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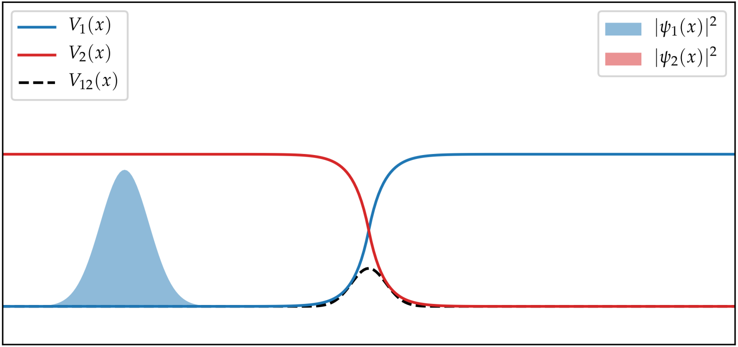
Quantum entanglement from uncoupled classical trajectories

Johan E. Runeson

Group of Prof. J. O. Richardson

Wavepacket branching (Tully I)



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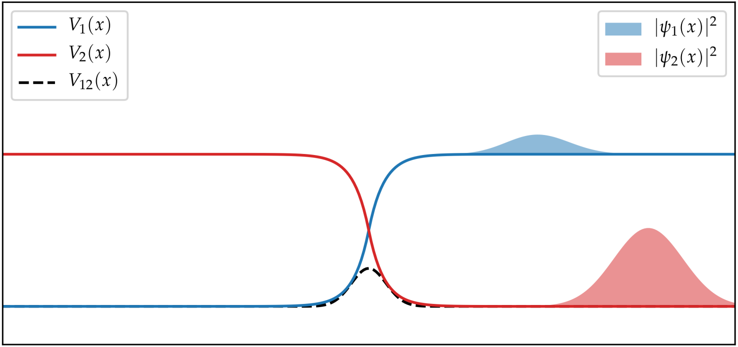


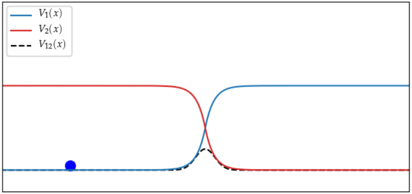
Before: $\underbrace{\psi_{L,1}(x)|1\rangle}_{\text{Product state}}$ After: $\underbrace{\psi_{R,1}(x,t)|1\rangle + \psi_{R,2}(x,t)|2\rangle}_{\text{Entangled state}}$

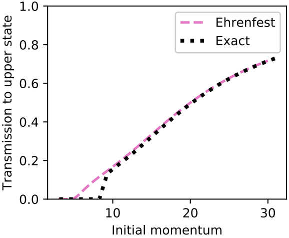
Ehrenfest dynamics: no branching

$$|\psi\rangle = c_1|1\rangle + c_2|2\rangle$$

$$\begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \end{pmatrix} = -\frac{\mathrm{i}}{\hbar}\hat{V}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\dot{x} = p/m, \quad \dot{p} = -\frac{\partial}{\partial x}\langle\psi|\hat{V}|\psi\rangle$$





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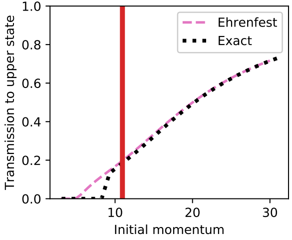
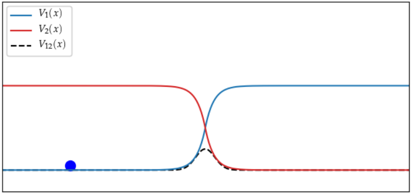
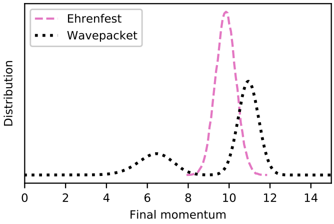
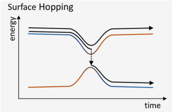




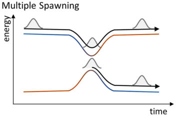


Existing ways to describe branching

Figs: Crespo-Otero & Barbatti (2018)



- Surface hopping (Tully, JCP 1990)
- Coupled trajectories
  - MC Ehrenfest (Shalashilin, Faraday Discuss. 2011)
  - Exact factorization (Min, Agostini & Gross, PRL 2015)
  - Ab-initio multiple spawning (Curchod & Martinez, PRL 2015)
  - QCLE (Kelly, van Zon, Schofield & Kapral, JCP 2012)
  - Bohmian dynamics (Curchod & Tavernelli, JCP 2013)
  - ...



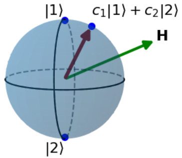
- Forward-backward IVR (Miller, J. Phys. Chem A, 2009)

$$C_{AB}(t) \sim \int dx_0 dp_0 dx_0' dp_0' C_t \, \mathrm{e}^{i(S_t(p,q)-S_t(p',q'))} \langle p_0, q_0 | A | p_0', q_0' \rangle \langle p_t', q_t' | B | p_t, q_t \rangle$$

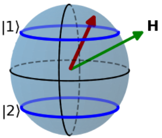
Possible with *classical* (deterministic, uncoupled, phaseless) trajectories?

Spin mapping

Ehrenfest ($\gamma = 0$)



Spin mapping ($\gamma \approx 0.732$)



- Same form of Hamiltonian as MMST mapping (Meyer & Miller 1979, Stock & Thoss 1997)

$$\hat{V} \mapsto \frac{1}{2}\sum_n V_{nn}(X_n^2 + P_n^2 - \gamma) + \sum_{n \neq m} V_{nm}(X_n X_m + P_n P_m)$$

- Original MMST: $\gamma = 1$, typically $0 < \gamma < 1$ most accurate

$$\gamma = 2|\boldsymbol{s}| - 1$$

$$|\boldsymbol{s}| \equiv \sqrt{\hat{\boldsymbol{s}}^2} = \sqrt{\frac{1}{2}\left(\frac{1}{2} + 1\right)} = \frac{\sqrt{3}}{2}$$

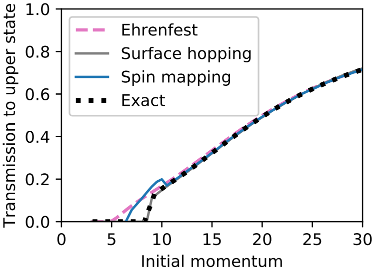
- Spin: $\gamma = \sqrt{3} - 1 \approx 0.732$ (Cotton & Miller, JCP 2013)
- When derived directly from spin:
  - ✓ robust to initial distribution
  - ✓ no zero-point energy leakage
  - ✓ total population $= 1$

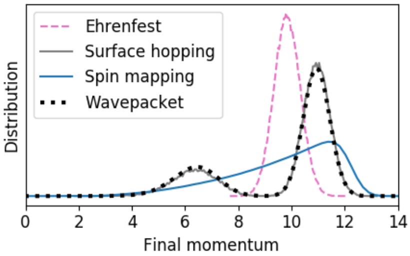
  (Runeson & Richardson, JCP 2019)
- Generalized to any number of levels (lower γ) (Runeson & Richardson, JCP 2020)

Results (one spin)

$$\mathrm{Tr}[\hat{\rho}\hat{A}] = \int \mathrm{d}^2\boldsymbol{s}\,\rho(\boldsymbol{s})A(\boldsymbol{s})$$

$$\boxed{\mathrm{Tr}[\hat{\rho}(t)\hat{A}] \approx \int \mathrm{d}^2\boldsymbol{s}\,\rho(\boldsymbol{s}_t)A(\boldsymbol{s})}$$





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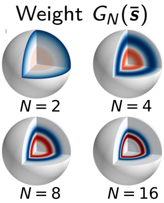
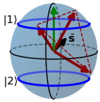
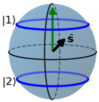
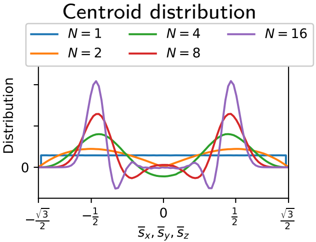
Path integral of spins

$$
\begin{aligned}
\mathrm{Tr}[\hat{\rho}\hat{A}] &= \int \mathrm{d}^2\boldsymbol{s}\,\rho(\boldsymbol{s})A(\boldsymbol{s}) \\
&= \int\cdots\int \left(\prod_{k=1}^{N}\mathrm{d}^2\boldsymbol{s}_k\right) \color{red}{\mathrm{Tr}\left[\prod_{k=1}^{N}\hat{w}(\boldsymbol{s}_k)\right]} \rho(\bar{\boldsymbol{s}})\,A(\bar{\boldsymbol{s}}) \\
&= \int \mathrm{d}^3\bar{\boldsymbol{s}}\,G_N(\bar{\boldsymbol{s}})\rho(\bar{\boldsymbol{s}})A(\bar{\boldsymbol{s}})
\end{aligned}
$$



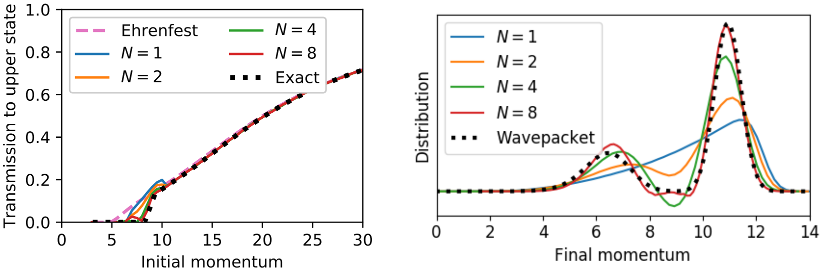
$\int\cdots\int$ 

$= \int$ 



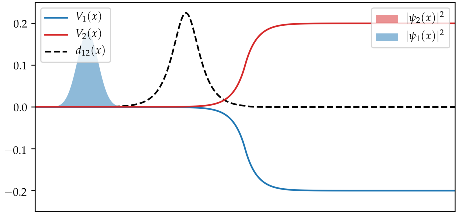
Results (N spins)

$$\mathrm{Tr}[\hat{\rho}(t)\hat{A}] \approx \int \mathrm{d}^3\bar{\mathbf{s}}\; G_N(\bar{s})\rho(\bar{\mathbf{s}}_t)A(\bar{s})$$



Quantum entanglement from classical trajectories,
Runeson & Richardson, *submitted* (2021), arXiv:2105.02075

Harder problem: Recrossing (Tully III)



Before: $\psi_{L,1}(x)|1\rangle$, After: $\psi_{L,1}(x,t)|1\rangle + \psi_{L,2}(x,t)|2\rangle + \psi_{R,1}(x,t)|1\rangle$

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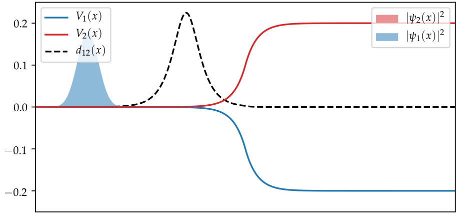

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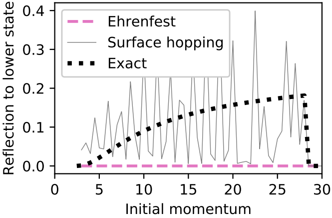

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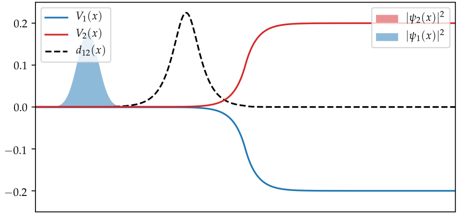

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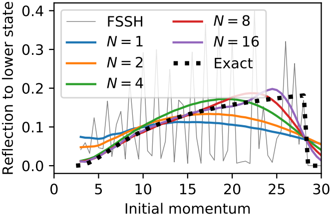

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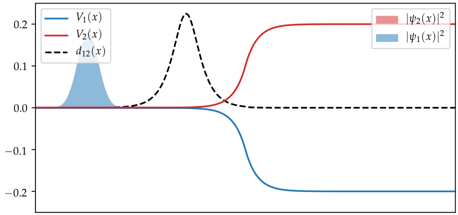

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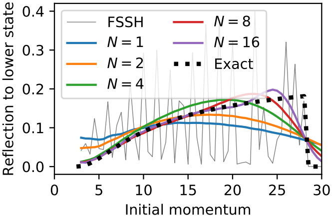

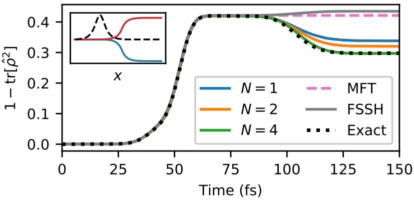

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Conclusions

- Quantum effects (branching, entanglement) using classical mechanics
- Opens up for a new class of nonadiabatic methods

Acknowledgements

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