Bipolar Quantum Trajectory Dynamics

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Photo: the Millau viaduct

Trajectory interpretation of quantum mechanics

- Semiclassical approximation: long history (*JWKB*, *etc*.)
  - Statistical ensemble of classical trajs that "carry" quantum info. (complex amplitude)
  - Semiclassical trajs cross
- Other (***exact***) traj. interpretation by Madelung, Bohm…
  - *Quantum Potential Q* guides trajectory dynamics
  - Quantum Trajectory Methods *QTM* (see *Bob Wyatt*'s book)
    - *"Analytical" QTM* → physical insight
    - *"Synthetic" QTM* → to actually solve TDSE
  - Quantum trajs do not cross

Bohmian wavefunction and "*the node problem*"

- ***Unipolar*** amplitude / phase decomposition:

$$\psi = R(x,t)\exp\left[iS(x,t)/\hbar\right]$$

- $R(x,t)$ and $S(x,t)$ are smooth ***if*…**
  - slowly varying potential $V(x)$
  - no interference
- Interferences give rise to:
  - non classical-like oscillations in $R(x,t)$ and $S(x,t)$
  - numerical difficulties in *QTM*: "*the node problem*"
- *Classical correspondence* not satisfied
- ☞ Solution: ***bipolar*** decomposition of the wavefunction… ☞

Bipolar decomposition of the wave function

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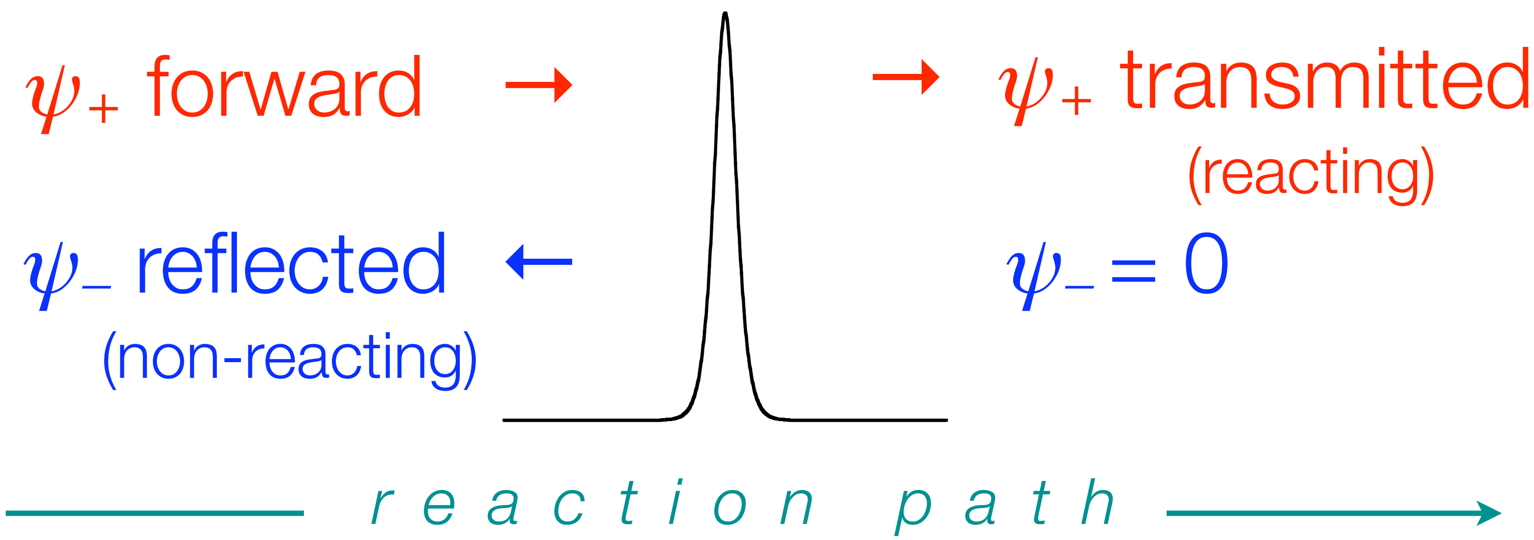
$$\psi = \psi_+ + \psi_-$$



- $\psi_\pm$ are traveling waves moving in opposite directions
- $\psi_\pm$ are well-behaved, "classical-like" waves
- $\psi_\pm$ (***exact***) correspond to (approx) semiclassical waves
- ψ "nasty" interferences result from…

…superposition of well-behaved ψ_+ and ψ_-

Bipolar quantum trajectories

- Amplitude / phase decomposition of $\psi_\pm$

$$\psi_\pm = R_\pm \exp\left(iS_\pm / \hbar\right)$$

- $Q_\pm \to 0$ in classical limit
- $Q_\pm$ is small even in quantum limit!
- Quantum trajectories obtained from $V_{\text{eff}} = V + Q_\pm$
- Quantum trajs associated with bipolar waves are well-behaved and classical-like

Bipolar wave packets

Bill Poirier

- Initially, bipolar treatment for ***delocalized stationary*** wave functions $\phi^E = \phi_+^E + \phi_-^E$
- Bipolar treatment extended to ***localized time-dependent*** wave packets; much more complicated (caustics, *etc*)!
- Localized time-dependent wave packets expanded over stationary states:

$$\psi = \psi_+ + \psi_- \qquad \psi_\pm(x,t) = \int_0^\infty a(E)\,\phi_\pm^E(x,t)\,dE$$

- Apply $\int dE$ to time-evolution eq. for the $\phi_\pm$'s – get rid of all dependence on E (see *Bill Poirier* papers)

… ☞

Bipolar wave packets: *time evolution eq.*

Coupled wave packets with "unusual" coupling term:

$$i\hbar\frac{\partial\psi_\pm}{\partial t} = \hat{H}\psi_\pm \pm \frac{V'}{2}\left(\Psi_+ - \Psi_-\right)$$

$$\boxed{V' \equiv \partial V/\partial x}$$

$$\Psi_\pm(x,t) = \int_{-\infty}^{x} \psi_\pm(x',t)\,dx'$$

- Can be directly integrated over time to get $\psi_\pm(x,t)$
- Coupling $\sim V' \to 0 \quad as \quad x \to \pm\infty$
- Opposite ± couplings $\Rightarrow \psi_\pm$ is solution of H:

$$i\hbar\partial\psi/\partial t = \hat{H}\psi \qquad \psi = \psi_+ + \psi_-$$

- *N.B.* Ψ_Δ is also (independent) solution of H:

$$i\hbar\partial\Psi_\Delta/\partial t = \hat{H}\Psi_\Delta \qquad \Psi_\Delta = \Psi_+ - \Psi_-$$

Bipolar wave packets: *properties*

- (1) Perfect ***asymptotic separation*** at $t = t_0$ and $t = t_f$
  - requires initial momentum > 0
- (2) Well ***localized*** $\psi_\pm(x,t)$ and $\Psi_\pm(x,t)$ at all t
  - requires initial momentum > 0
- (3) ***Node-free*** components $\psi_\pm(x,t)$ at all t
  - (no formal proof for this condition)

Bipolar wave packets: *fixed-grid methods*

$$i\hbar\partial\psi/\partial t = \hat{H}\psi \qquad i\hbar\partial\Psi_\Delta/\partial t = \hat{H}\Psi_\Delta$$

- ***Propagate separately*** ψ and Ψ_Δ
  - At $t = 0$, $\psi = \psi_+ =$ Gaussian and $\psi_- = 0$
  - At $t = 0$, $\Psi_\Delta =$ complex *erf* function
  - Crank-Nicholson algorithm
  - Get ψ_+ and ψ_- from $\boxed{\psi_\pm = \psi \pm \partial\Psi_\Delta/\partial x}$
- Alternatively, one can ***solve the coupled eqs*** for ψ_+ and ψ_-

$$\boxed{i\hbar\frac{\partial\psi_\pm}{\partial t} = \hat{H}\psi_\pm \pm \frac{V'}{2}\Psi_\Delta}$$

  - time-dependent Crank-Nicholson (nb of steps x 2)
  - or Runge-Kutta

Bipolar quantum trajectories: *motion eqs*

$$i\hbar \frac{\partial \psi_\pm}{\partial t} = \hat{H}\psi_\pm \pm \frac{V'}{2}\Psi_\Delta$$

$$\psi_\pm = R_\pm \exp\left(iS_\pm/\hbar\right)$$

$$\Psi_\Delta = \int_{-\infty}^{x}\left(\psi_+ - \psi_-\right)dx'$$

Lagrangian ref.-frame

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{p_\pm}{m}\frac{\partial}{\partial x}$$

$$\Downarrow$$

Momentum field

$$p_\pm = \frac{\partial S_\pm}{\partial x}$$

- Density eqs

$$\frac{d\rho_\pm}{dt} = -\frac{\rho_\pm}{m}p'_\pm \pm \lambda_\pm(x,t)$$

- +/– transfer rates (dissipation)

$$\boxed{\lambda_\pm(x,t) = \frac{V'}{\hbar}\rho_\pm^{1/2}\,\mathrm{Im}\left[\Psi_\Delta e^{-iS_\pm/\hbar}\right]}$$

- *N.B.* combined continuity ***not*** satisfied: $\lambda_\mp \neq -\lambda_\pm$

Bipolar quantum trajectories: *motion eqs*

$$\Downarrow$$

- Phase eqs

$$\frac{dS_\pm}{dt} = \frac{p_\pm^2}{2m} - V(x,t) - Q_\pm(x,t) \mp Q_{\Delta\pm}(x,t)$$

- Quantum potential

$$\boxed{Q_\pm(x,t) = -\frac{\hbar^2}{2m}\frac{R''_\pm}{R_\pm}}$$

- Off-diagonal quantum potential

$$\boxed{Q_{\Delta\pm}(x,t) = \frac{V'}{2}\rho_\pm^{-1/2}\,\mathrm{Re}\left[\Psi_\Delta\, e^{-iS_\pm/\hbar}\right]}$$

- Newtonian eqs

$$\boxed{\frac{dp_\pm}{dt} = -\frac{\partial}{\partial x}\left(V + Q_\pm \pm Q_{\Delta\pm}\right)}$$

- ☞ classical force + quantum force + off-diag. force

"*Analytical*" quantum trajectories

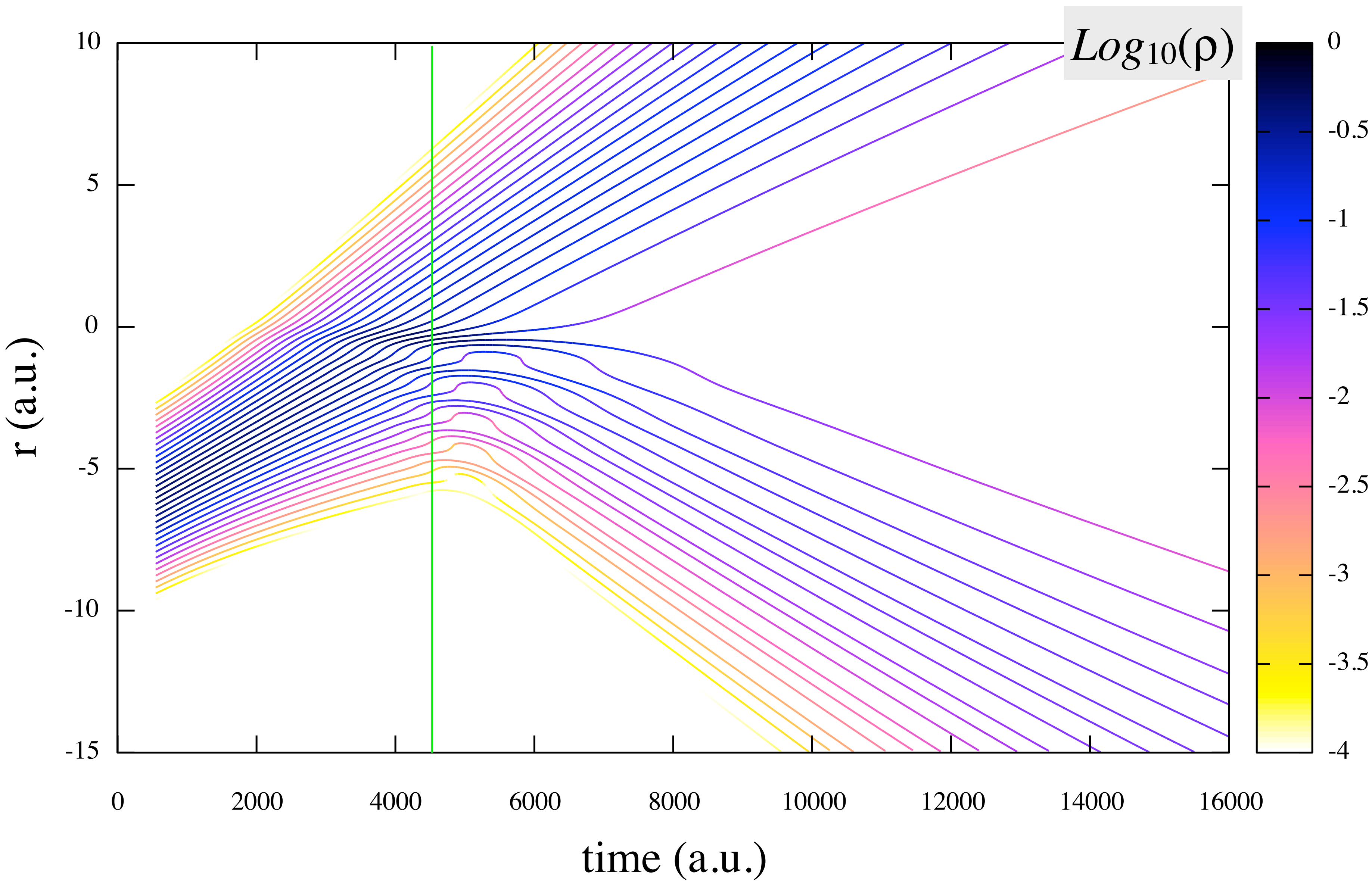
- Obtain ψ_+ and ψ_- from a fixed-grid method
- Get momenta $p_\pm = \partial S_\pm / \partial x$
- Propagate trajectories $dr_\pm/dt = p_\pm/m$
- All quantities such as $p_\pm$, $Q_\pm$, *etc*. are
  - (1) computed on the fixed grid
  - (2) spline-interpolated at trajectory positions

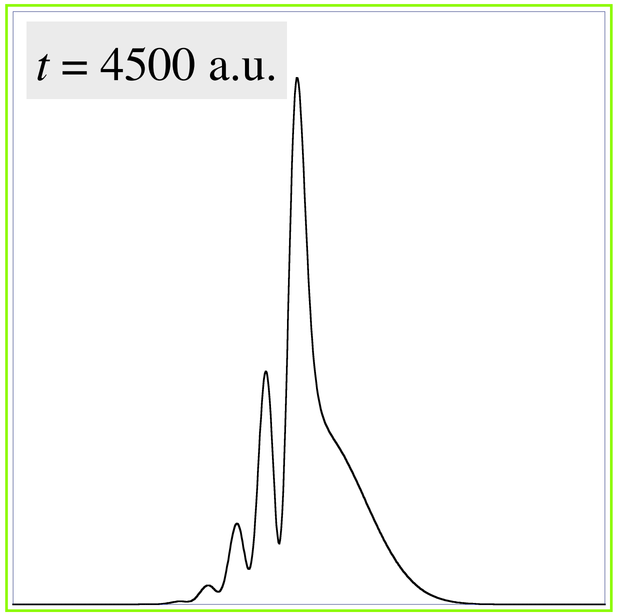
Outline and goals

- Numerical validation of bipolar decomposition
  - (1) asymptotic separation
  - (2) well-localized $\psi_\pm$ and $\Psi_\pm$
  - (3) node-free components $\psi_\pm$
- Propagation of bipolar wave packets by standard grid method
- Extract "*analytical*" quantum trajs $r(t)$ from wave-packet
- Analysis of trajs: look at density, quantum forces, *etc*.
  $\rightarrow$ *adds a new dimension to the dynamics*
- Propagate "*synthetic*" quantum trajs

Eckart barrier: ***unipolar** quantum trajectories*

- energy ~ above barrier
- proton mass

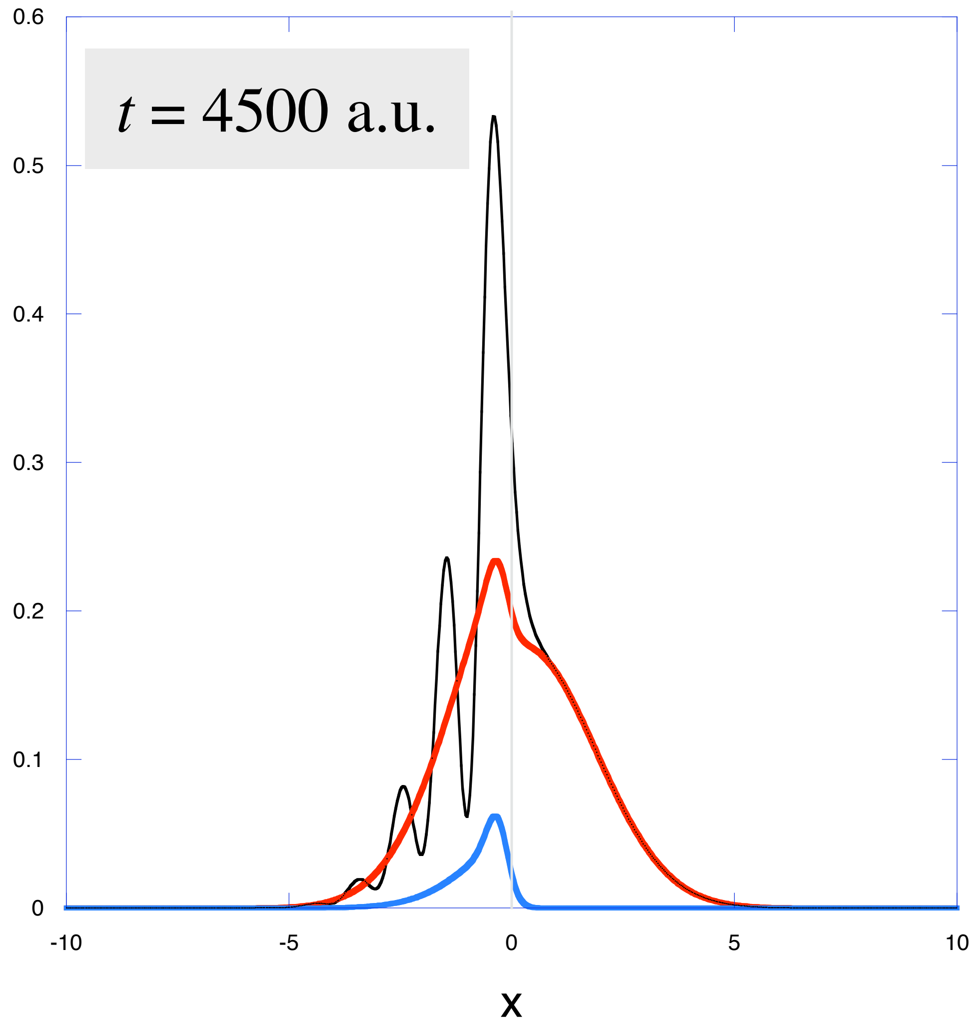


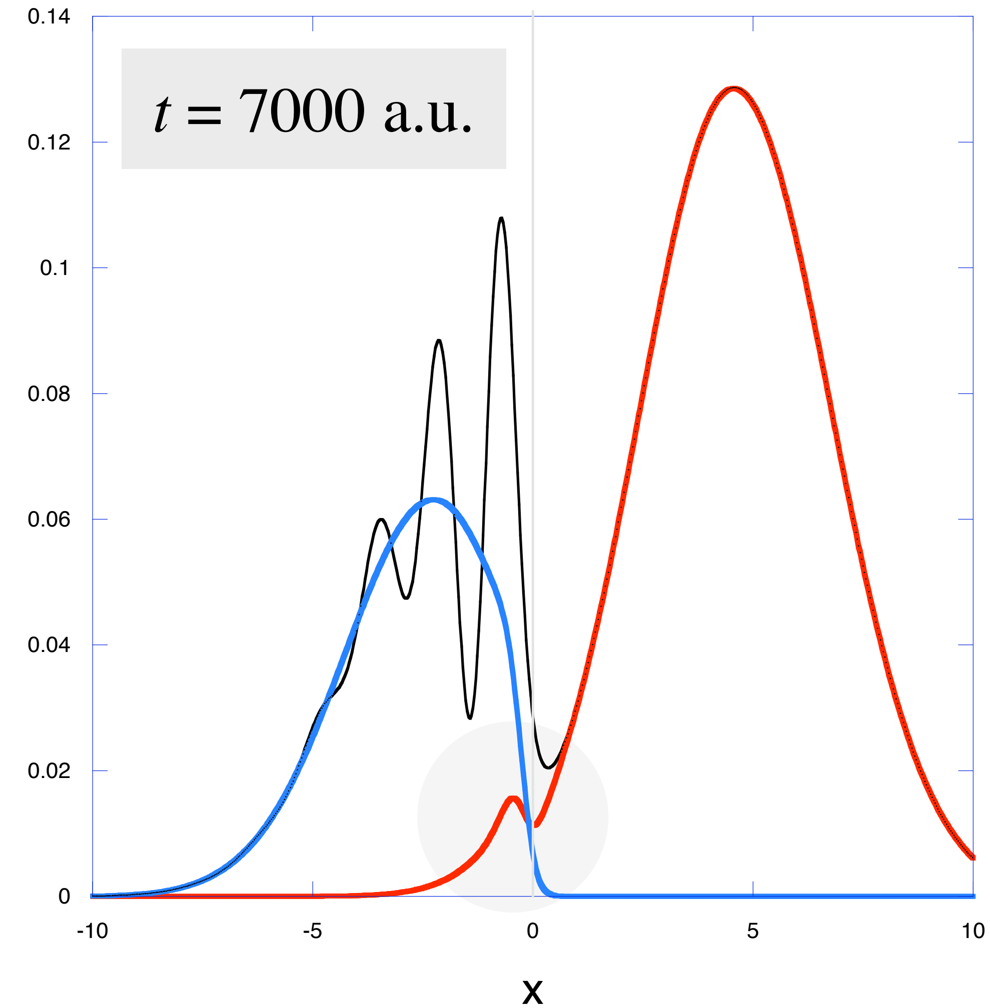


- Interferences ⇒ reflected trajectories show “avoided crossings”
- Distorted trajectories are difficult or impossible to compute

Eckart barrier: *bipolar wave packets*

ψ_- initially 0, grows in 2 stages

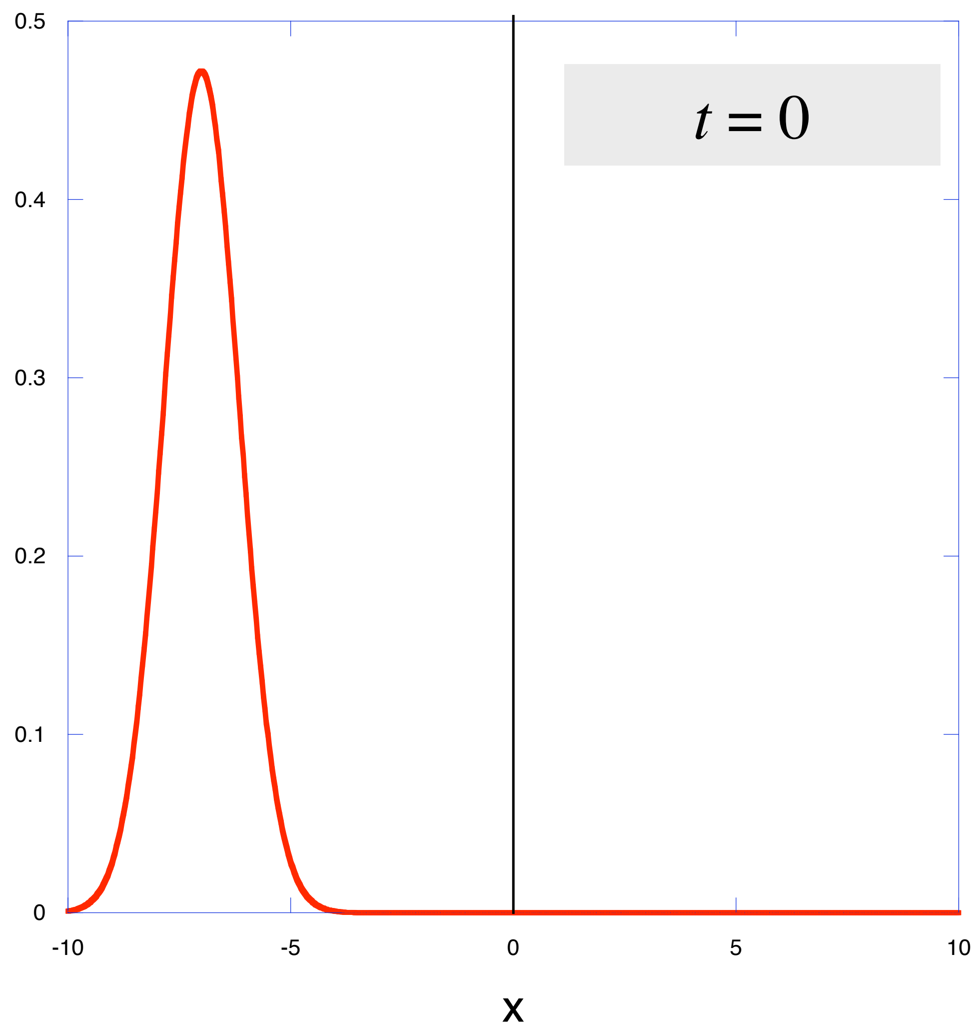


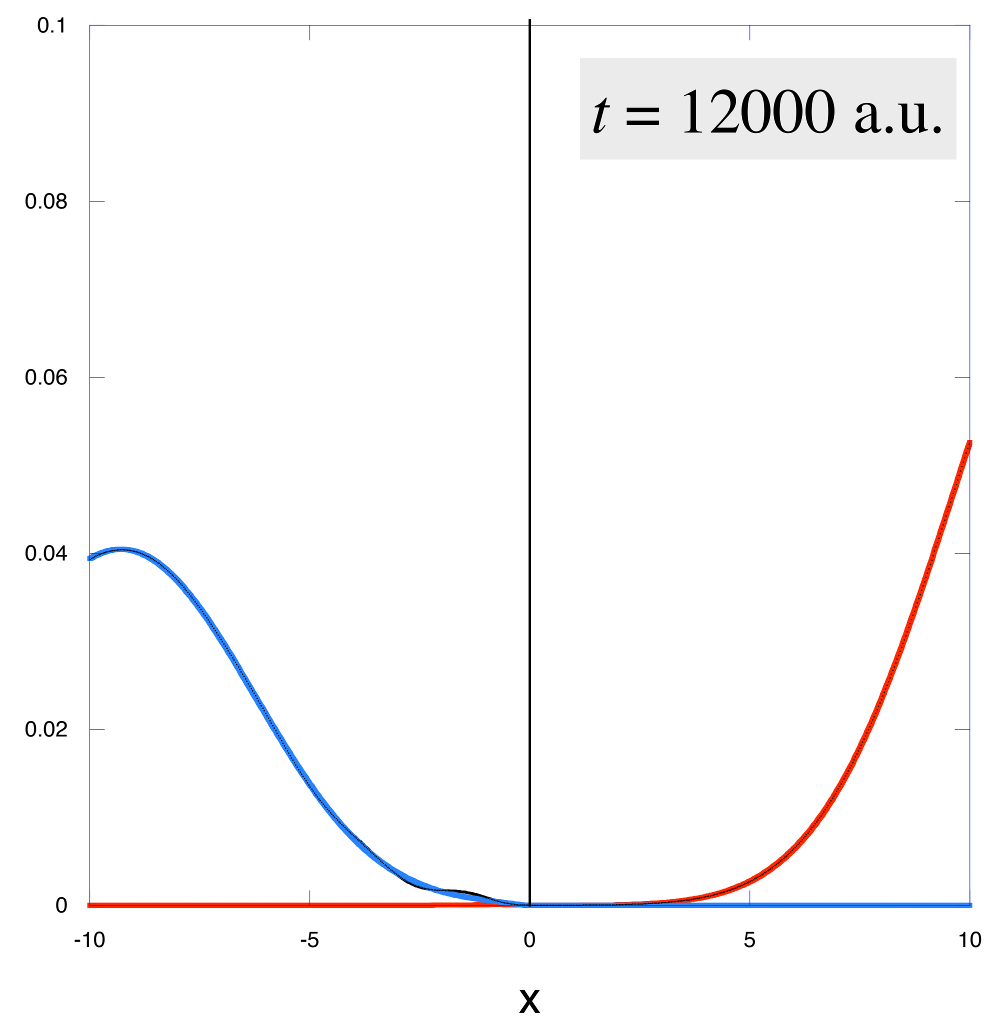


- ψ_- stays in place
- ψ_- disperses & moves to the left

ψ_+ shows a "spur", that feeds ψ_-

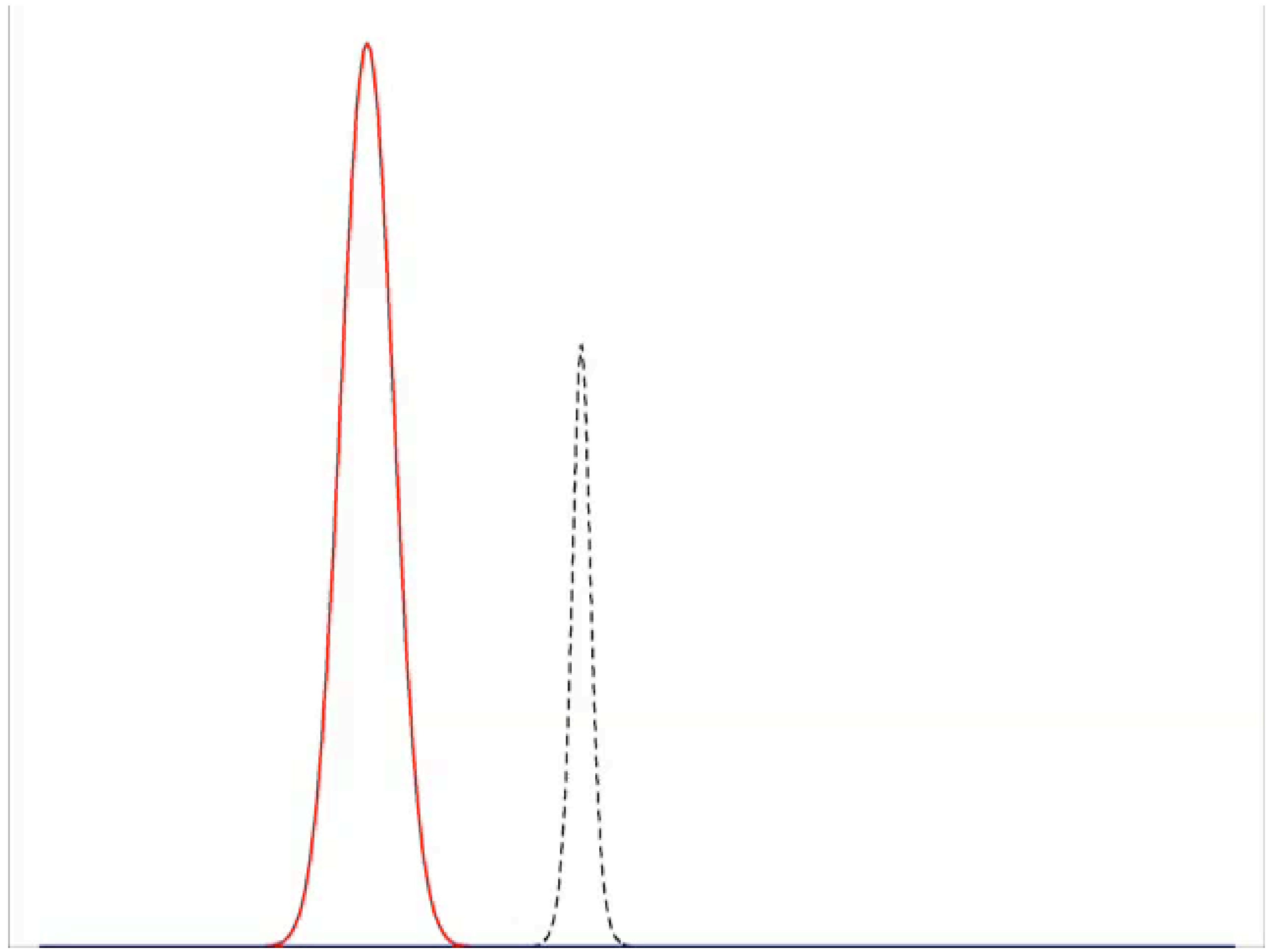
Eckart barrier: *bipolar wave packets*



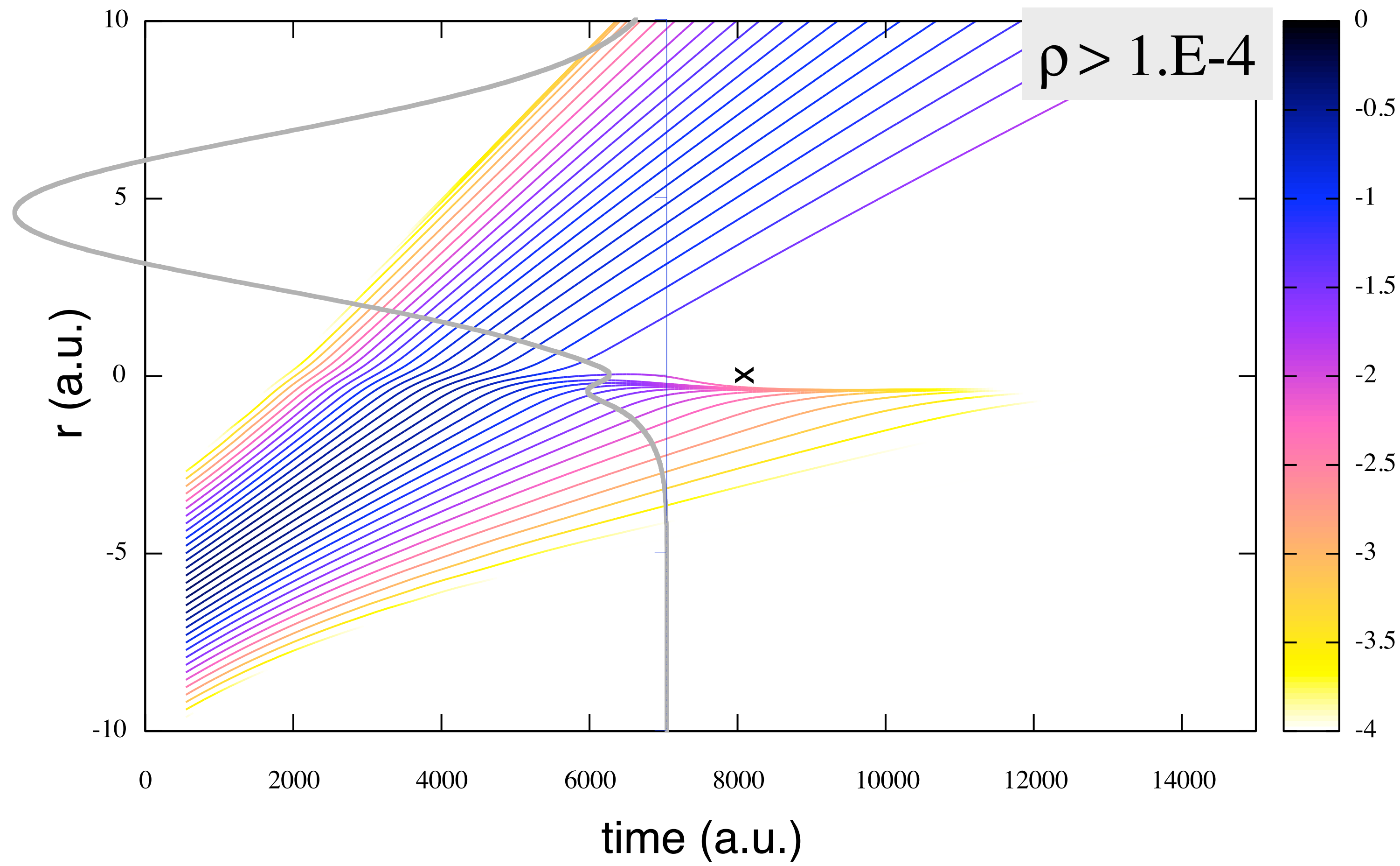


- $\psi_\pm$ localized and smooth *vs.* ψ interferences
- $\psi_+ \sim$ Gaussian-like evolution
- At large time ψ_+ and $\psi_- \sim$ separated Gaussians

Eckart barrier: *bipolar wave packets*

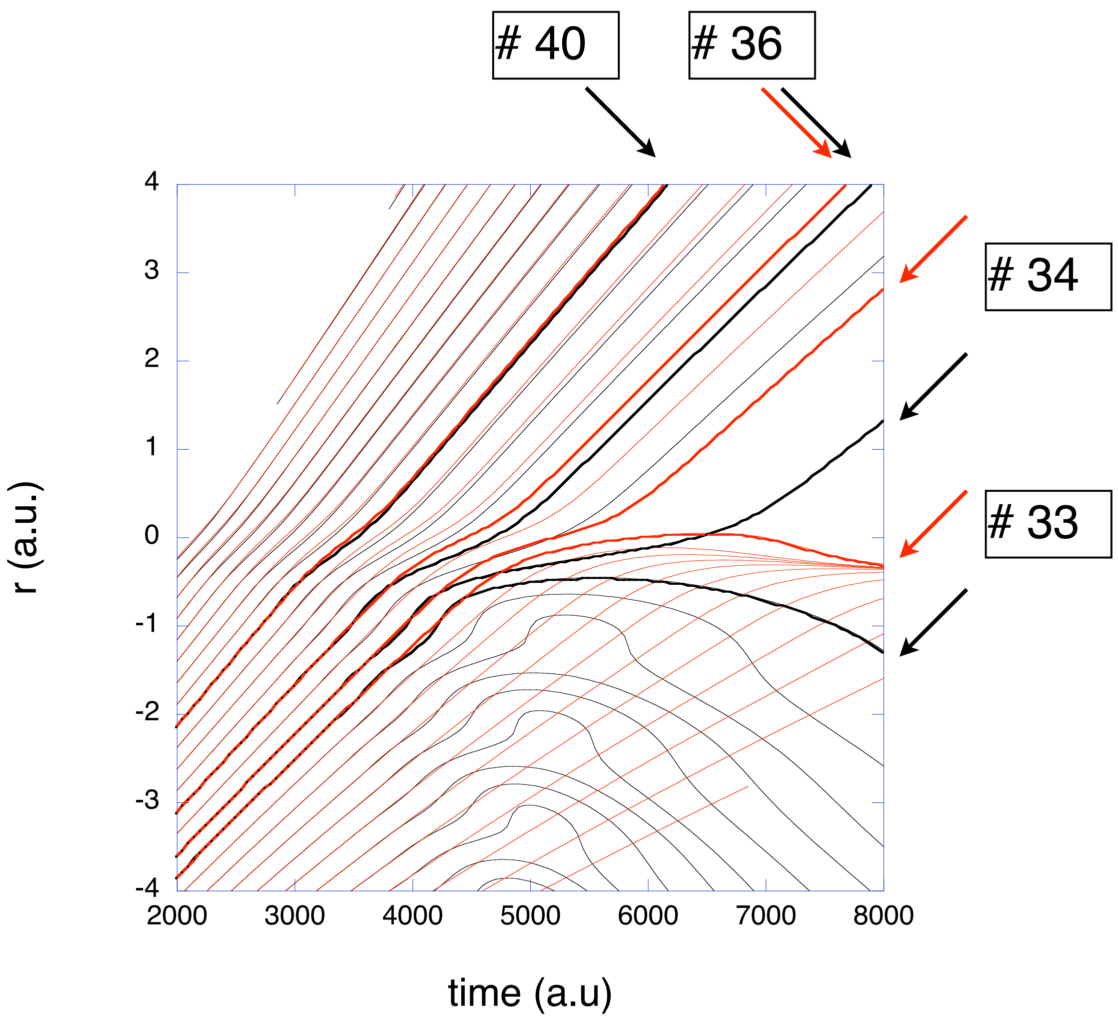


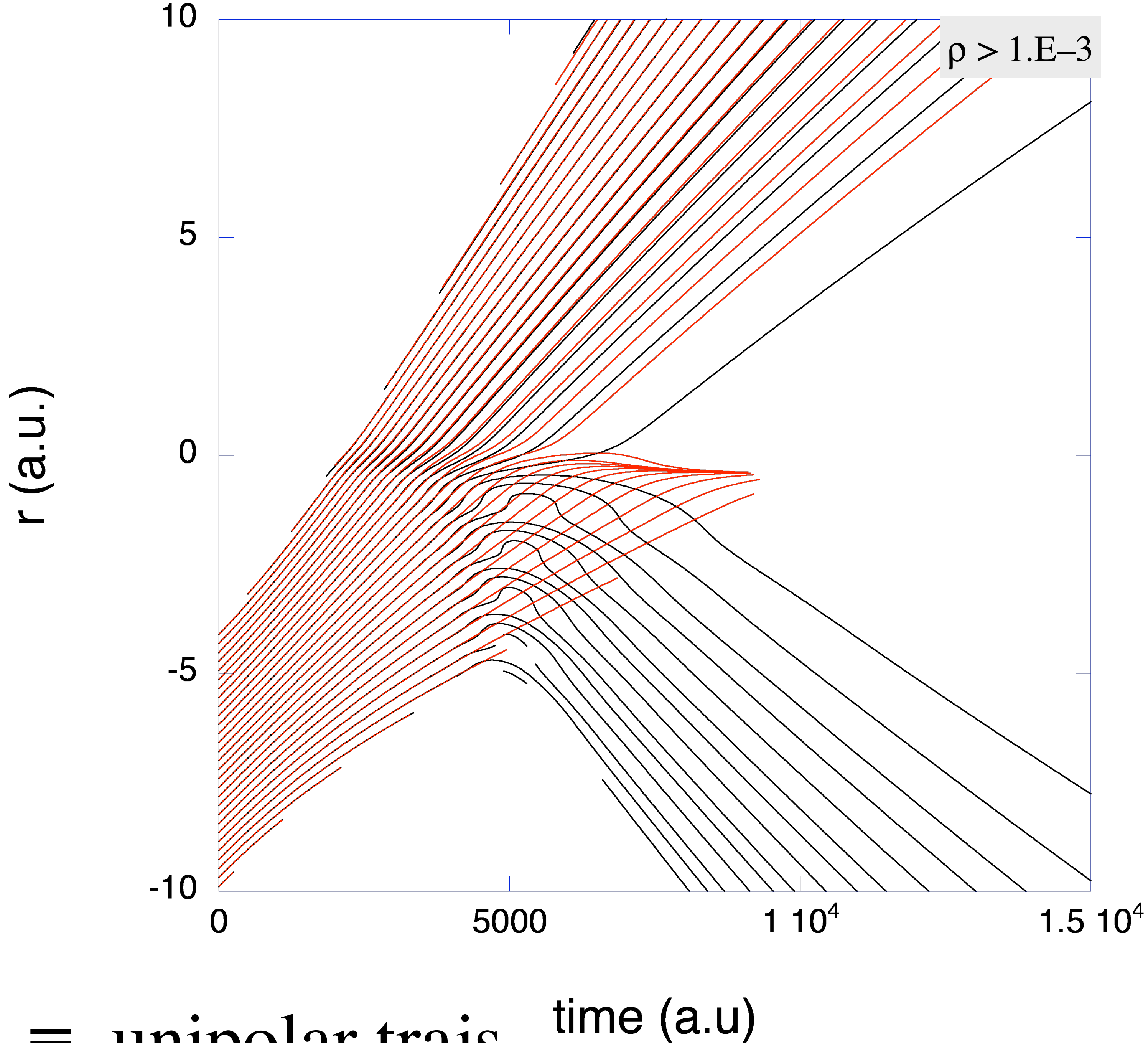
Forward (+) quantum trajectories



- Well-behaved *transmitted* trajs – no "avoided crossings"
- Unexpected (but well-behaved) *reflected* trajs
- Reflected trajs coalesce ~ caustic shape
- Reflected trajs vanish as time ↗

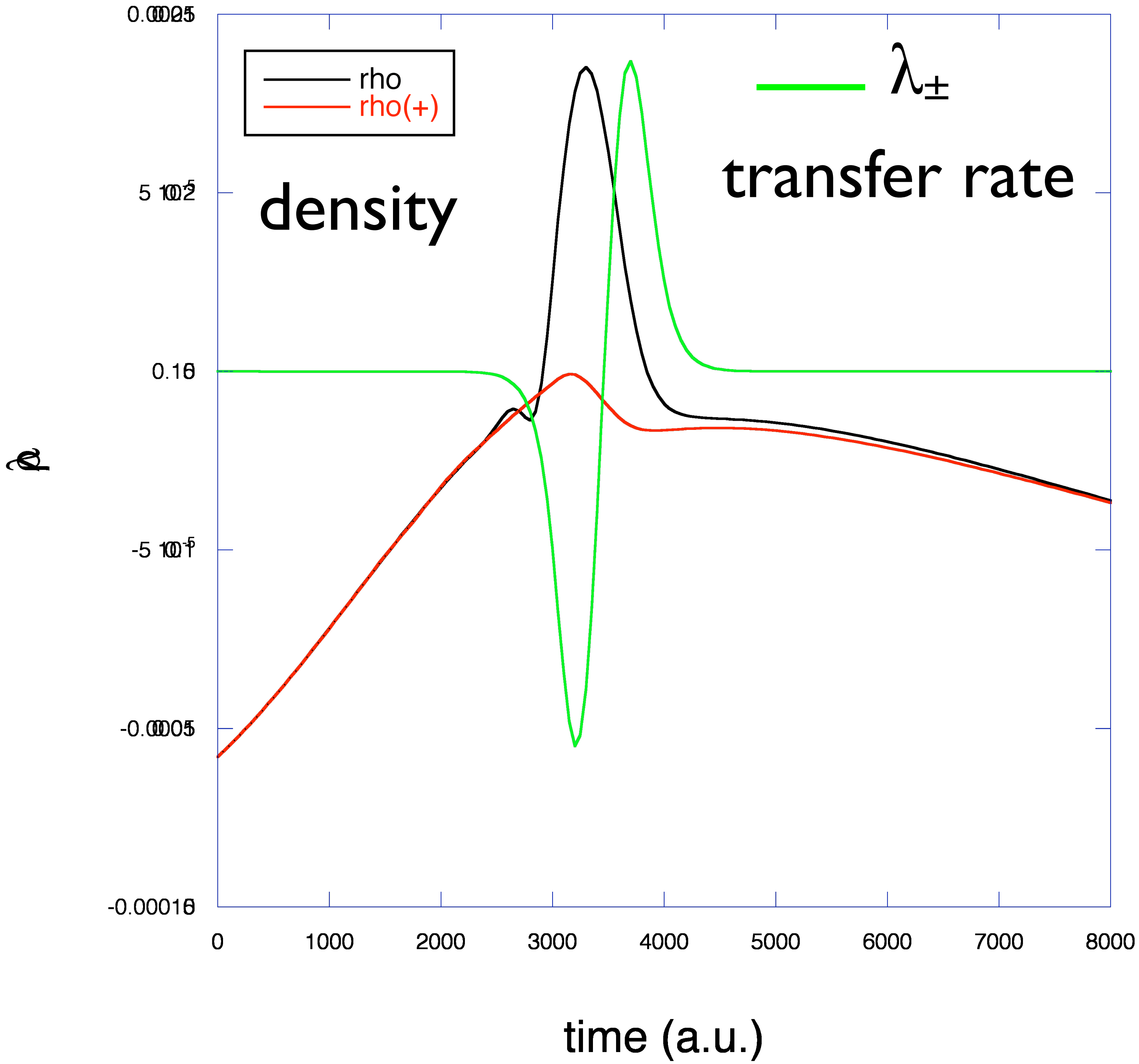
Forward (+) *vs.* unipolar trajectories



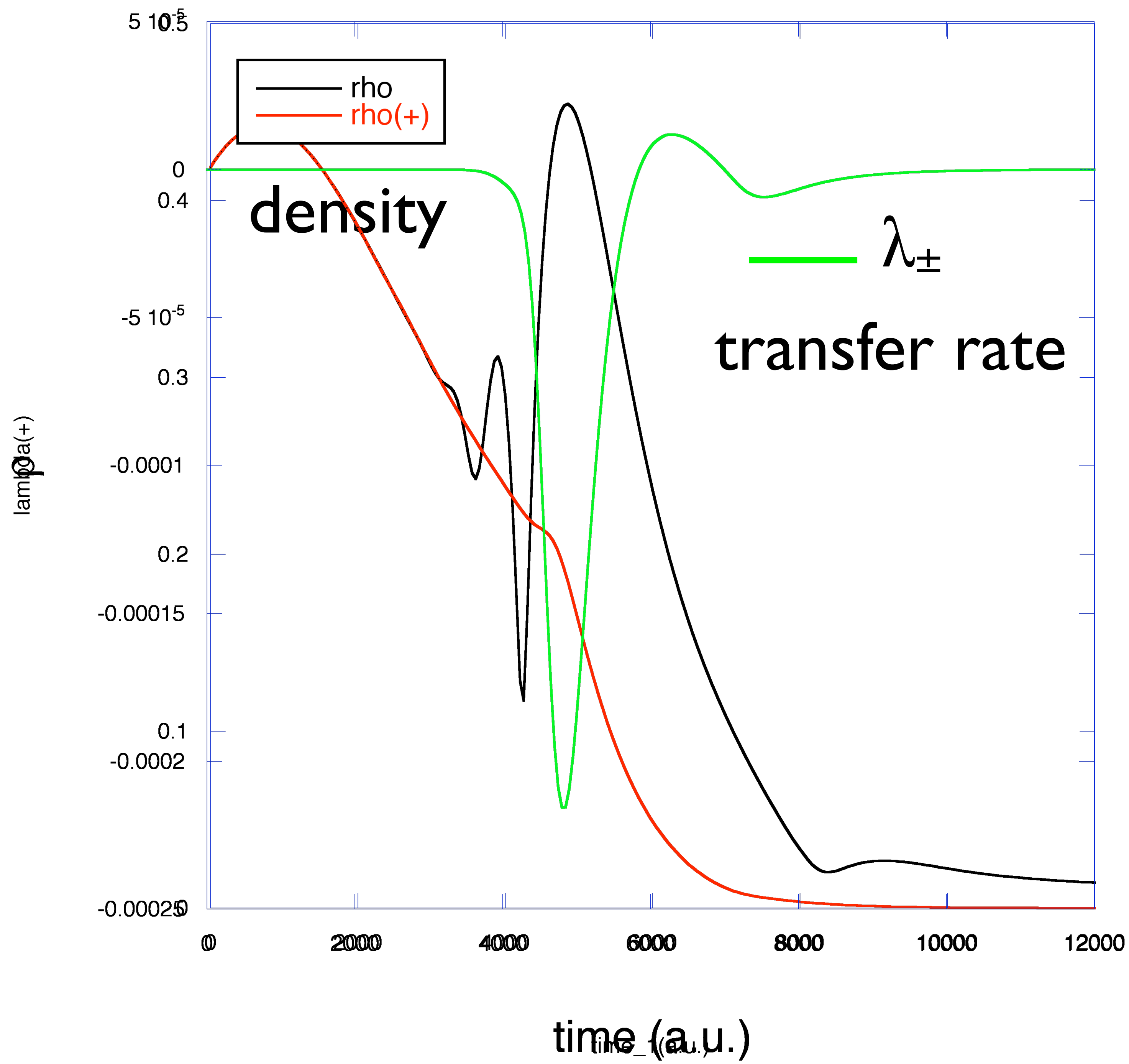


- *Transmitted* trajs almost ≡ unipolar trajs
- *Reflected* trajs totally ≠ unipolar trajs

Forward (+) *vs.* unipolar: *transmitted traj. # 40*

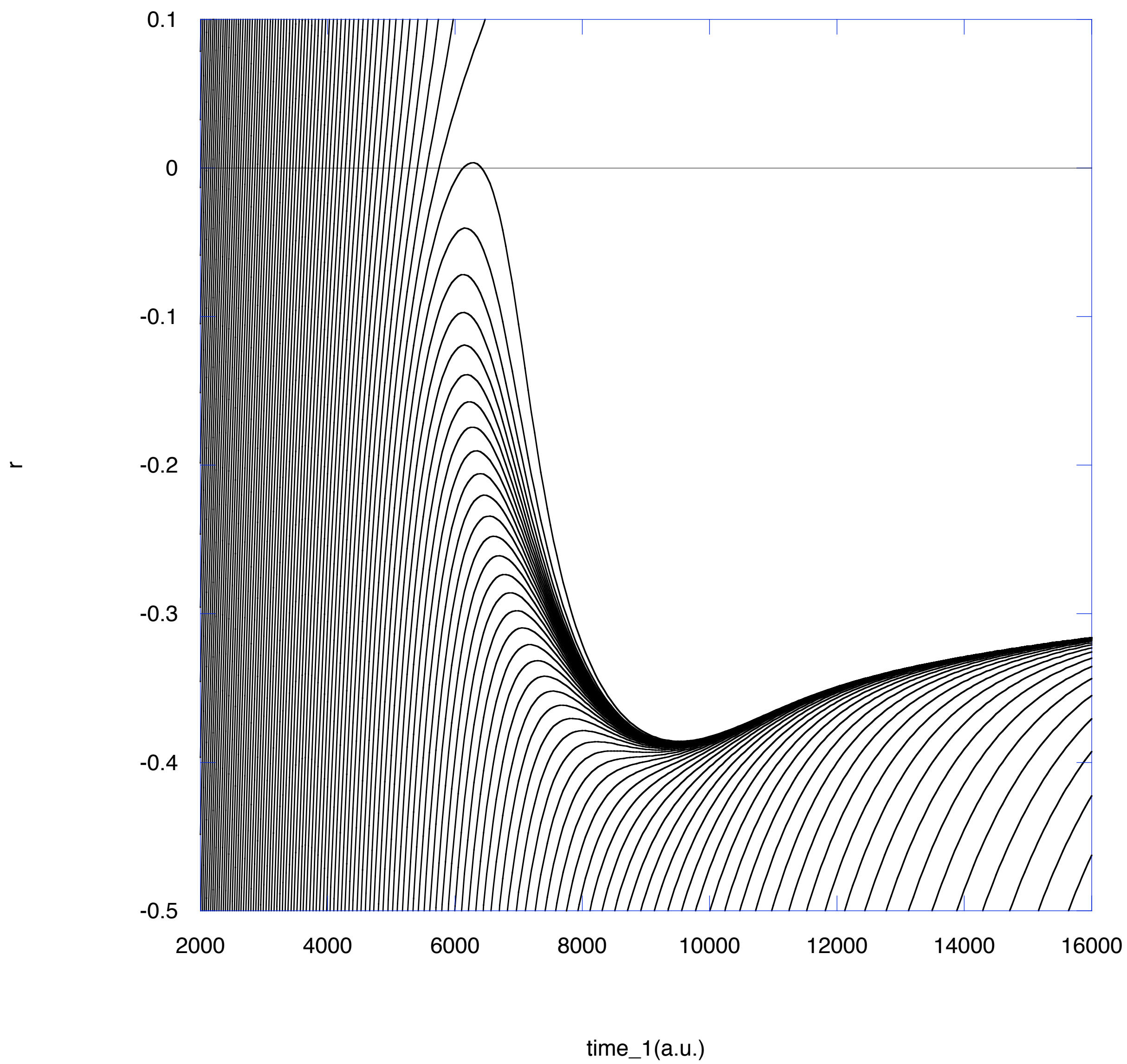


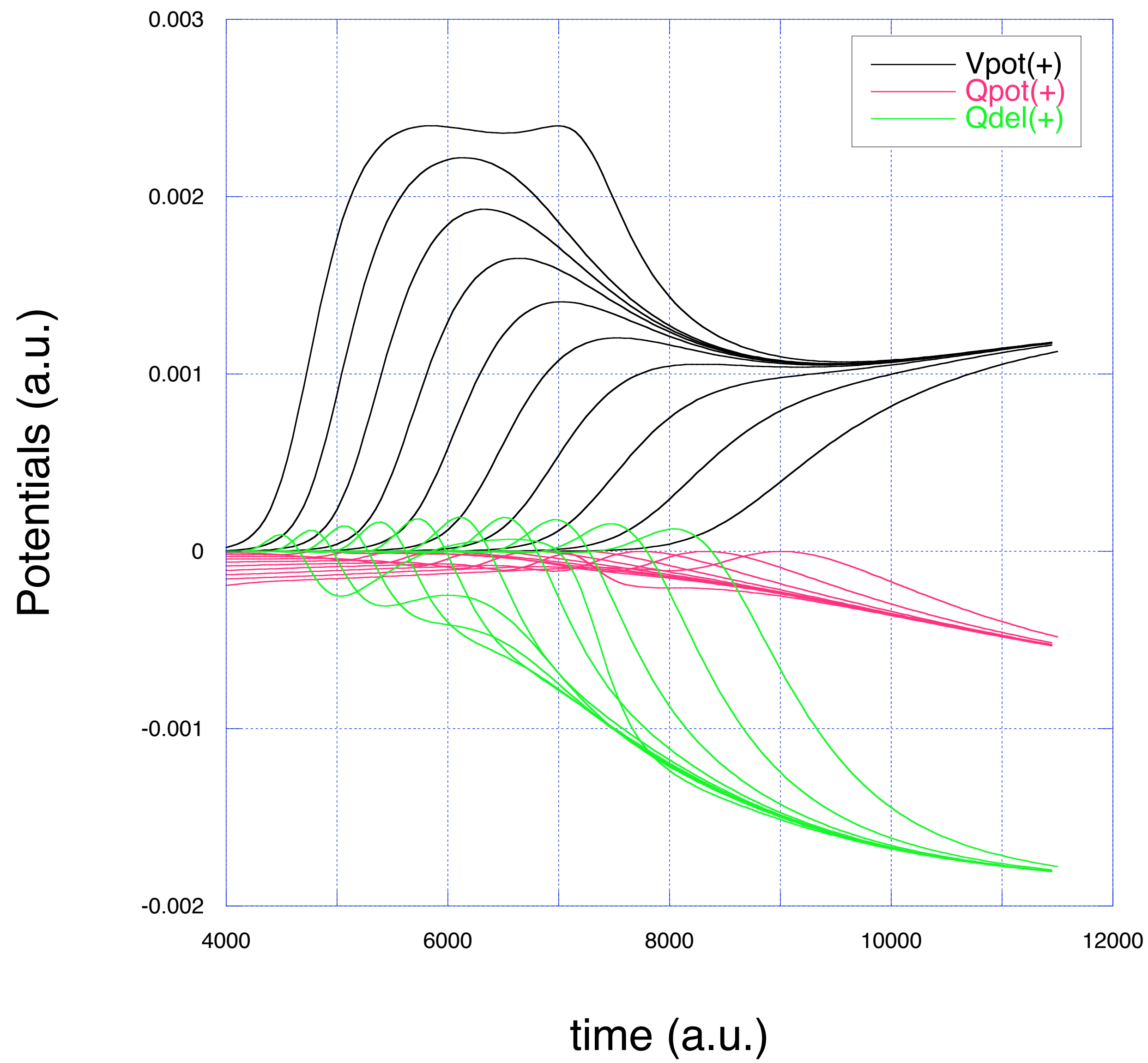
Forward (+) *vs* unipolar: *reflected traj. # 33*



Caustic-shape of reflected (+) trajs

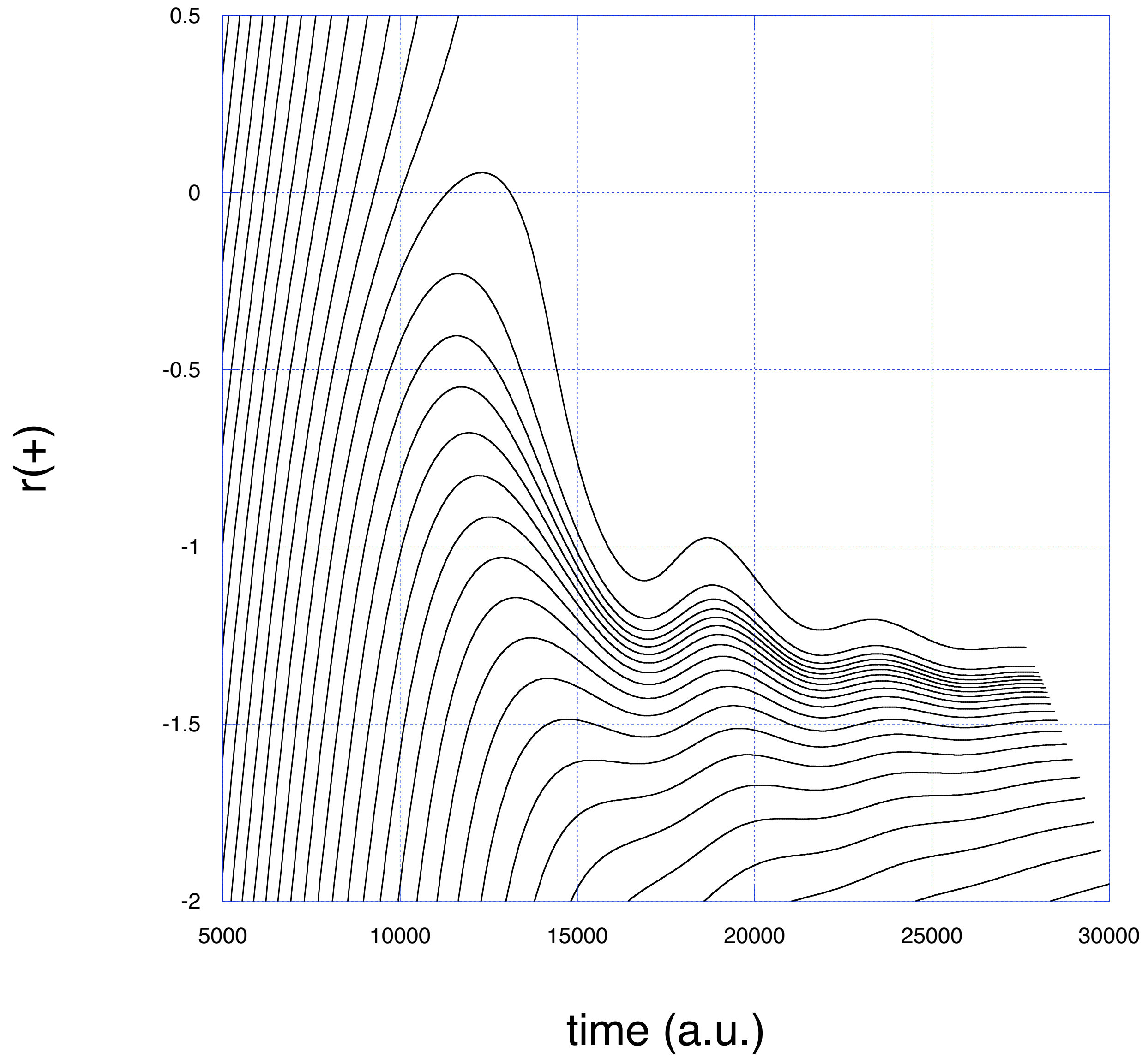
Why are (+) trajs not reflected away

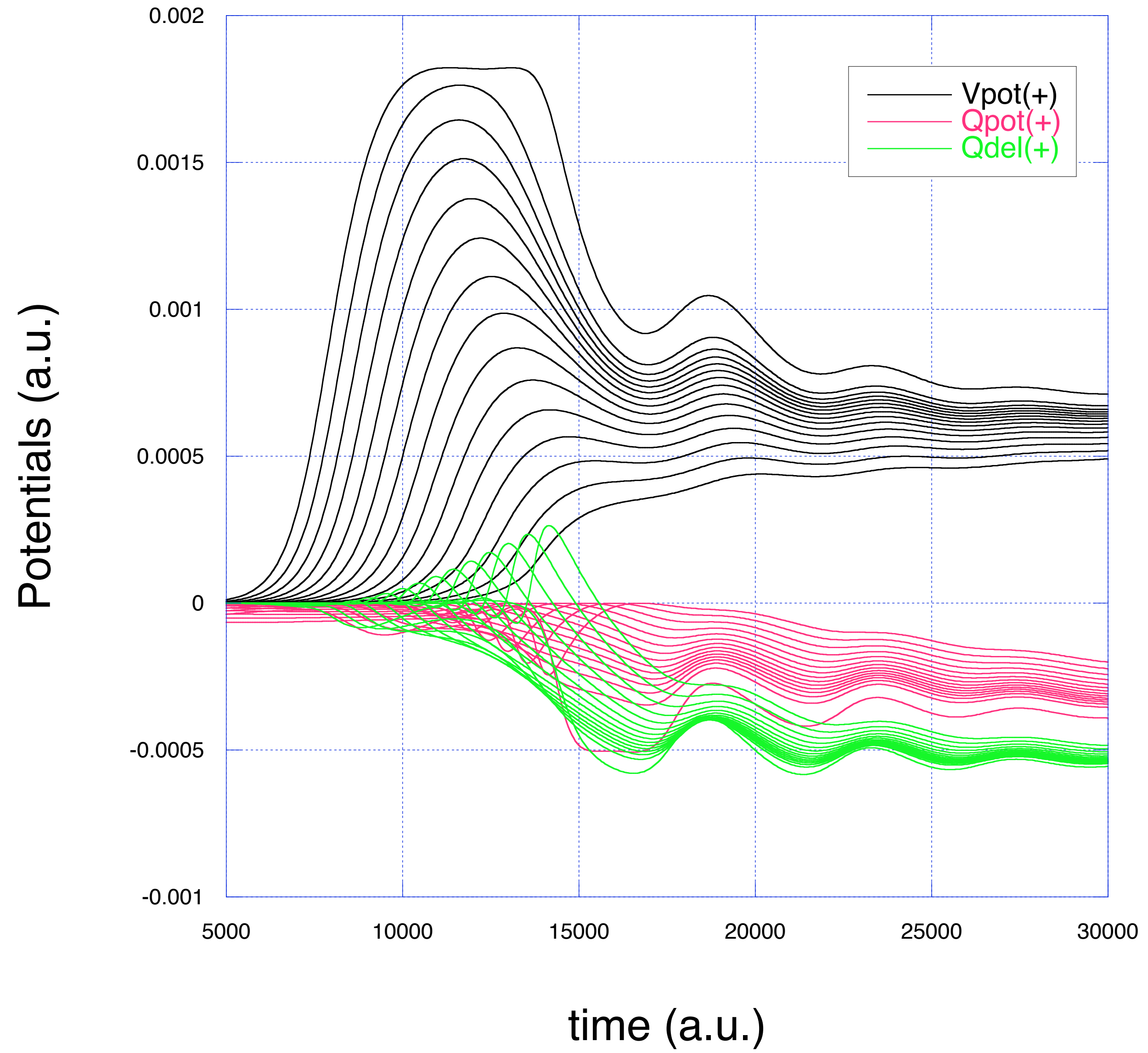




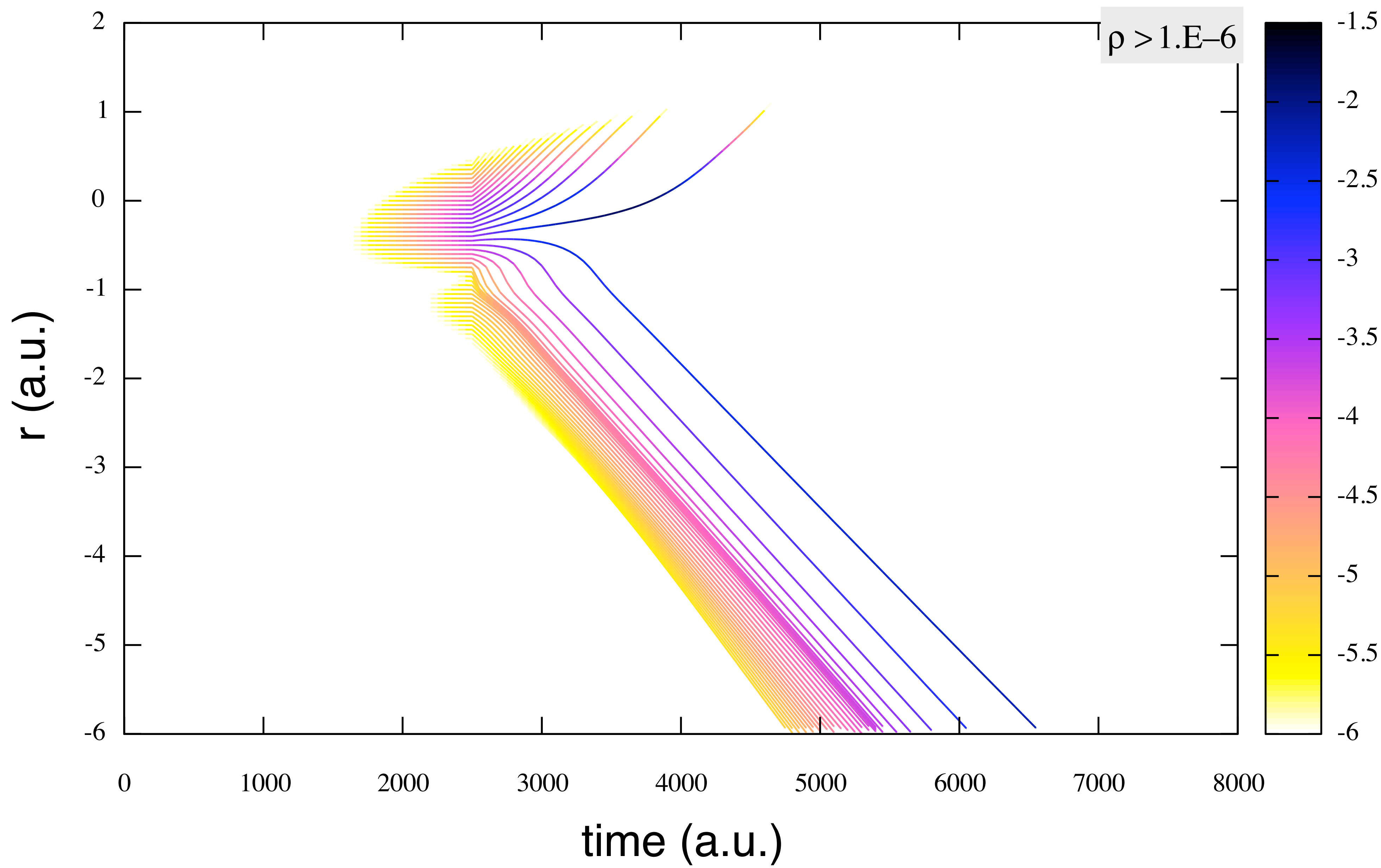
- Quantum potential Q_+ is small
- Quantum potential $Q_{\Delta+}$ "compensates" for classical potential V

More caustic-shape reflected (+) trajs

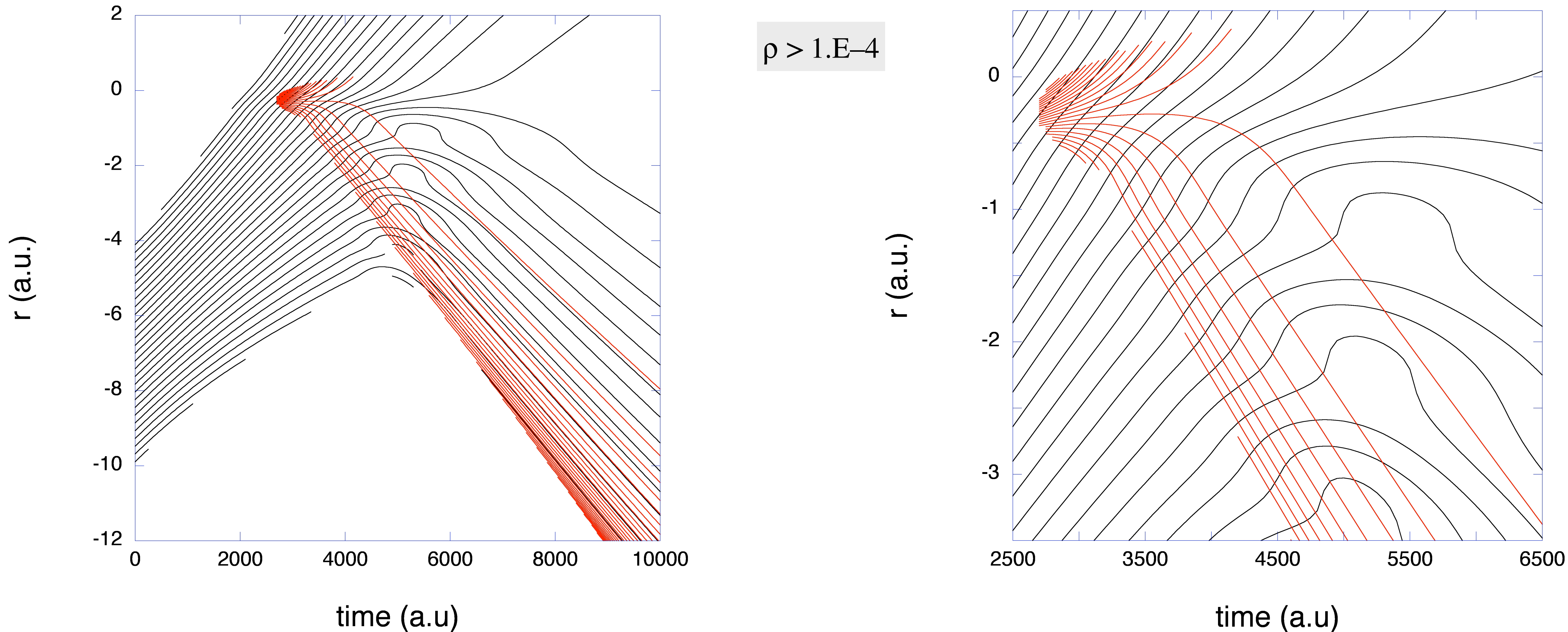




Backward (–) quantum trajectories

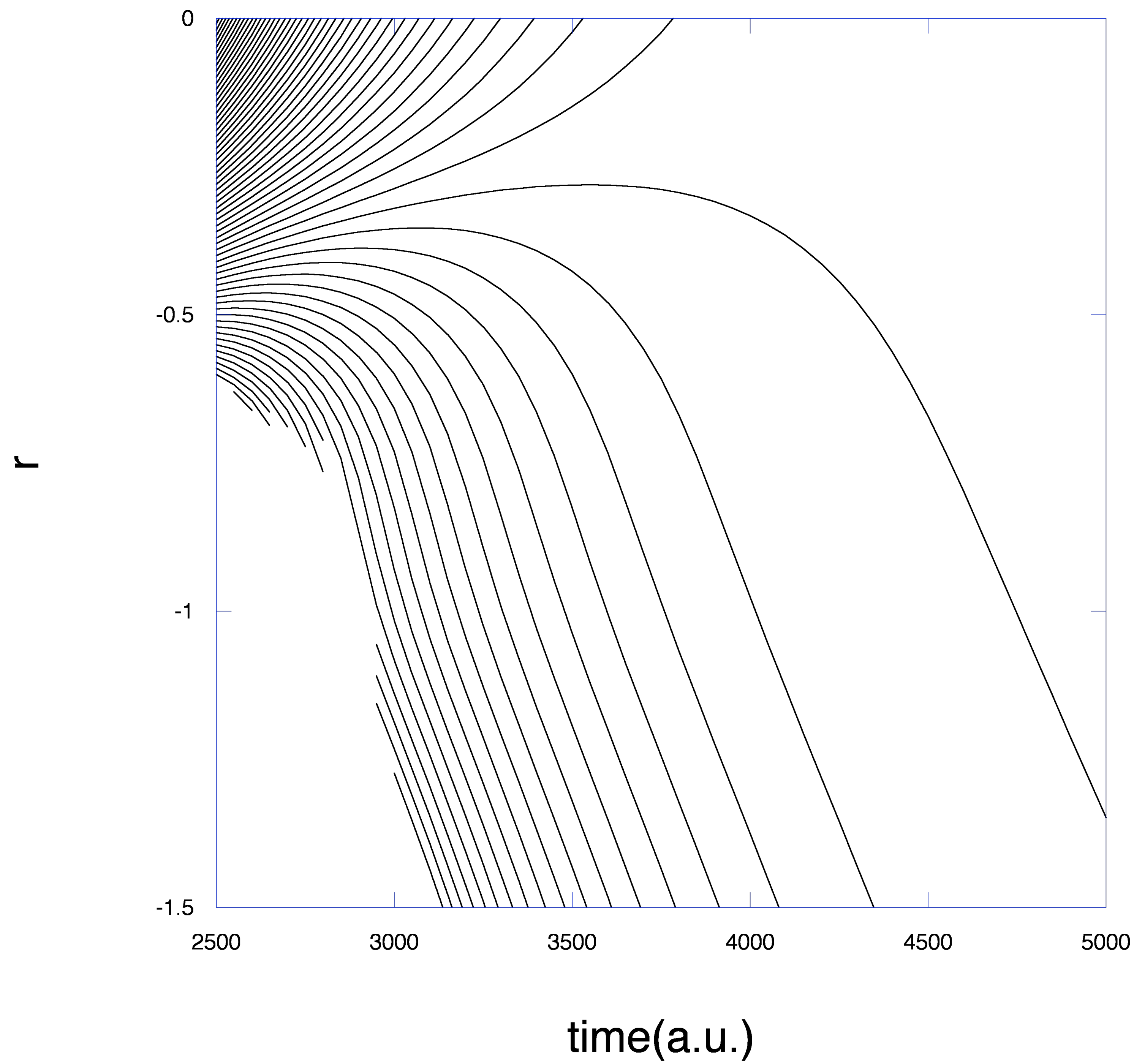


Backward (–) quantum trajectories



- well behaved trajs
- no “avoided crossing”
- *reflected* trajs “fan out”
- *transmitted* trajs vanish as time ↗

Backward (–) quantum trajectories



- Very regular trajectories

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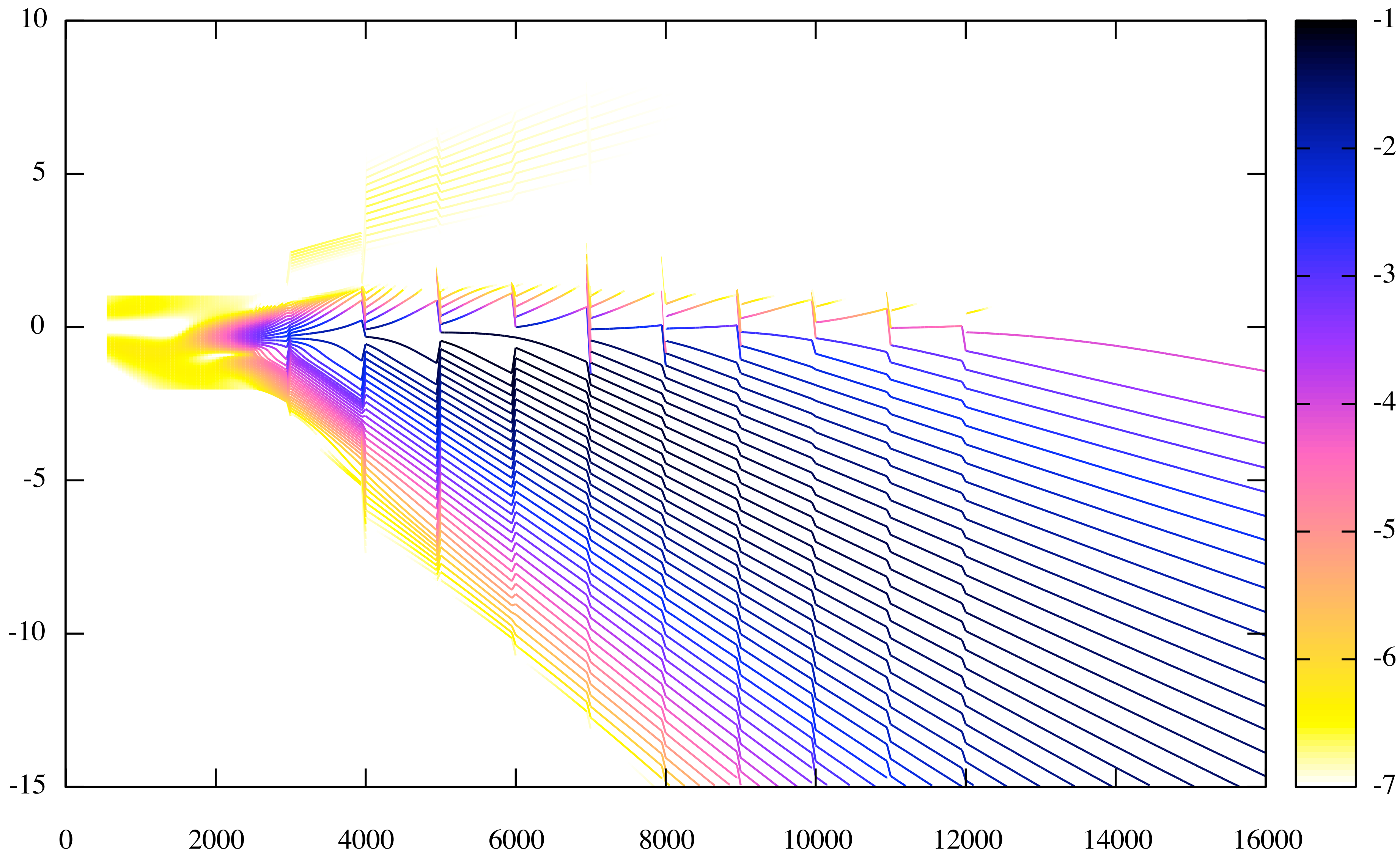
Backward (–) quantum trajs: *“fan out” effect*



- At each time $t = n * 1000$, trajs are “restarted” in order to sample the ψ_- wave packet

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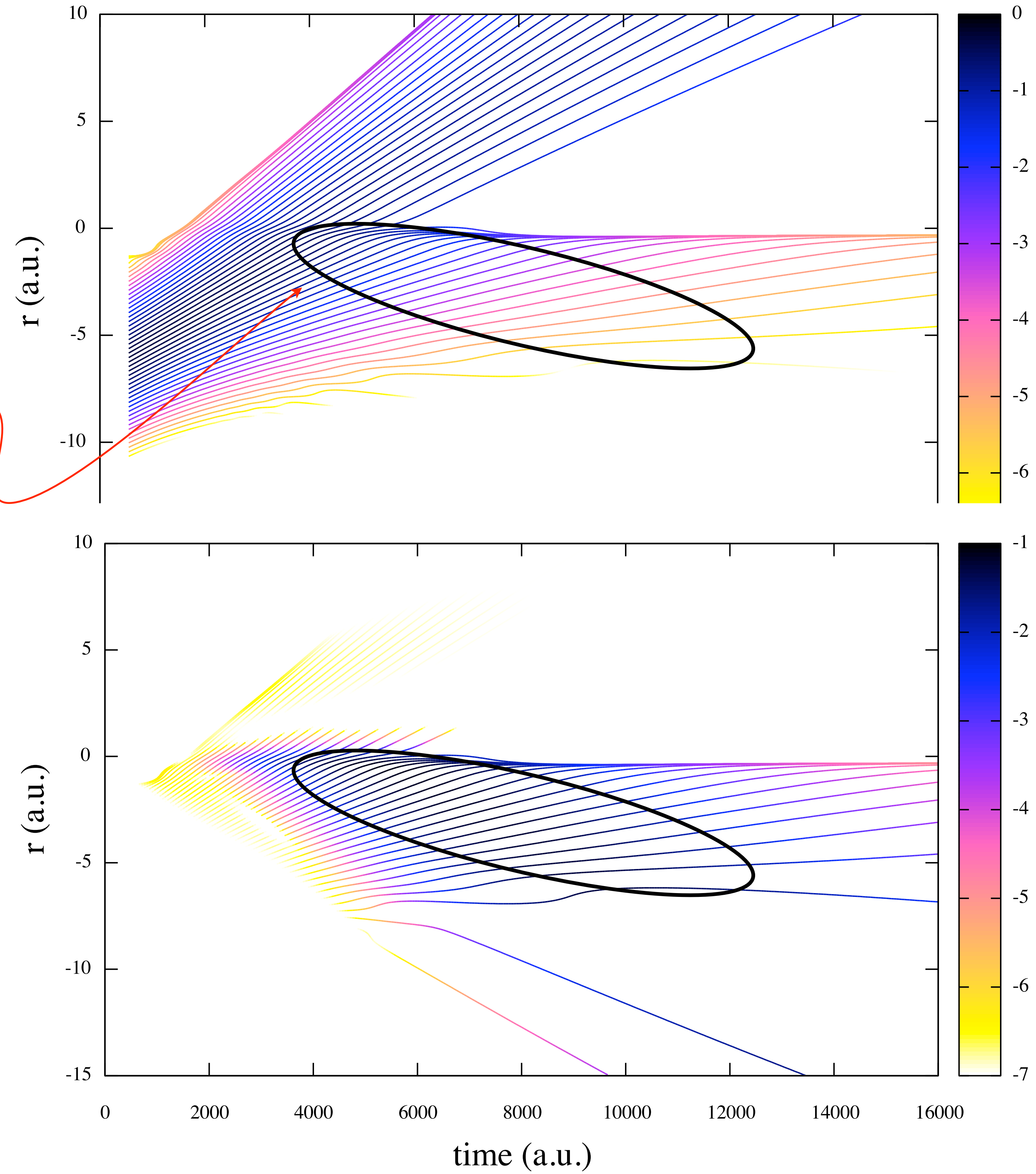
(–) density on (+) trajectories

Zone of (+) → (–) transition

(+) trajectories carrying (–) density



“*Synthetic*” bipolar quantum trajectories

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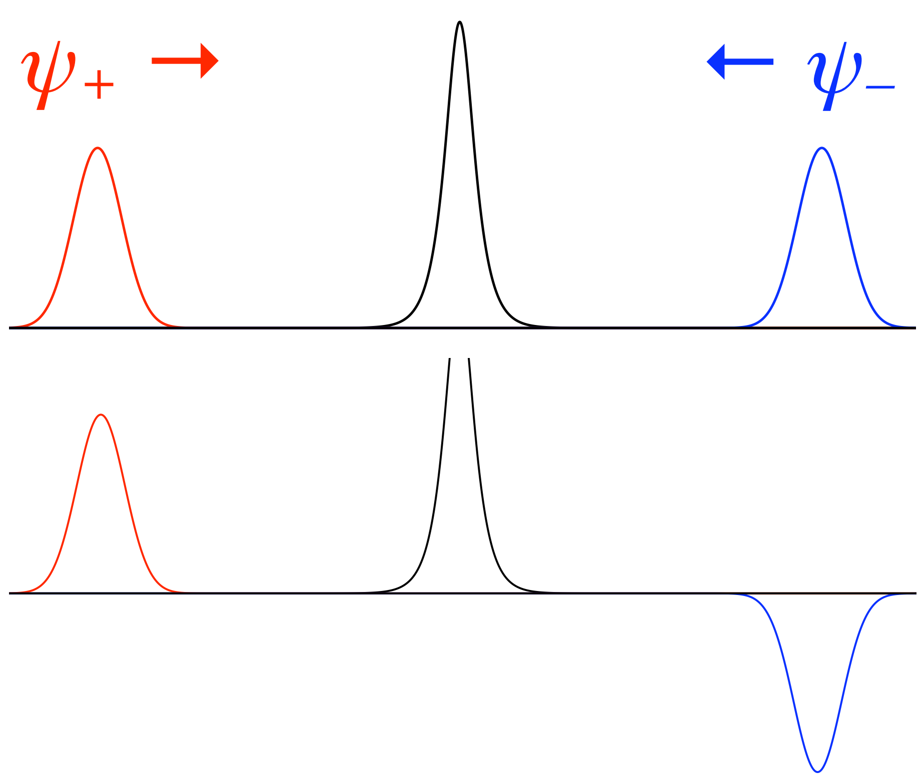
- *Synthetic* trajectories are *actually propagated*
- Difficulties related to (–) trajectories:
  - $\psi_-(t=0) = 0 \rightarrow$ how does one choose initial (–) trajs?
  - strong “inflation” effect $\rightarrow$ drives trajs out of coupling zone
- Solution: use sym. & antisym. combinations of ψ_+ and ψ_-



At time $t = 0$

$$\left| \begin{array}{l} \psi_1 = \psi_+ + \psi_- \\ \psi_2 = \psi_+ - \psi_- \end{array} \right.$$

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"*Synthetic*" bipolar quantum trajectories

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- Propagate quantum trajectories for ψ_1 and ψ_2
- From ψ_1 and $\psi_2 \rightarrow$ one can derive ψ_+ and ψ_- at any time
- *n.b.* (ψ_{1-}, ψ_{2-}) are mirror images of (ψ_{1+}, ψ_{2+})

"*Synthetic*" (1+) and (2+) densities

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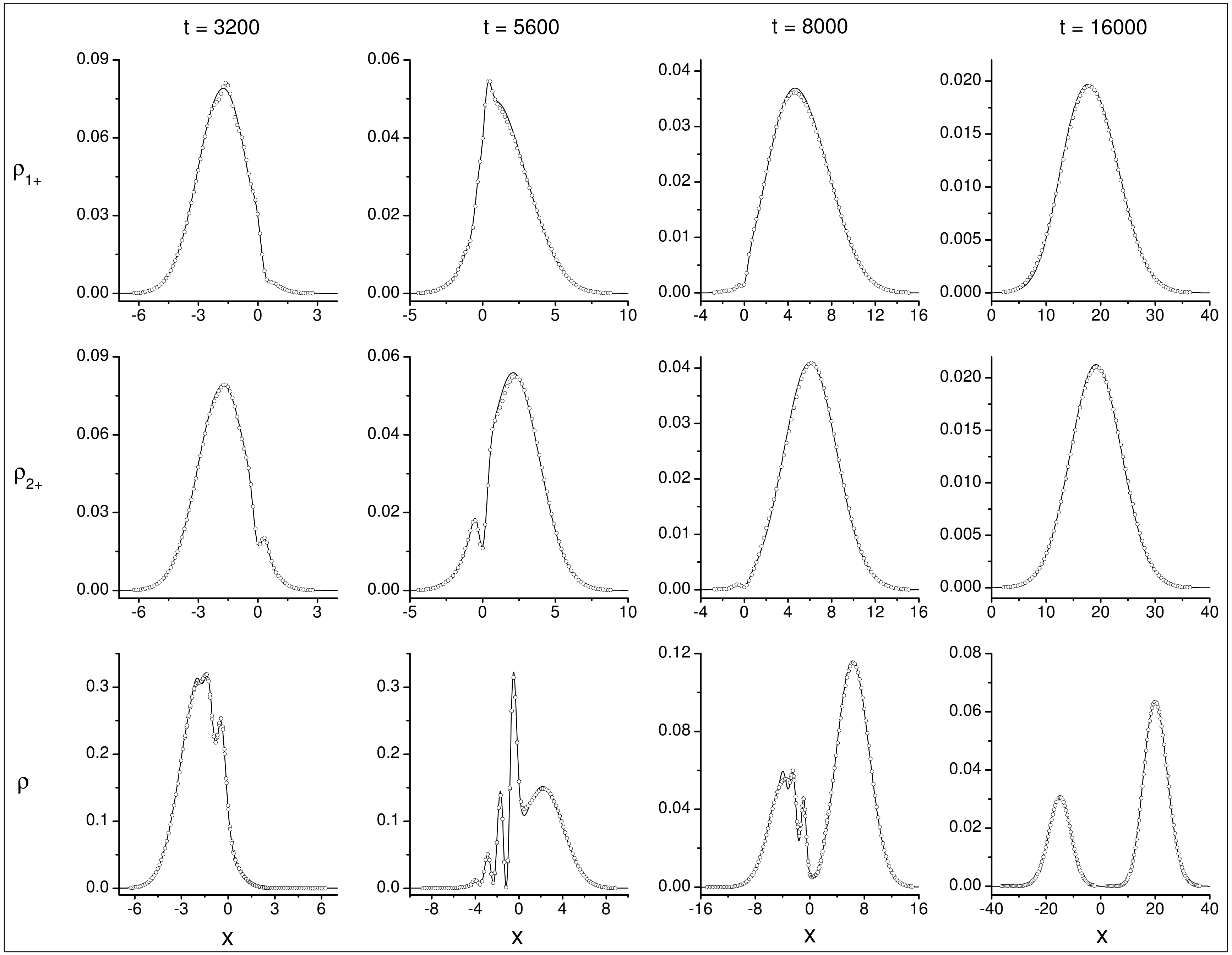
ρ_{1+}

ρ_{2+}

ρ



- Densities are obtained from synthetic trajectories and compared with fixed-grid wave packets

“*Synthetic*” (1+) and (2+) densities

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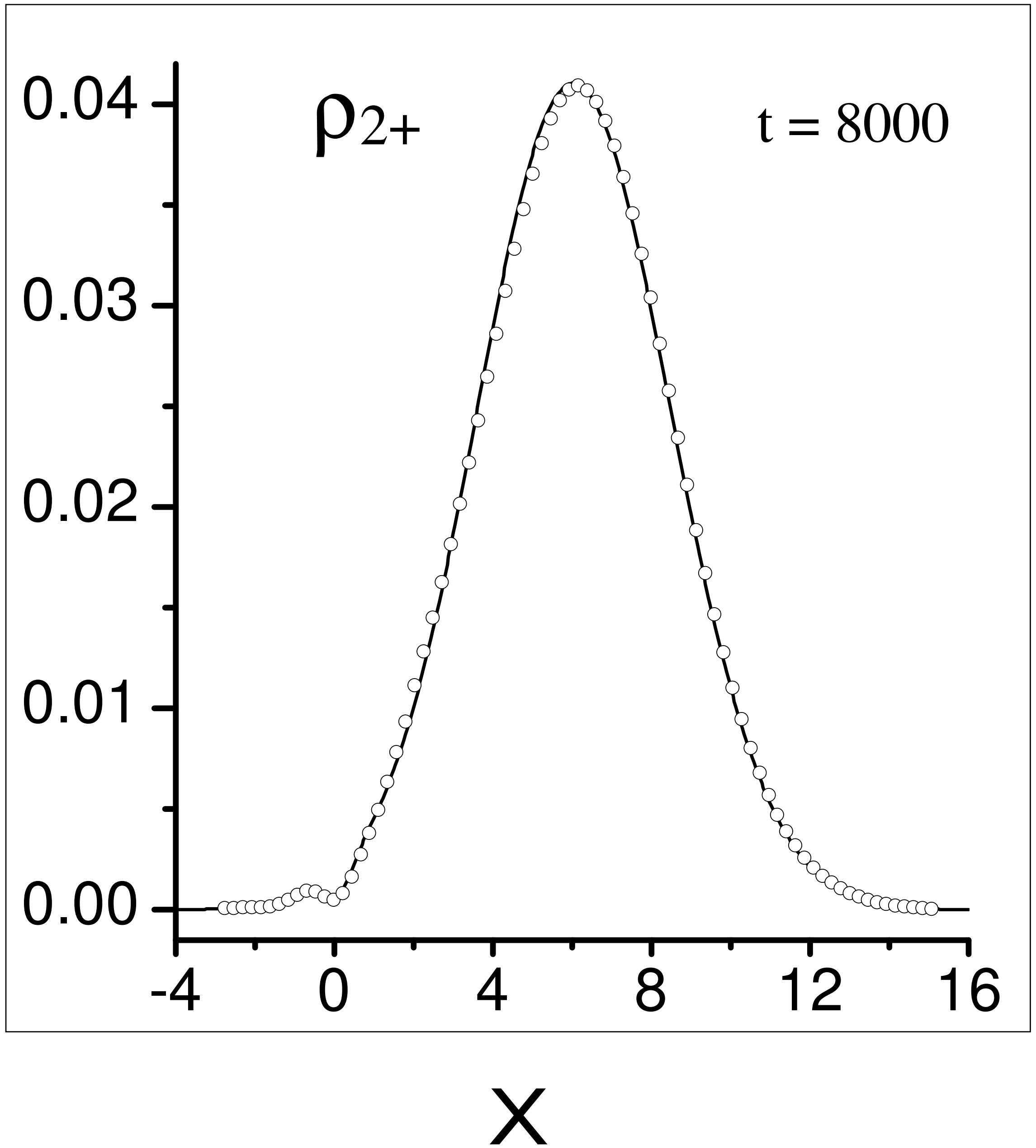

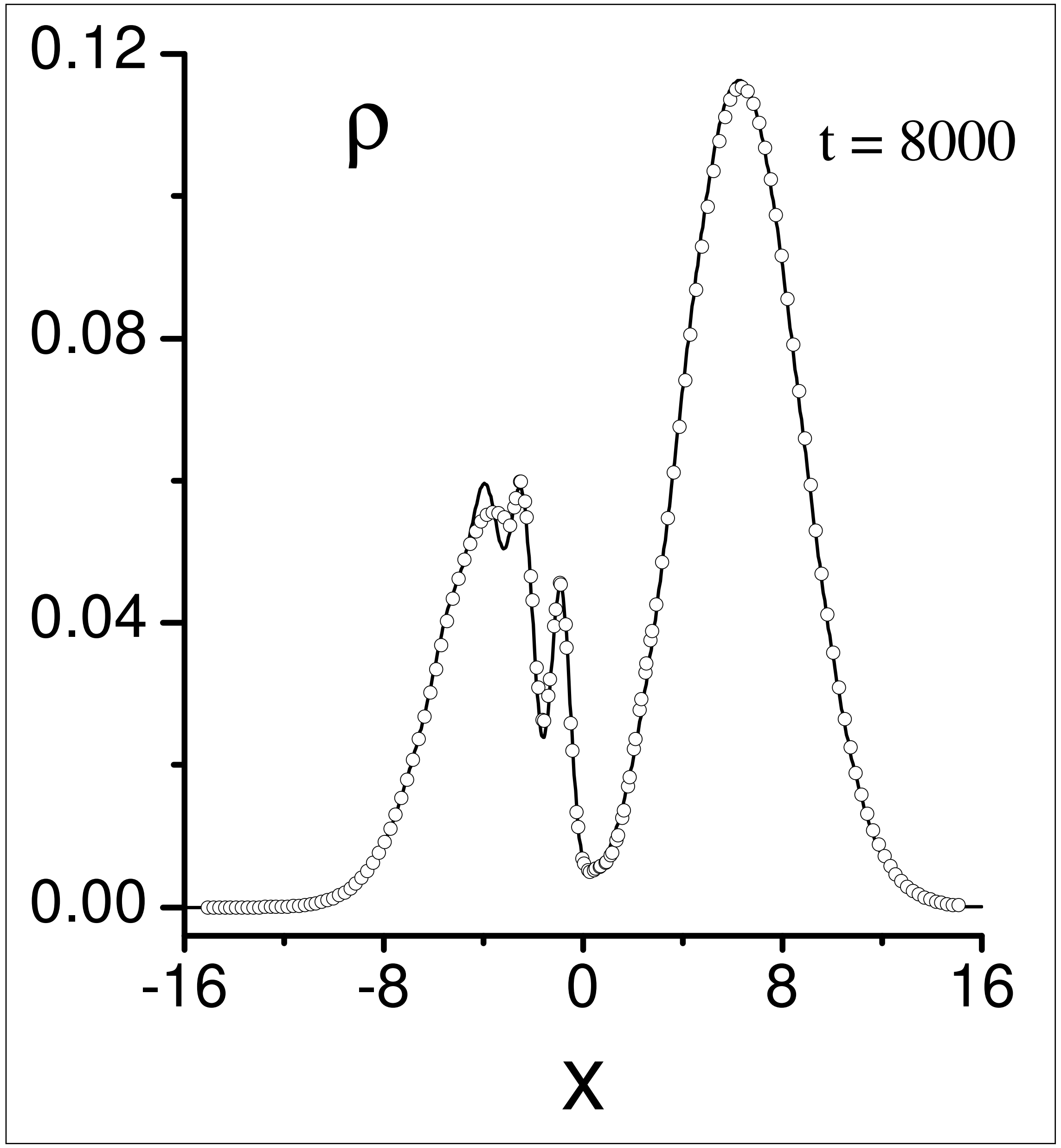

Summary

- Propagation of bipolar wave packets by fixed-grid method
- Well-behaved "*analytical*" quantum trajs
- Analysis of trajs *adds a new dimension to the dynamics*
- Propagation of "*synthetic*" quantum trajs

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Thank you…

- …for your attention
- Bill Poirier
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- CNRS and Univ. Montpellier for €€€