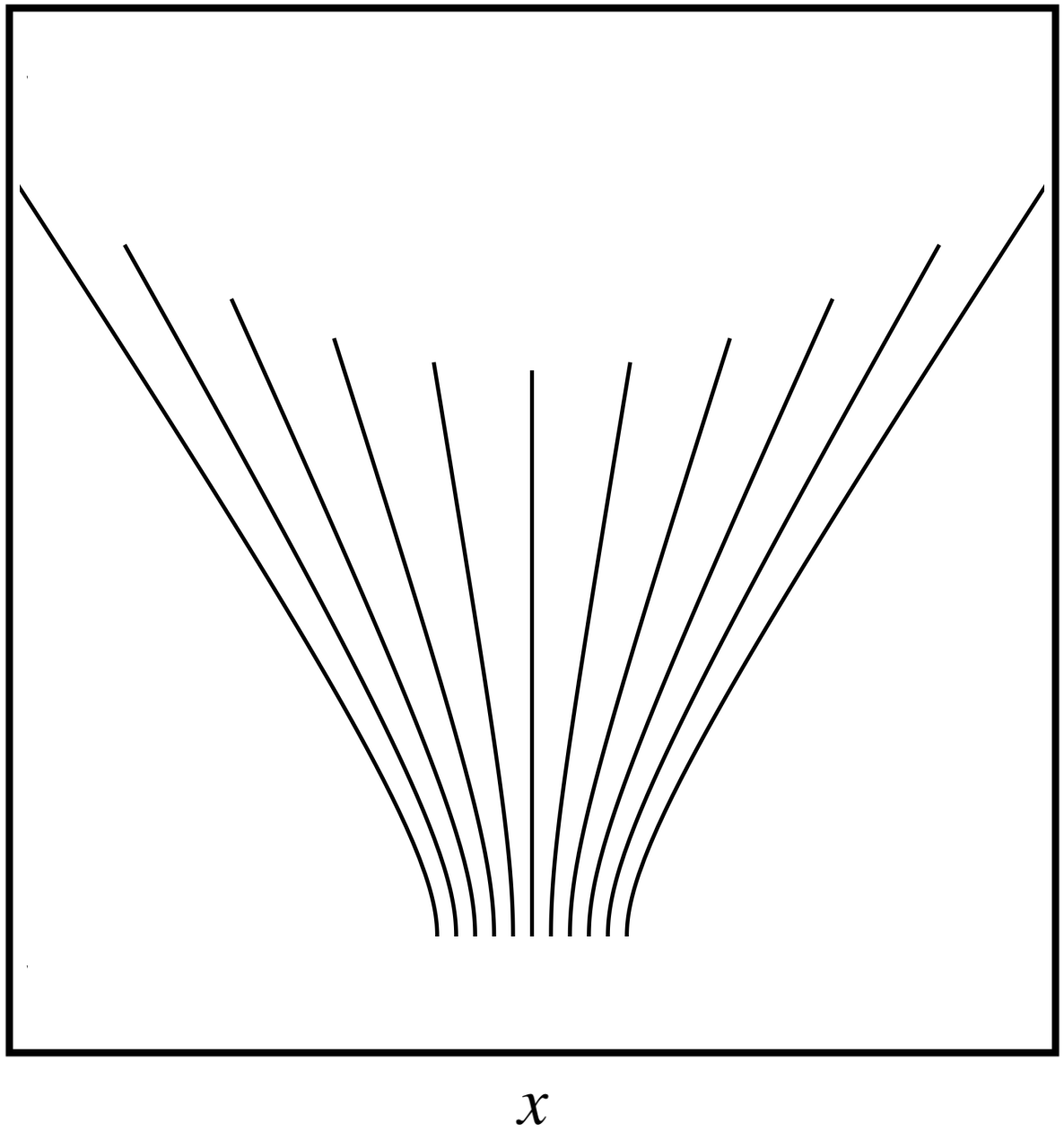
  - Non-physical negative-energy solutions.
  - The temporal part of the four-current density is:

$$j^0=\frac{i\hbar}{2mc}\left(\Phi^*\frac{\partial}{\partial t}\Phi-\Phi\frac{\partial}{\partial t}\Phi^*\right)$$

  - j^0 is ***not*** positive-definite in general.
  - The four-current density j^α is ***not*** time-like in general.
- Our approach is "natural," because it involves action-extremizing trajectories.
  - *All of above issues seem to be avoided in our relativistic trajectory-based approach!!*
  - Why? Precisely *because* of the C conservation law!

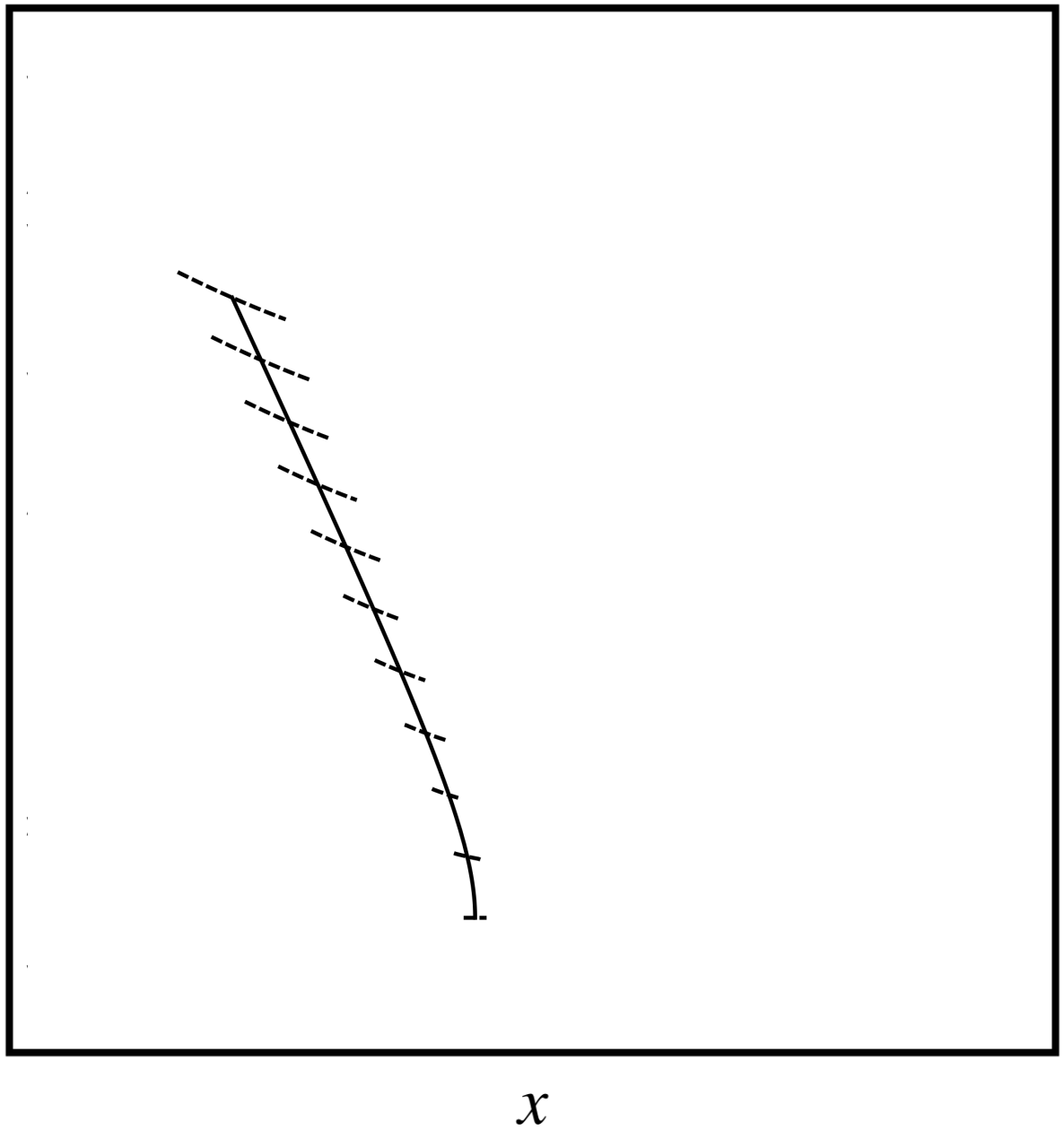
Relativistic Trajectory Equation

Gaussian Wavepacket



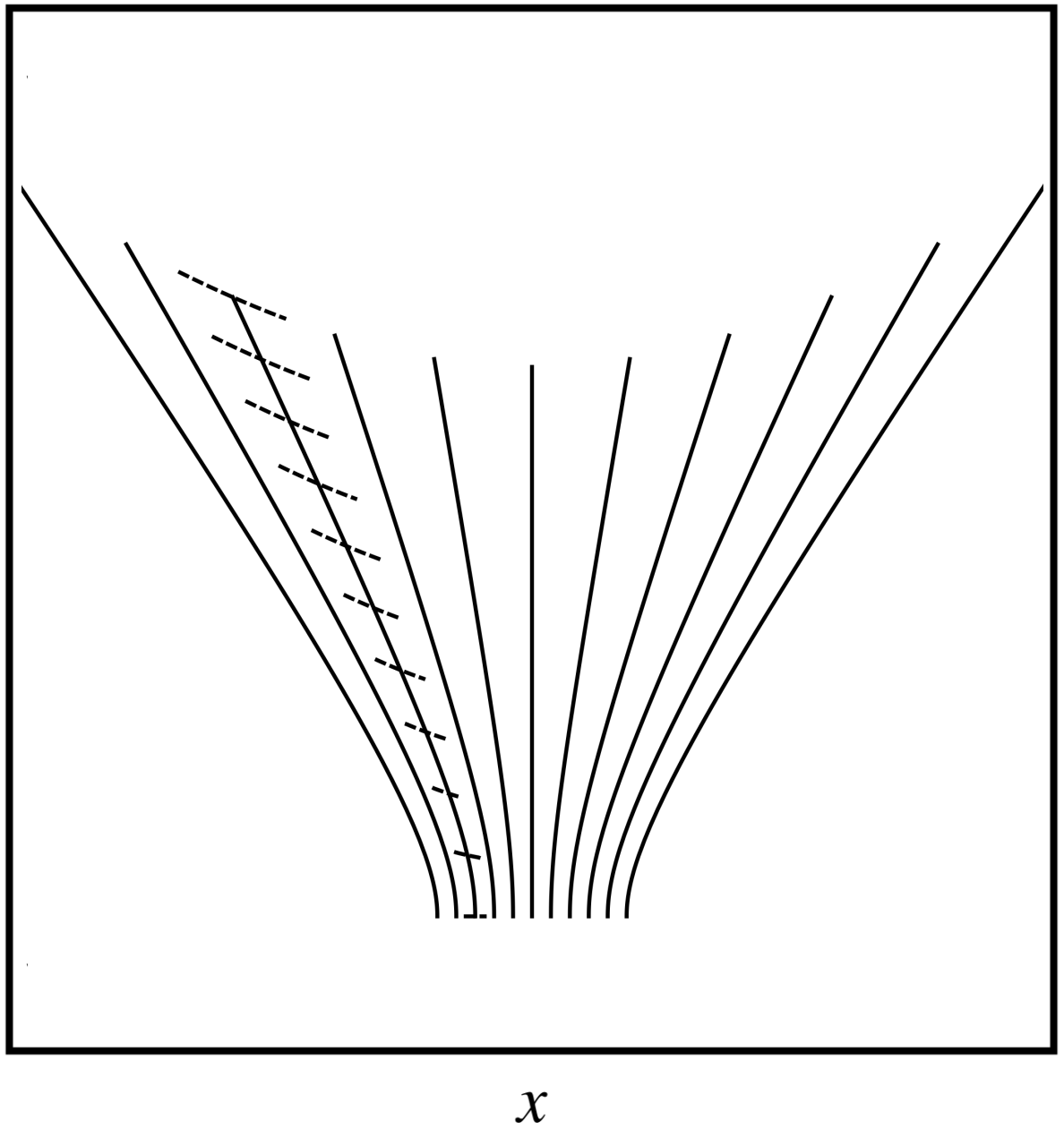
- Relativity demands that space and time be treated on an equal footing, so *t must be a dep. var*.
- The ensemble of quantum trajectories are *contours* of a "global spacelike" coord., $C(x,t)$.
- Conversely, there ought to be a "global time-like coordinate", $\mathcal{T}(x,t)$.
- The contours of $\mathcal{T}(x,t)$ provide *simultaneity* for accelerating particles.

Simultaneity for Accelerating Particles (1+1)



• According to relativity theory, *local* simultaneity can be defined for accelerating particles, but *global* simultaneity can not.

Simultaneity for Accelerating *Quantum* Particles (1+1)



- The system now consists of an *ensemble* of quantum trajectories.
- Each trajectory has its own local simultaneity segments.

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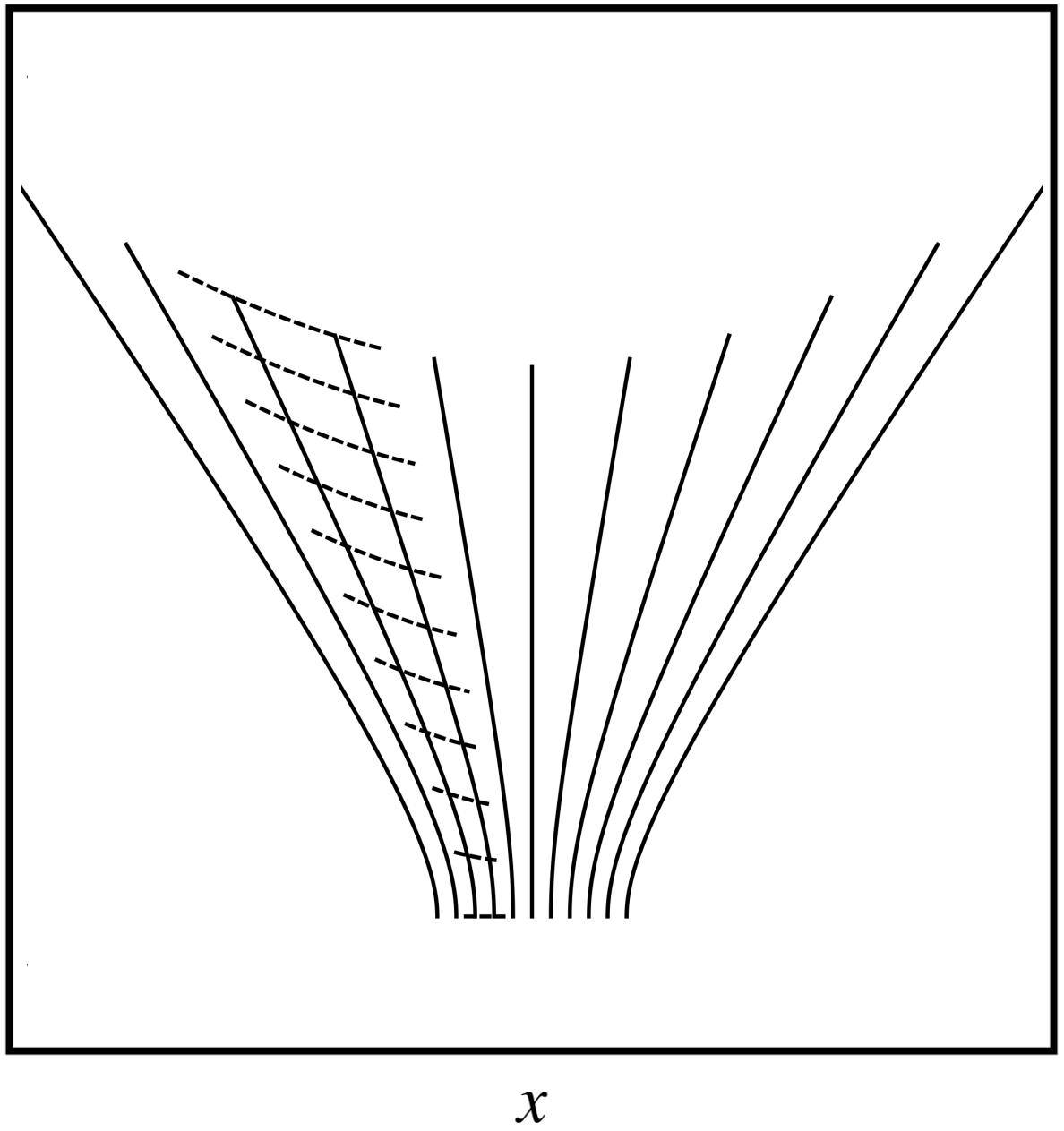
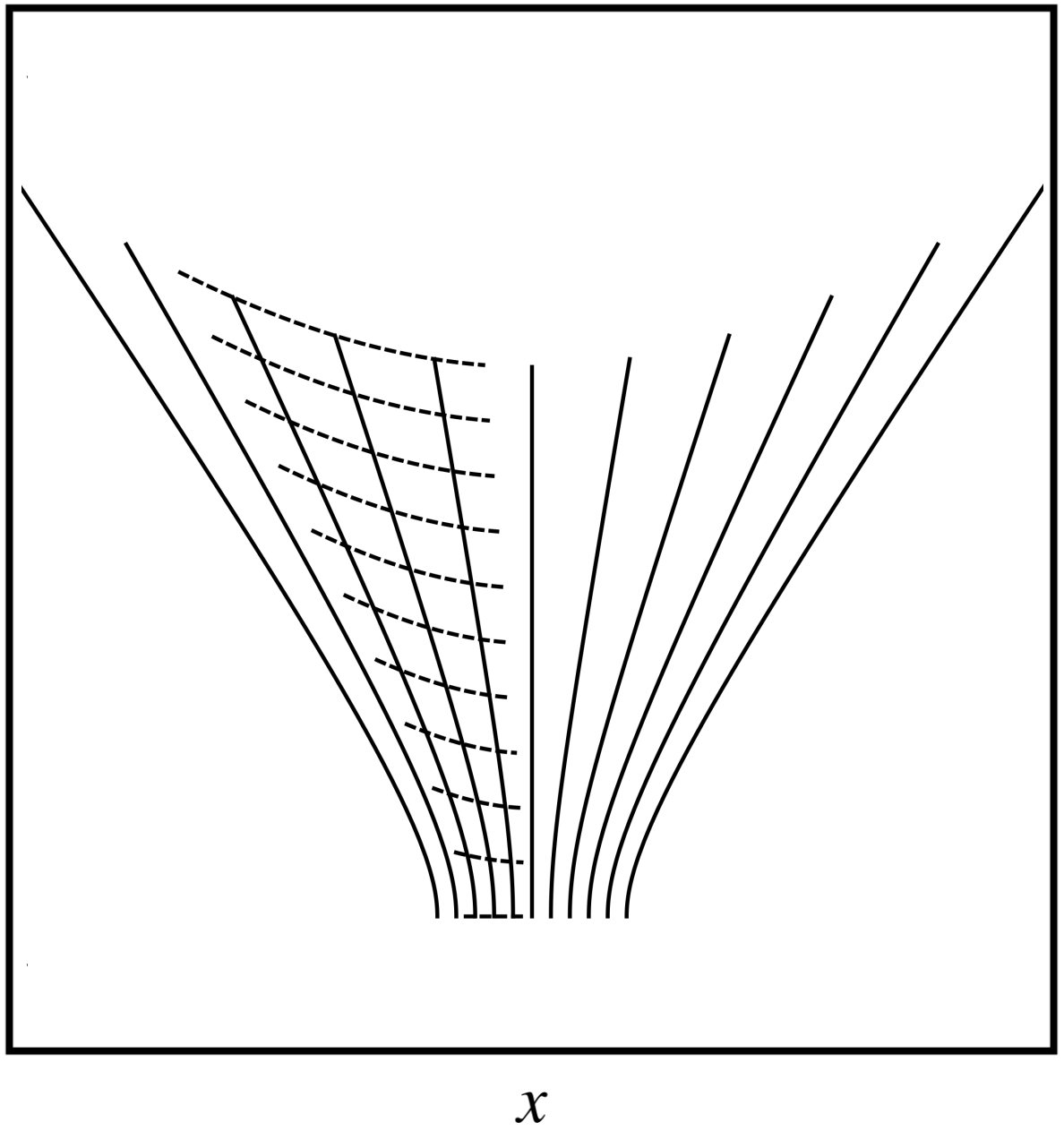


- The system now consists of an *ensemble* of quantum trajectories.
- Each trajectory has its own local simultaneity segments.
- Gluing all of these together, we can construct *global* simultaneity submanifolds.

Simultaneity for Accelerating *Quantum* Particles (1+1)



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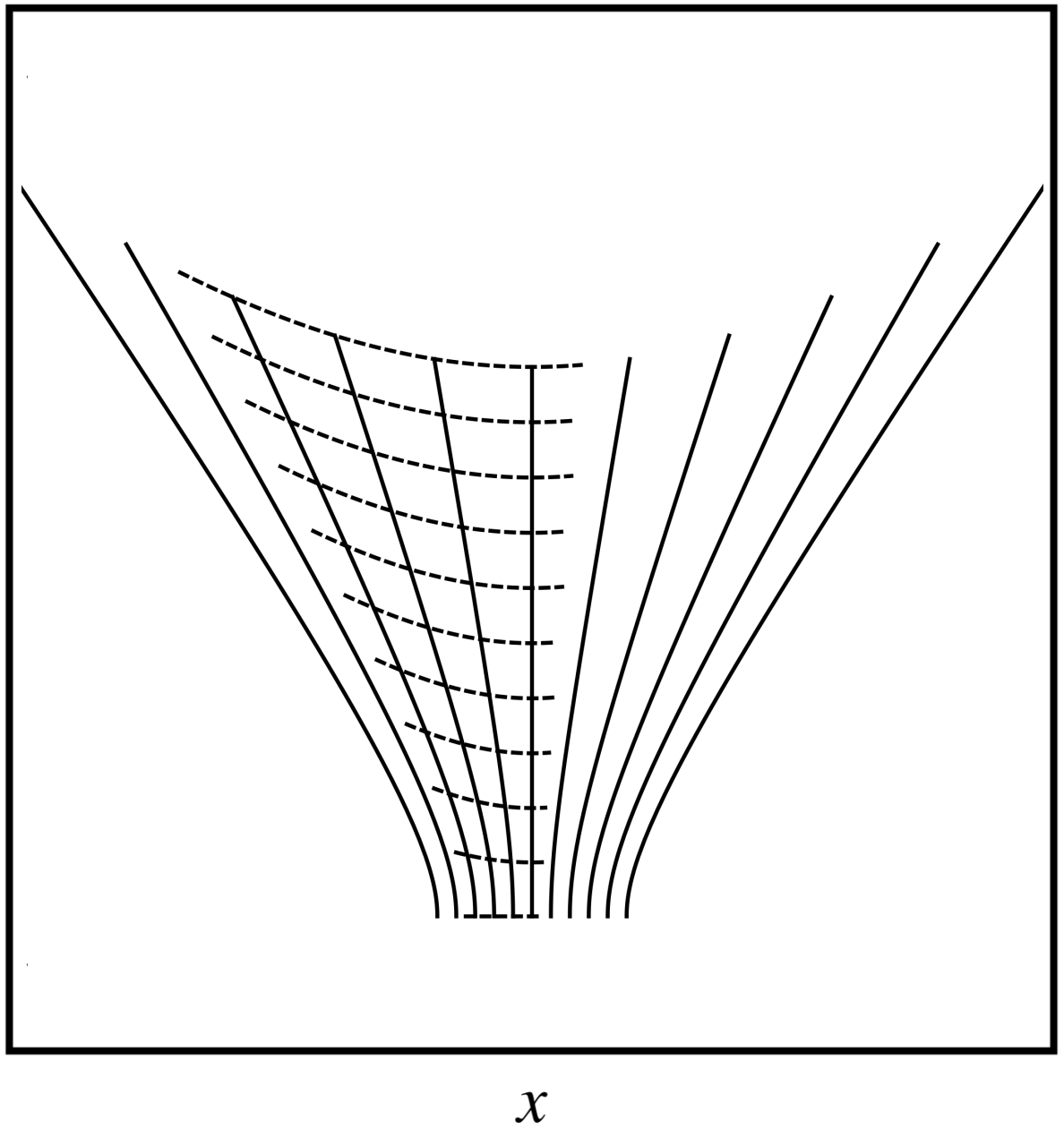

- The system now consists of an *ensemble* of quantum trajectories.
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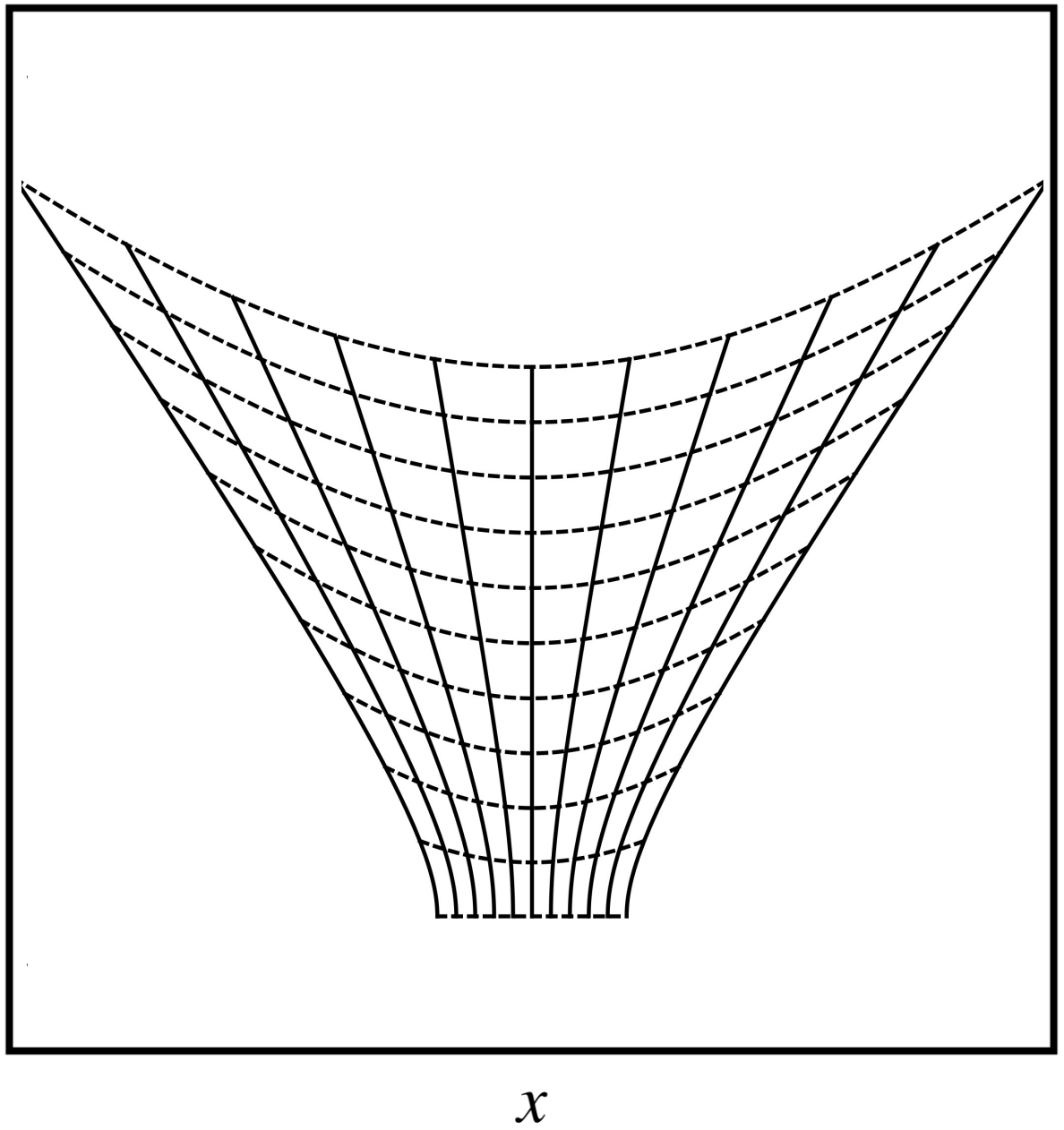
Relativistic Trajectory Equation

Simultaneity for accelerating particles



- The contours of $\mathcal{T}(x,t)$ restores the relativistic notion of *simultaneity*, for accelerating particles.
- *However*, this does not work for just any velocity field…
- …a necessary condition is that *the C conservation law must be satisfied!*

Some "Have You Tried?" Questions:

- Bound eigenstate calculations: yes
- 1D wavepacket calculations: yes
- Multidimensional generalization: yes
- Mixed quantum classical methods: yes, but need help
- Quantum capture probabilities: yes, but need help
- Spin generalization: yes
- Relativistic conservation laws: yes
- Relativistic "Gaussian" wavepackets: yes
- Lorentz-transformed wavepackets: yes
- Single-particle Dirac equation: working on it
- Multiple-particle Dirac equation: definitely need help
- Others working on cosmology, but still could use some help

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- Sergei Tretiak

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- Texas Tech University
- Texas Advanced Computing Center

All of You !!

Continuous vs. Discrete MIW

Continuous MIW	Discrete MIW
continuous ensemble, $x(C,t)$	discrete ensemble, $x_i(t)$
exact solution of PDE	approximate discretization
unique dynamical law	dynamical law unspecified
action extremization principle	unclear at present
invariance/symmetry principle	unclear at present
relativistic generalization	unclear at present
Heisenberg/many-D/spin	under development
probability measure required	probability arises naturally
natural classical limit	natural classical limit
no trajectory crossing	no trajectory crossing

Relativistic Trajectory Theory

Motivated by Two Questions:

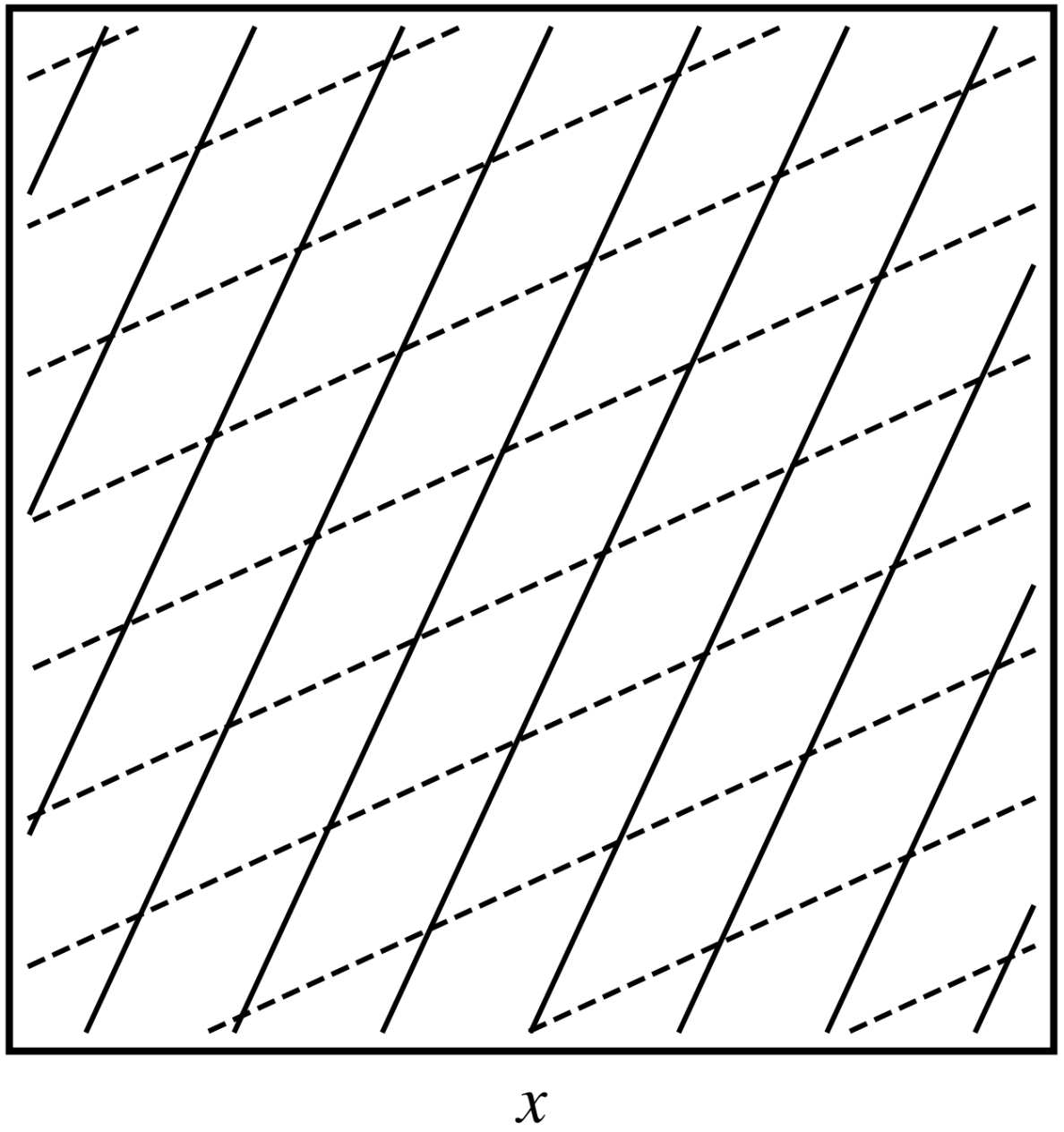
1. *What is the Schroedinger equation the non-relativistic limit of ?*

   Dynamics

2. *Why does relativity theory provide no notion of* global *simultaneity for accelerating particles?*

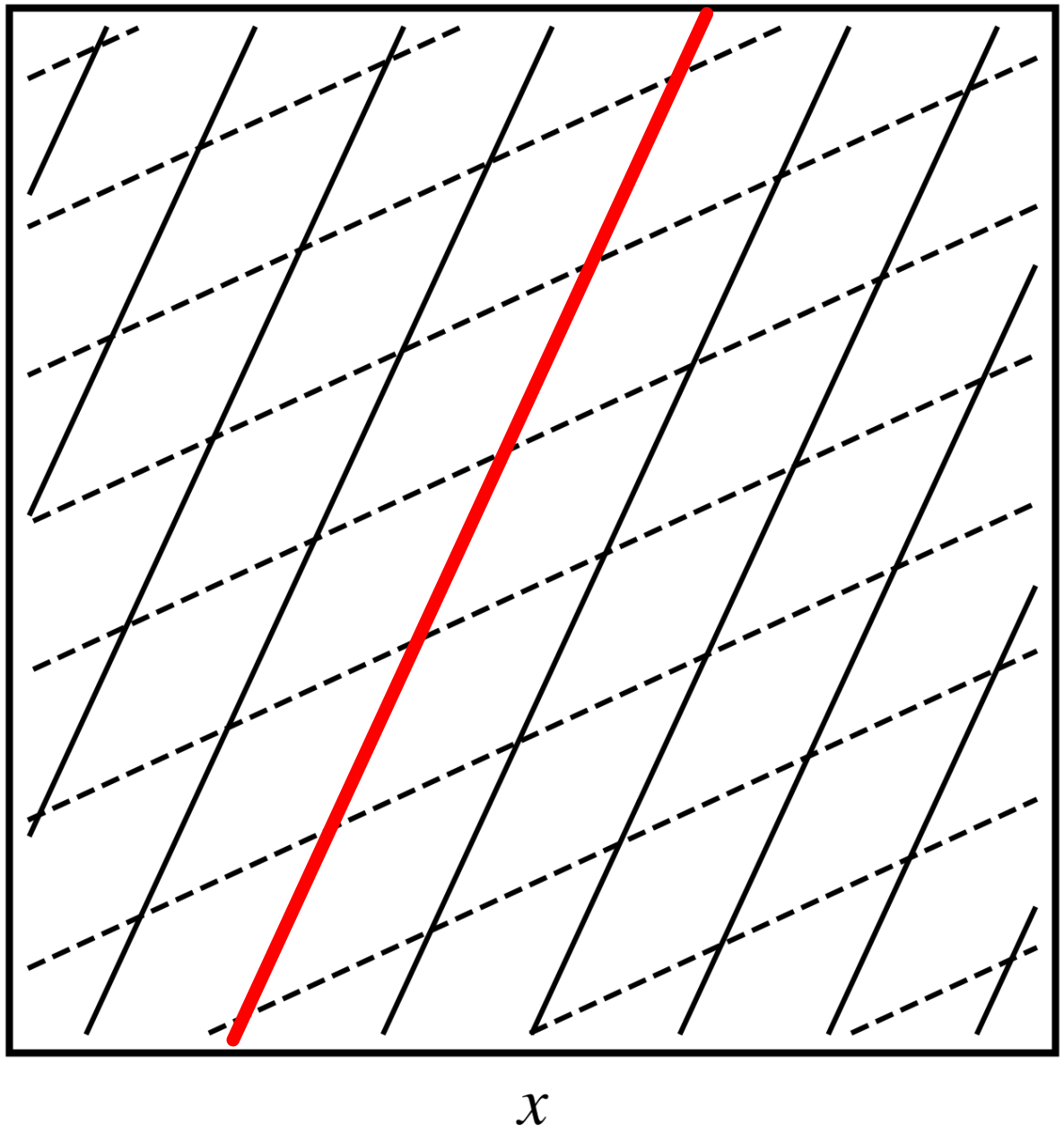
   Kinematics

Einsteinian Relativity (1+1)



• Simultaneity well-defined for a given inertial observer, but, *depends* on observer.

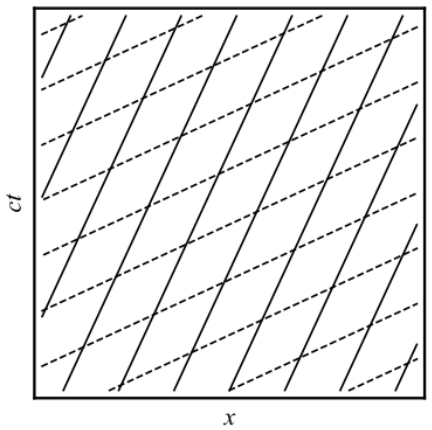
Einsteinian Relativity (1+1)



- Simultaneity well-defined for a given inertial observer, but, *depends* on observer.
- A single inertial particle (red curve) suffices to define an entire (ct', x') inertial frame (whose contours are the dashed and solid lines, respectively.)

Quantum Accelerated and Quantum Inertial Motion (1+1)

- Even for a single relativistic ***free*** particle, quantum forces can give rise to ***quantum accelerated motion***, i.e. curved quantum trajectories and simultaneity submanifolds.
- As a special case, a single relativistic free particle can also undergo ***quantum inertial motion***, when Q=0 everywhere.
  - Trajectories are parallel straight lines, corresponding to contours of Lorentz-transformed x'.
  - "Simultaneity submanifolds" are also parallel straight lines, corresponding to ct'



- This corresponds to the SR notion of an **inertial frame.**

Spacetime of a Relativistic Quantum Particle

- The *spacetime* of a single relativistic spin-zero particle is represented by a 4D Reimannian manifold, which is presumed *flat*.
- A global inertial frame can be defined. The inertial coordinates are: $x^\alpha = (ct, \mathbf{x})$ $\alpha = 0,1,2,3$
- Define the Minkowski metric tensor:

$$\tilde{\eta} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- The proper time is defined as:

$$d\tau^2 = -\frac{1}{c^2}\,\eta_{\alpha\beta}\,dx^\alpha dx^\beta$$

Ensemble Time and Natural Coords

- Simultaneity submanifolds are contours of a scalar function, called the *ensemble time* λ
- Define a system of *natural coordinates*:

$$X^\mu = \left(c\lambda, C^i\right)$$

where C^i are the trajectory labels. For now, we allow arbitrary reparametrizations: $\lambda \rightarrow \lambda' = \lambda'(\lambda)$ and $\mathbf{C} \rightarrow \mathbf{C}' = \mathbf{C}'(\mathbf{C})$

- The metric tensor of the natural coordinates and that of the inertial coordinates are related by:

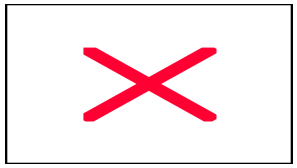
$$g_{\mu\nu} = \eta_{\alpha\beta} \frac{\partial x^\alpha}{\partial X^\mu} \frac{\partial x^\beta}{\partial X^\nu} \qquad \tilde{g} = \begin{pmatrix} g_{00} & \mathbf{0} \\ \mathbf{0} & \tilde{\gamma} \end{pmatrix}$$

- Note that the metric tensor is *block-diagonal*.
- Define:

$$g = \det\left(\tilde{g}\right) \qquad \gamma = \det\left(\tilde{\gamma}\right)$$

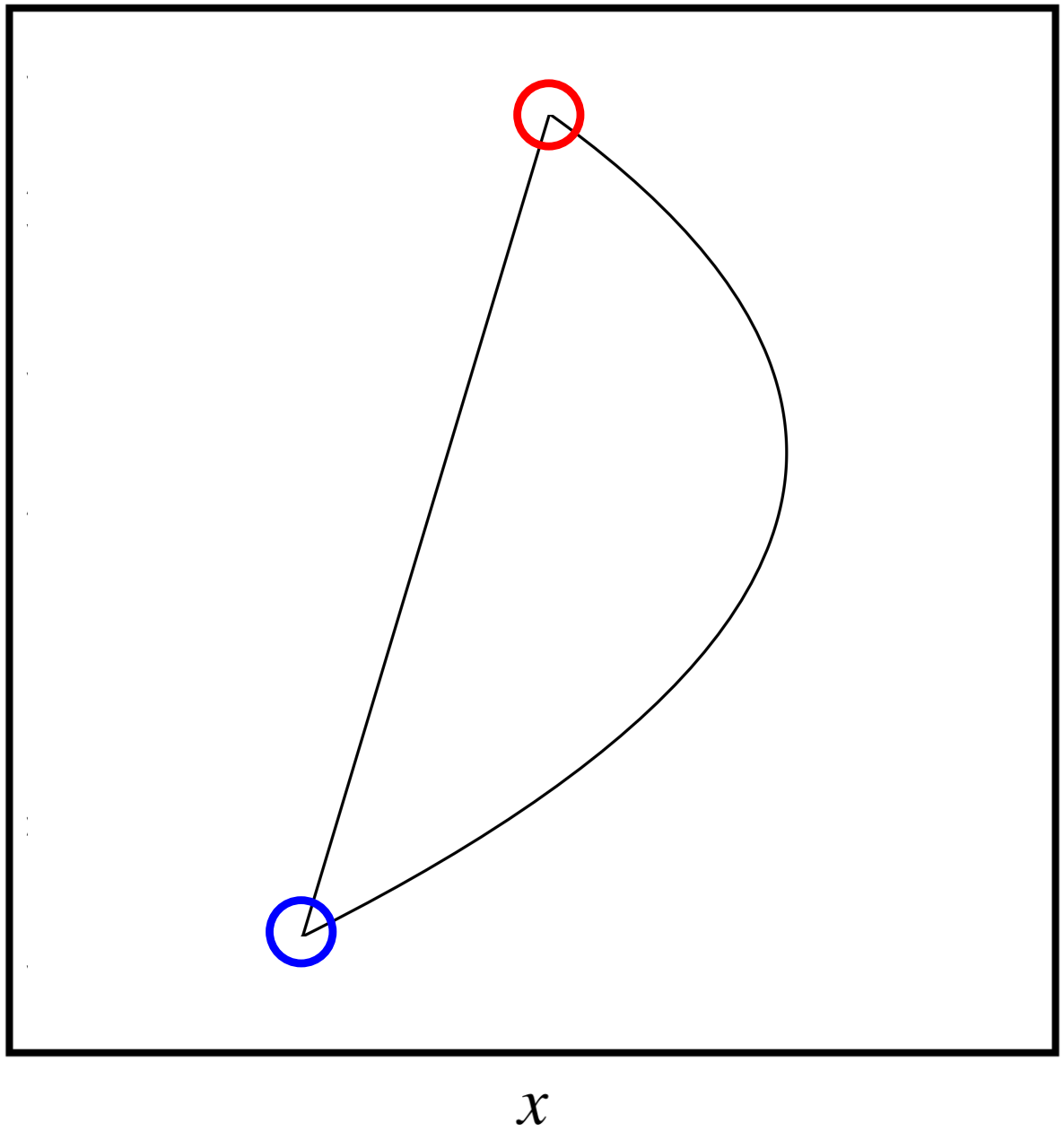
Ensemble Time and the Generalized Twin "Paradox"

- Simultaneity submanifolds are contours of a scalar time-like function, called the *ensemble time,* λ
- *Is it possible to take* proper time τ *to be an ensemble time,* λ *?*
  - In general, *NO*, this is not possible.
  - The relation between τ and λ can be found from the metric tensor:



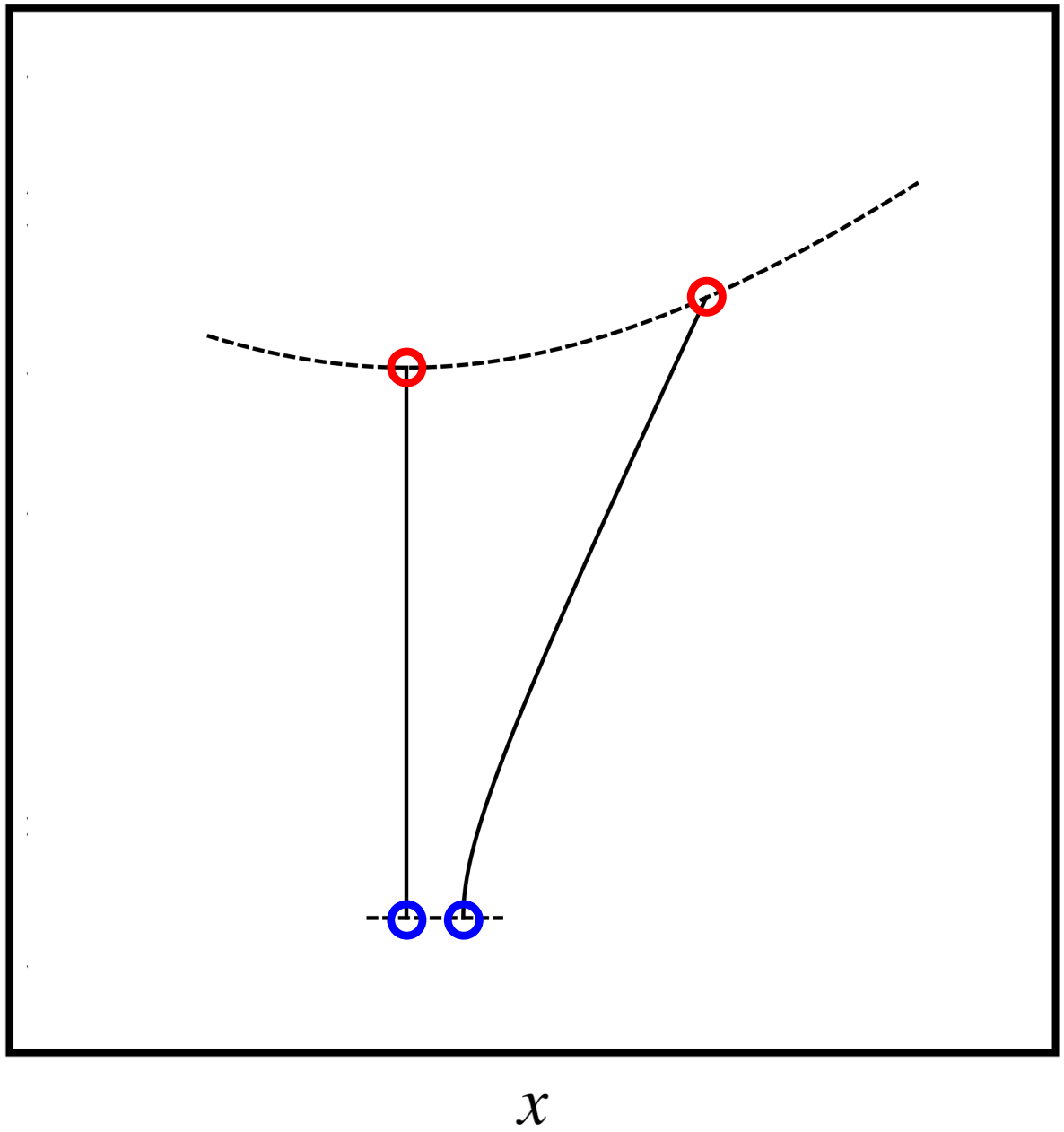
  - Note: g_{00} is *negative*, in keeping with the -+++ metric signature.
- The difference between τ and λ gives rise to the *generalized (quantum) twin paradox.*

Regular Twin "Paradox"



- Two "twin" observers cross paths at the blue circle event.
- Left twin: inertial motion; right twin: accelerated motion
- Right twin is *younger* when paths recross at the red circle event.

Generalized (Quantum) Twin "Paradox"



- Two "copies" of the same observer follow two, non-crossing paths.
- Both agree that the two blue circle events occur simultaneously.
- Both also agree that the two red circle events occur simultaneously.
- One trajectory has experienced less elapsed proper time than the other.

Ensemble Proper Time, & the Relativistic Quantum Potential

- Of all choices of ensemble time coordinates, λ , one choice is special. We call it the *ensemble proper time*, denoted $\mathcal{T}$.
- There is a close connection between $\mathcal{T}$ and Q, the (relativistic) quantum potential:

$$\frac{d\tau}{d\mathcal{T}} = \tau_{\mathcal{T}} = \exp\left[-\frac{Q}{mc^2}\right]$$

- Note: $\mathcal{T}$ reduces to τ, in the limit of quantum inertial motion.
- *Note: Q itself plays a dynamical role, and not just its gradient, the quantum force!*
  - Reminiscent of the *gravitational potential*.

Ensemble Proper Time, & the Relativistic Quantum Potential

- Gravitational potential vs. quantum potential (weak-field limit)

$$-\left(1+2\frac{m\Phi}{mc^2}\right)\approx g_{00}\approx-\left(1-2\frac{Q}{mc^2}\right)$$

- Note: Q can be either positive *OR* negative!
- When $Q > 0$ (classically allowed), $d\tau < d\mathcal{T}$
  - The passage of the proper time for a given trajectory is **slower** than that of an inertial trajectory (time *dilation*).
- When $Q < 0$ (classically forbidden), $d\tau > d\mathcal{T}$
  - The passage of the proper time for a given trajectory is **faster** than that of an inertial trajectory (time *compression*).

Relativistic Derivation

Dynamical PDE (eqs. of motion)

- By extremizing the action, we obtain the equation of motion for the trajectory ensemble.

$$\frac{\partial^2 x^\alpha}{\partial \mathcal{T}^2} = \exp\left[-\frac{2Q}{mc^2}\right]\frac{f^\alpha}{m} - \frac{1}{mc^2}\frac{\partial Q}{\partial \mathcal{T}}\frac{\partial x^\alpha}{\partial \mathcal{T}}$$

- PDE is fourth order in **C**, second order in $\mathcal{T}$, *but* treats all inertial coordinates x^α on equal footing.
- Choosing uniformizing coordinates:

$$Q = -\frac{\hbar^2}{2m}\gamma^{-1/4}\frac{\partial}{\partial C^i}\left[\gamma^{1/2}\gamma^{ij}\frac{\partial}{\partial C^j}\gamma^{-1/4}\right], \qquad f^\alpha = -\frac{\partial x^\alpha}{\partial C^i}\gamma^{ij}\frac{\partial}{\partial C^j}Q$$

Classical Hamiltonian Form for the 1D TISE ODE

Turns out to be identical to Ostrogradski Approach...

- Search for a quantum Hamiltonian form to describe the 1D TISE ODE for $x(t)$.
  - Fourth-order ODE equivalent to four coupled 1st order ODEs
  - Incredibly, *these can be written as ordinary* ***classical*** *Hamilton's equations* for a two degree of freedom system!)

$$\dot{x} = \frac{\partial H}{\partial p} \; ; \; \dot{p} = -\frac{\partial H}{\partial x} \; ; \; \dot{r} = \frac{\partial H}{\partial s} \; ; \; \dot{s} = -\frac{\partial H}{\partial r}$$

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$$s = m\dot{x} \; ; \; r = \frac{\hbar^2 \ddot{x}}{4m^2 \dot{x}^4} \; ; \; p = m\dot{x} + \frac{\hbar^2}{4m}\left(\frac{\dddot{x}}{\dot{x}^4} - \frac{2\ddot{x}^2}{\dot{x}^5}\right)$$

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1D Time-Independent Hamiltonian
Completely Integrable Form

- Original Hamiltonian form:

$$H(x,\, p,\, r,\, s) = \frac{s(2p - s)}{2m} + V(x) - \frac{2r^2 s^4}{m\hbar^2}$$

- Canonical transform (free particle case):

$$X = x + rs/\,p \quad ; \quad P = p \quad ; \quad r' = rp \quad ; \quad s' = s/\,p$$

$$H(X,P,r',s') = \frac{P^2}{2m} h(r',s'), \quad \text{where}$$

$$h(r',s') = s'(2 - s') - 4r'^2 s'^4/\hbar^2 = \text{const}$$

  - $H(X,P,r',s')$ is now *completely separable/integrable*.
  - $X(t)$ is now *linear* for free particles (even with interference), and otherwise *smoothly varying* with $V(x)$.

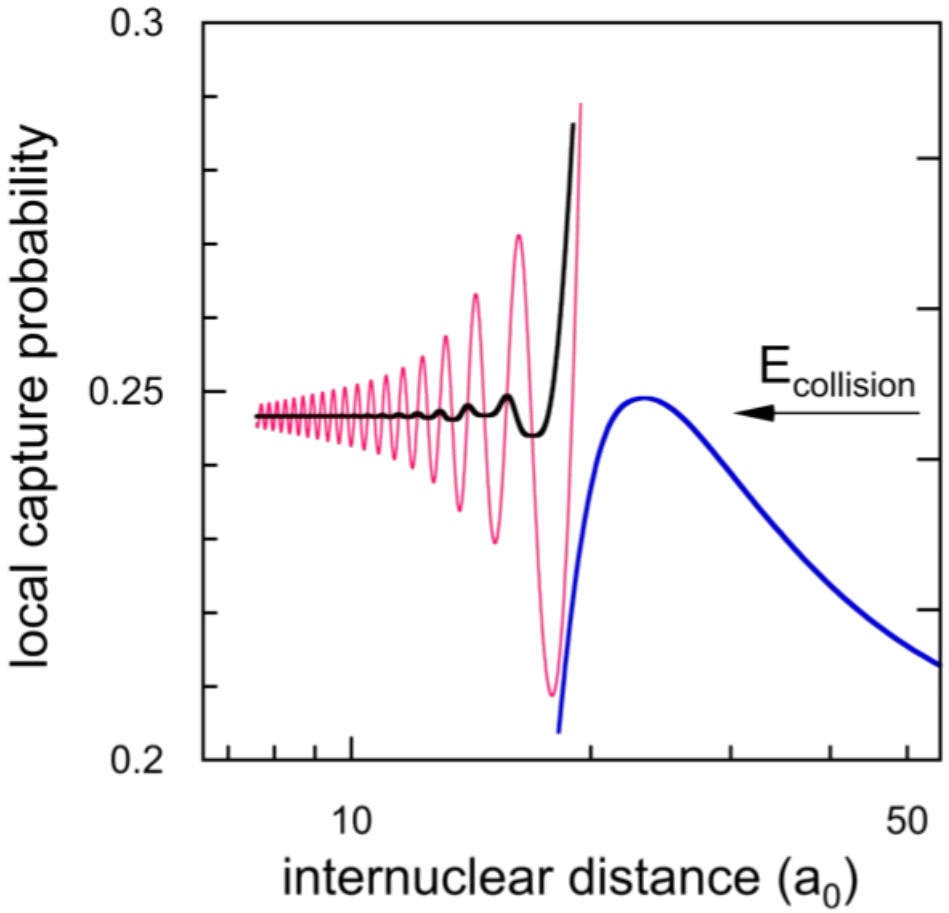
Revised Quantum Trajectory Convergence

Completely Integrable Form

- New form for P_T is now suggested:

$$P_T = 2\hbar k / (\hbar k + P) \quad \text{where} \quad \hbar k = \sqrt{2m\left[E - V(X)\right]}$$

- Yields much better results when applied to Li+CaH:



Bohmian trajectories

Substituting $\psi(x,t) = R(x,t)e^{iS(x,t)/\hbar}$ (R, S real) into

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + V(x,t)\psi$$

gives

$$\begin{aligned} R_t + \frac{S_x R_x}{m} + \frac{RS_{xx}}{2m} &= 0\,, \\ S_t + \frac{S_x^2}{2m} + V(x,t) - \frac{\hbar^2}{2m}\frac{R_{xx}}{R} &= 0\,. \end{aligned}$$

Bohmian trajectories are obtained by solving

$$m\frac{dx}{dt} = S_x\,.$$

This gives us a one parameter family of trajectories $x(t, C)$ where C is some trajectory label.

The change of coordinates

Change spatial coordinate from x to C. To avoid confusion, do a full change of coordinates from (x, t) to (C, s) with $t = s$ (derivatives with respect to t are at constant x, derivatives with respect to s are at constant C). Writing x' for $\frac{\partial x}{\partial C}$

$$\begin{cases} \frac{\partial}{\partial C} &= x' \frac{\partial}{\partial x} \\ \frac{\partial}{\partial s} &= \frac{S_x}{m} \frac{\partial}{\partial x} + \frac{\partial}{\partial t} \end{cases}$$

The R equation

The R equation becomes

$$R_s + \frac{R}{2}\frac{\partial}{\partial x}\left(\frac{\partial x}{\partial s}\right) = 0 \;\Rightarrow\; R_s + \frac{R}{2x'}\frac{\partial^2 x}{\partial C \partial s} = 0 \;\Rightarrow\; R_s + \frac{R}{2x'}\frac{\partial x'}{\partial s} = 0\,.$$

Mutliplying by $2Rx'$ we have $\frac{\partial}{\partial s}(R^2 x') = 0$ implying $R^2 x'$ is a function of C alone,

$$R^2 x' = f(C)\,.$$

Parametrizations

C can be taken to be the value of the trajectory at time 0, $C = x(0)$, in which case $f(C) = R(0, C)^2$. It is equally valid to take C to be any monotone increasing function of $x(0)$; C can take values in either a finite or an infinite interval. Given 2 parametrizations, C_1 and C_2,

$$f_1(C_1)\frac{dC_1}{dC_2} = f_2(C_2)\ .$$

A convenient choice is

$$C = \int_{-\infty}^{x_0} R(0, x_0)^2 dx_0\ .$$

In this parametrization C takes values from 0 to 1, and $f(C) = 1$ (assuming we are working with normalized wave packets).

The S equation

In the new parametrization

$$R^2 = \frac{1}{x'} .$$

This allows us to write the quanutm force in terms of the kinematic quantity x'. and to write a PDE for $x(C, s)$. Differentiating the S equation with respect to x gives

$$m\left(\frac{S_{xt}}{m} + \frac{S_x S_{xx}}{m^2}\right) + V_x(x, s) - \frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left(\frac{R_{xx}}{R}\right) = 0 .$$

Moving to the new coordinates and simplifying this gives

$$m\frac{\partial^2 x}{\partial s^2} + V_x(x, s) + \frac{\hbar^2}{4m}\left(\frac{x''''}{x'^4} - 8\frac{x'' x'''}{x'^5} + 10\frac{x''^3}{x'^6}\right) = 0 .$$

This is the modified Newton equation.