# Semiclassical approach for interacting fermionic systems: interference and echos in the Hubbard model

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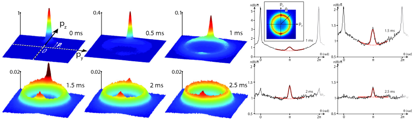
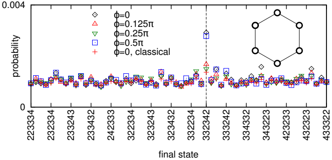
March 18, 2015

- Coherent backscattering




[cf. F. Jendrzejewski, K. Müller, J. Richard, A. Date, T. Plisson, P. Bouyer, A. Aspect and V. Josse, PRL **109** 195302 (2012)]




[TE, J. Dujardin, A. Argüelles, P. Schlagheck, K. Richter and J. D. Urbina, PRL **112** 140403 (2014)]

→ talk by Peter Schlagheck (Fr. 11h)

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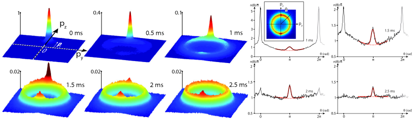

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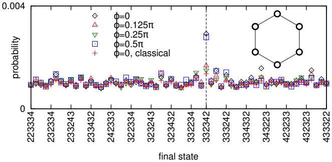


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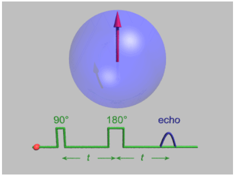
→ talk by Peter Schlagheck (Fr. 11h)

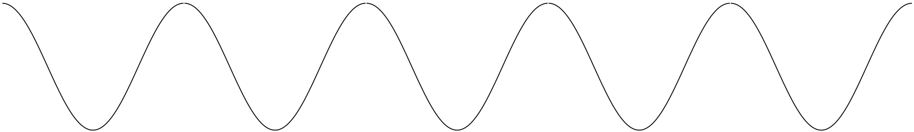
- Echoes:




[cf. http://en.wikipedia.org/wiki/Spin_echo]

?

# Fermionic Hubbard model



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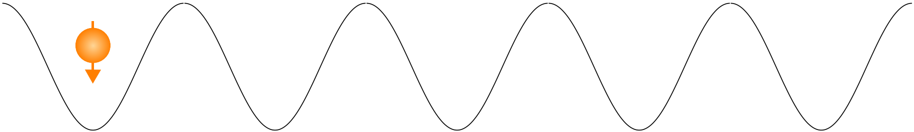
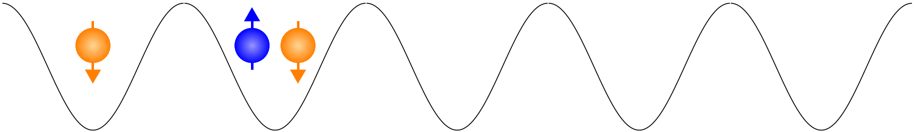


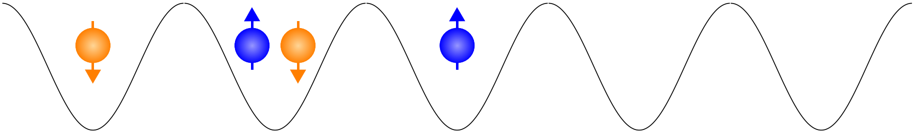
$$|\mathbf{n}\rangle = \quad \hat{c}^{\dagger}_{1\downarrow} |0,0,0,0,0,0,0,0,0,0\rangle$$

# Fermionic Hubbard model



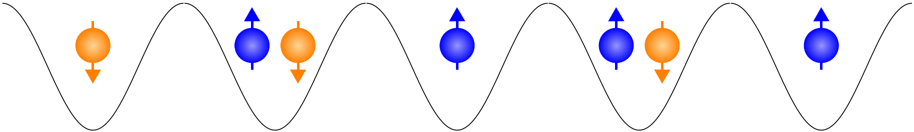
$$|\mathbf{n}\rangle = \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\downarrow}\,|0,1,0,0,0,0,0,0,0,0\rangle$$

# Fermionic Hubbard model



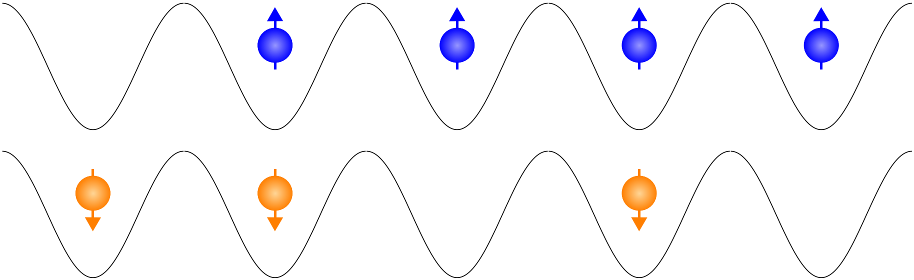
$$|\mathbf{n}\rangle = -\hat{c}^{\dagger}_{3\uparrow}|0,1,1,1,0,0,0,0,0,0\rangle$$

# Fermionic Hubbard model



$$|\mathbf{n}\rangle = \qquad |0, 1, 1, 1, 1, 0, 1, 1, 1, 0\rangle$$

# Fermionic Hubbard model



## Hamiltonian

$$\hat{H} = \sum_j \Big\{ \sum_{\sigma=\uparrow,\downarrow} \Big[ \epsilon_j \hat{c}^\dagger_{j\sigma}\hat{c}_{j\sigma} - J\left(\hat{c}^\dagger_{j\sigma}\hat{c}_{j+1\sigma} + \hat{c}^\dagger_{j+1\sigma}\hat{c}_{j+1\sigma}\right)\Big] + U\hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}\hat{c}_{j\uparrow}$$
$$+ \kappa\left(\hat{c}^\dagger_{j,\downarrow}\hat{c}_{j+1,\uparrow} - \hat{c}^\dagger_{j+1,\downarrow}\hat{c}_{j,\uparrow}\right) + \kappa^*\left(\hat{c}^\dagger_{j+1,\uparrow}\hat{c}_{j,\downarrow} - \hat{c}^\dagger_{j,\uparrow}\hat{c}_{j+1,\downarrow}\right)\Big\}$$

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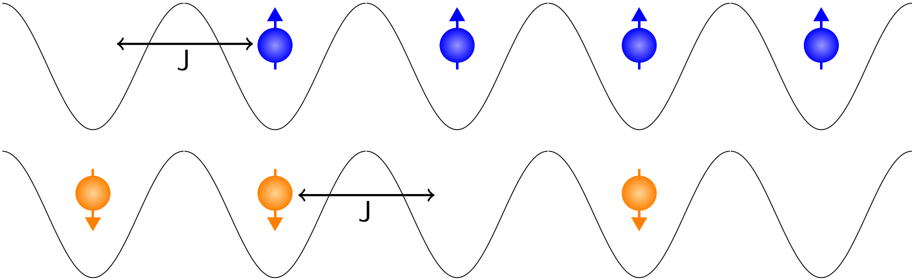


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$$+ \kappa \left( \hat{c}^\dagger_{j,\downarrow} \hat{c}_{j+1,\uparrow} - \hat{c}^\dagger_{j+1,\downarrow} \hat{c}_{j,\uparrow} \right) + \kappa^* \left( \hat{c}^\dagger_{j+1,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}^\dagger_{j,\uparrow} \hat{c}_{j+1,\downarrow} \right) \Bigg\}$$

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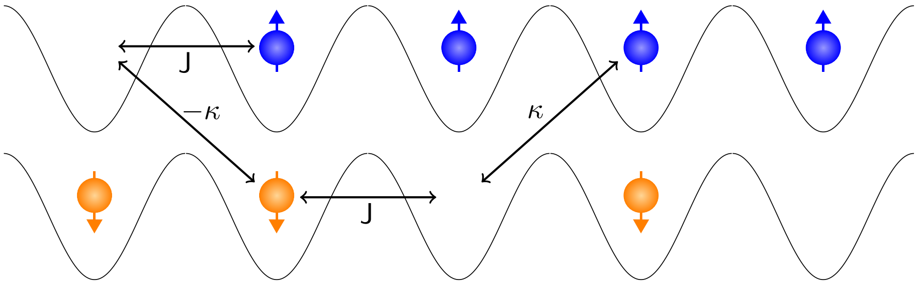


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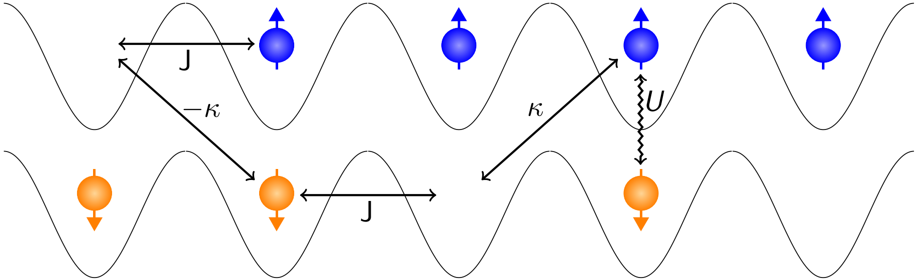


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$$\left. + \kappa \left( \hat{c}^\dagger_{j,\downarrow} \hat{c}_{j+1,\uparrow} - \hat{c}^\dagger_{j+1,\downarrow} \hat{c}_{j,\uparrow} \right) + \kappa^* \left( \hat{c}^\dagger_{j+1,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}^\dagger_{j,\uparrow} \hat{c}_{j+1,\downarrow} \right) \right\}$$

# Semiclassical theory

- Propagator in Fock basis: $K(\mathbf{n}, \mathbf{m}, t) = \left\langle \mathbf{n} \middle| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} \middle| \mathbf{m} \right\rangle$
- Construct Path integral

  $\rightarrow$ talk by Juan Diego Urbina (Fr. 11h30)

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## ⇒ Classical limit:

$$\hat{c}^{\dagger}_{j\sigma}\hat{c}_{j\sigma} \to \left|\phi_{j\sigma}(t)\right|^2,$$

$$\hat{c}^{\dagger}_{j\sigma}\hat{c}_{k\sigma'} \to \phi^{*}_{j\sigma}(t)\phi_{k\sigma'}(t)\mathrm{e}^{-\left|\phi_{j\sigma}(t)\right|^2-\left|\phi_{k\sigma'}(t)\right|^2} \prod_{(l,\sigma'')=(j,\sigma)}^{(k,\sigma')} \left(1-2\left|\phi_{l\sigma''}(t)\right|^2\right)$$

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- Stationary phase analysis $\Rightarrow$ Sum over classical trajectories

# Semiclassical propagator[1]

$$K(\mathbf{m},\mathbf{n},t) = \left\langle \mathbf{m} \left| \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} \right| \mathbf{n} \right\rangle \approx \sum_{\gamma:\mathbf{n}\to\mathbf{m}} \mathcal{A}_\gamma \mathrm{e}^{\frac{\mathrm{i}}{\hbar}R_\gamma + \mathrm{i}\mu_\gamma \frac{\pi}{2}}$$

Classical action: $R_\gamma = \int\limits_0^t \mathrm{d}t' \left[\hbar\boldsymbol{\theta}(t')\,\dot{\mathbf{J}}(t') - H^{(\mathrm{cl})}\left(\boldsymbol{\psi}^*(t'),\boldsymbol{\psi}(t')\right)\right]$

[1]TE, J. D. Urbina and K. Richter, Theor. Chem. Acc. **133**, 1563; arXiv:1409.4196

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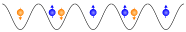
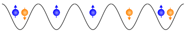
Classical trajectory $\gamma:\mathbf{n}\to\mathbf{m}$:



$$\left|\psi_{j\sigma}(0)\right|^2=n_{j\sigma}$$



$$\left|\psi_{j\sigma}(t)\right|^2=m_{j\sigma}$$

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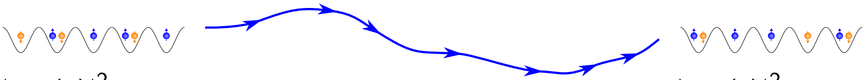

$\left|\psi_{j\sigma}(0)\right|^2 = n_{j\sigma}$ $\qquad$ $\left|\psi_{j\sigma}(t)\right|^2 = m_{j\sigma}$

$$\mathrm{i}\hbar\dot{\boldsymbol{\psi}} = \frac{\partial H^{(\mathrm{cl})}}{\partial \boldsymbol{\psi}^*}$$

Classical action: $R_\gamma = \int_0^t \mathrm{d}t' \left[\hbar\boldsymbol{\theta}\left(t'\right)\dot{\mathbf{J}}\left(t'\right) - H^{(\mathrm{cl})}\left(\boldsymbol{\psi}^*\left(t'\right), \boldsymbol{\psi}\left(t'\right)\right)\right]$

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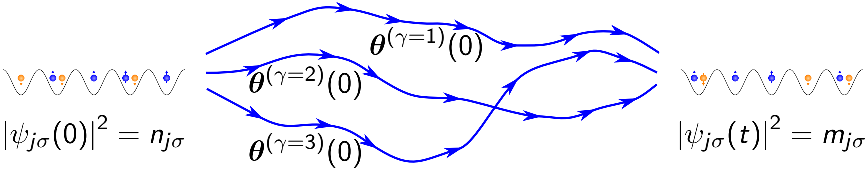


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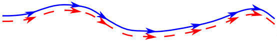
# Transition probability

$$P(\mathbf{n},\mathbf{m},t) = |K(\mathbf{n},\mathbf{m},t)|^2 = \sum_{\gamma,\gamma':\mathbf{m}\to\mathbf{n}} \mathcal{A}_\gamma \mathcal{A}^*_{\gamma'} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(R_\gamma - R_{\gamma'}) + \mathrm{i}\frac{\pi}{2}(\mu_\gamma - \mu_{\gamma'})}$$

- diagonal approximation $\gamma' = \gamma$:  $=: P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$

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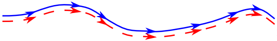
- diagonal approximation $\gamma' = \gamma$:  $=: P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$
- interference between time-reverse paths

$$\gamma' = \mathcal{T}\gamma$$

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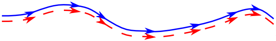
- diagonal approximation $\gamma' = \gamma$:  $=: P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$
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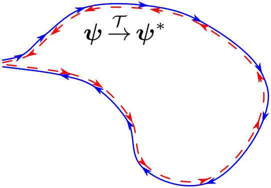
$$\gamma' = \mathcal{T}\gamma$$

$$R_\gamma - R_{\mathcal{T}\gamma} = 0$$

$\mathbf{n} = \mathbf{m}$



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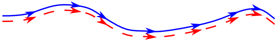
- diagonal approximation $\gamma' = \gamma$:  $=: P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$
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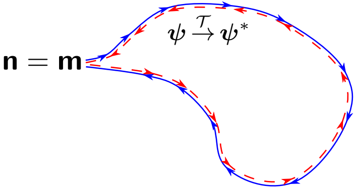
$\delta_{\mathbf{nm}} P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$



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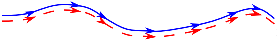
- diagonal approximation $\gamma' = \gamma$:  $=: P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$
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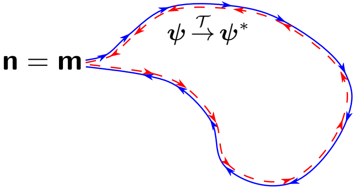


$$R_\gamma - R_{\mathcal{T}\gamma} = \hbar\pi \sum_j (n_{j\uparrow} - m_{j\uparrow})$$

$$\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \xrightarrow{\mathcal{T}} \begin{pmatrix} -\psi_\downarrow \\ \psi_\uparrow \end{pmatrix}^*$$

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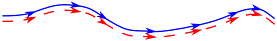
- diagonal approximation $\gamma' = \gamma$:  $=: P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$
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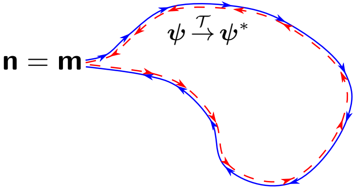
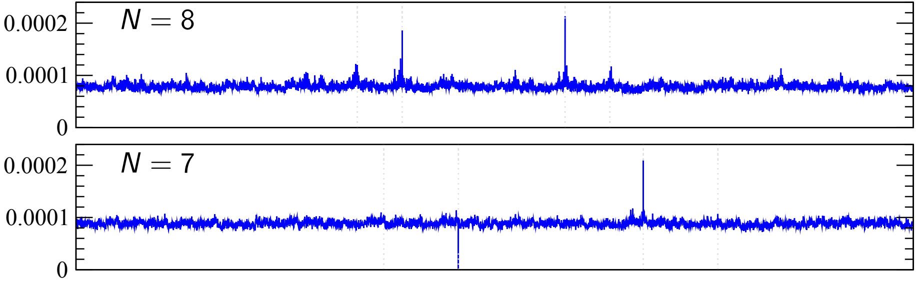


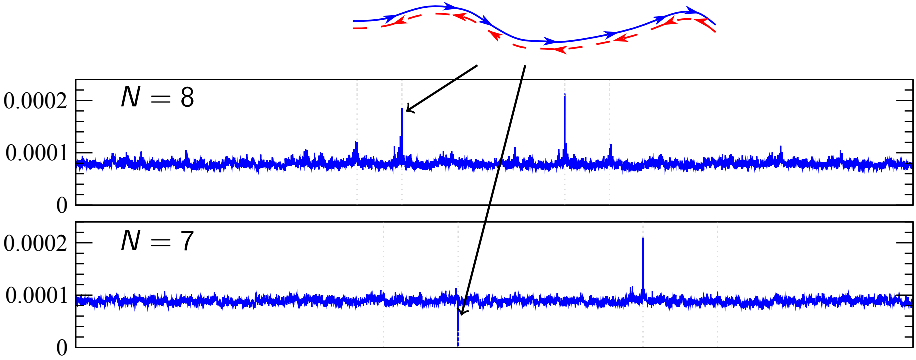

$$(-1)^N \delta_{\mathbf{n}_\uparrow \mathbf{m}_\downarrow} \delta_{\mathbf{n}_\downarrow \mathbf{m}_\uparrow} P_{\mathrm{cl}}(\mathbf{n},\mathbf{m},t)$$

$$\begin{pmatrix} \boldsymbol{\psi}_\uparrow \\ \boldsymbol{\psi}_\downarrow \end{pmatrix} \xrightarrow{\mathcal{T}} \begin{pmatrix} -\boldsymbol{\psi}_\downarrow \\ \boldsymbol{\psi}_\uparrow \end{pmatrix}^*$$

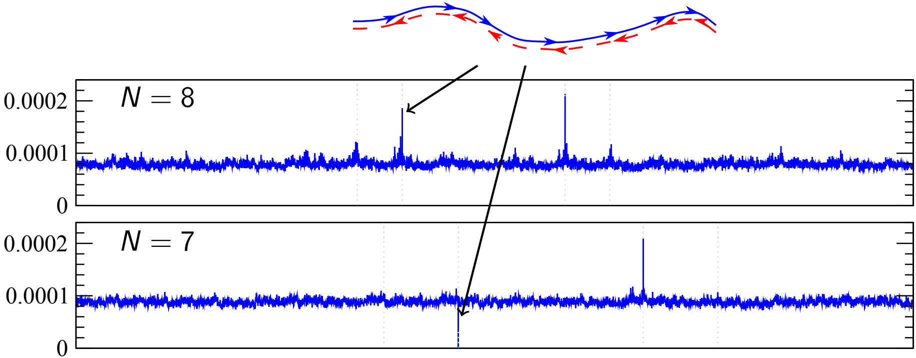
# Transition probability



# Transition probability



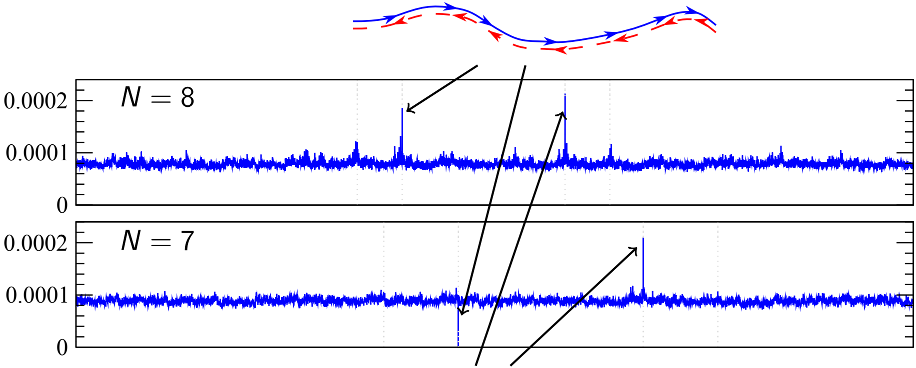
# Transition probability




$$\hat{H} = \sum_j \Bigg\{ \sum_{\sigma=\uparrow,\downarrow} \left[ \epsilon_j \hat{c}^\dagger_{j\sigma} \hat{c}_{j\sigma} - J \left( \hat{c}^\dagger_{j\sigma} \hat{c}_{j+1\sigma} + \hat{c}^\dagger_{j+1\sigma} \hat{c}_{j+1\sigma} \right) \right] + U \hat{c}^\dagger_{j\uparrow} \hat{c}^\dagger_{j\downarrow} \hat{c}_{j\downarrow} \hat{c}_{j\uparrow}$$

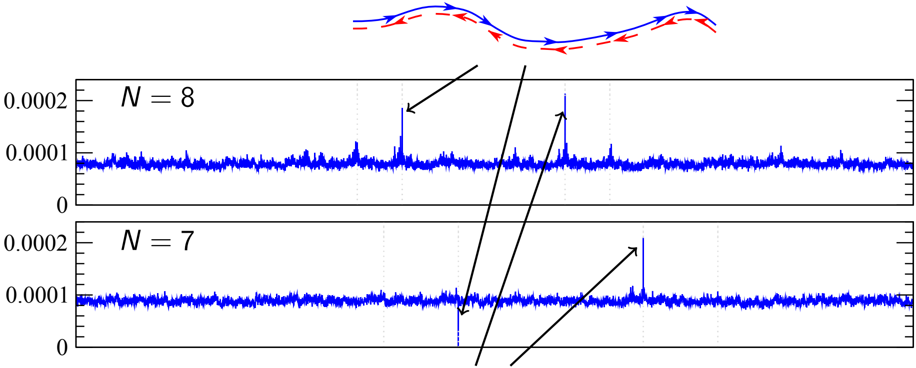
$$+ \kappa \left( \hat{c}^\dagger_{j,\downarrow} \hat{c}_{j+1,\uparrow} - \hat{c}^\dagger_{j+1,\downarrow} \hat{c}_{j,\uparrow} \right) + \kappa^* \left( \hat{c}^\dagger_{j+1,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}^\dagger_{j,\uparrow} \hat{c}_{j+1,\downarrow} \right) \Bigg\}$$

# Transition probability




symmetry under $\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \to \begin{pmatrix} \psi_\downarrow e^{i\arg(\kappa)} \\ \psi_\uparrow e^{-i\arg(\kappa)} \end{pmatrix}$

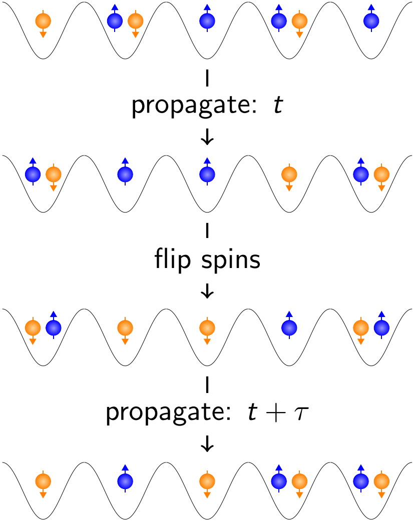
# Transition probability



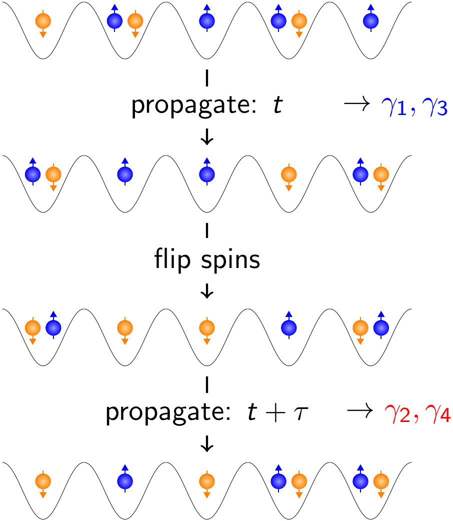

symmetry under $\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \to \begin{pmatrix} \psi_\downarrow e^{i\arg(\kappa)} \\ \psi_\uparrow e^{-i\arg(\kappa)} \end{pmatrix}$

**Every discrete (antiunitary) symmetry gives another peak/dip!**

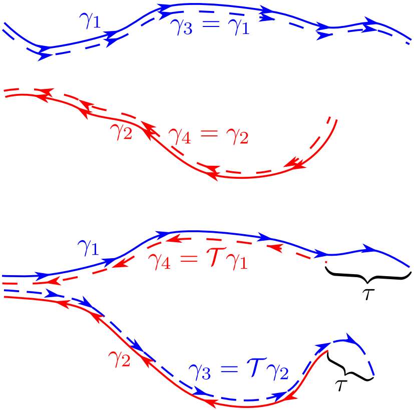
# Many-Body Spin Echo



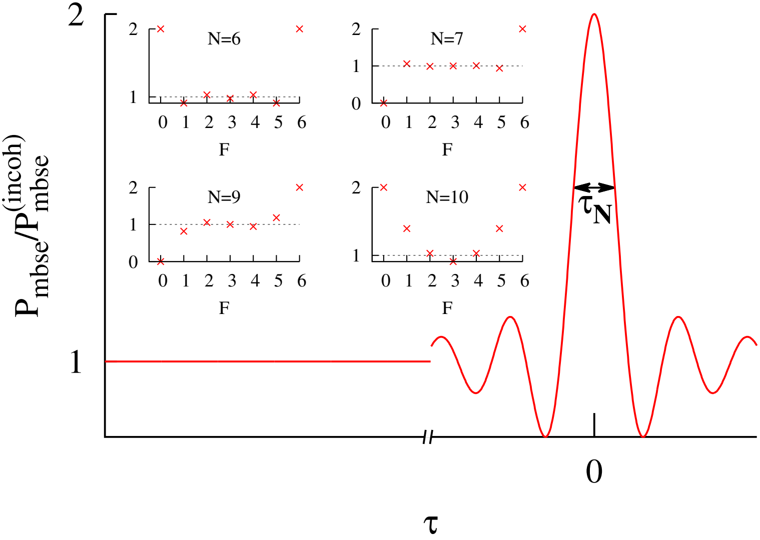
# Many-Body Spin Echo




4 trajectories:



# Many-Body Spin Echo



## Conclusion

[TE, J. D. Urbina and K. Richter, Theor. Chem. Acc. **133**, 1563 (2014); arXiv:1409.4196]

- Semiclassical theory for interacting Fermions in Fock space
- Successful prediction of interference phenomena in transition probability

[TE, J. D. Urbina and K. Richter, arXiv:1409.5684]

- Prediction of Many-Body Spin Echo

## Outlook

- Additional symmetries in Spin Echo
- Trace formula