Propagation of Bound States in Heisenberg XXZ Chains

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1. Model and Methods

- FM Heisenberg model

$$H = J_{xy} \sum_i \Delta S^z_i S^z_{i+1} + \frac{1}{2}(S^+_i S^-_{i+1} + S^-_i S^+_{i+1})$$

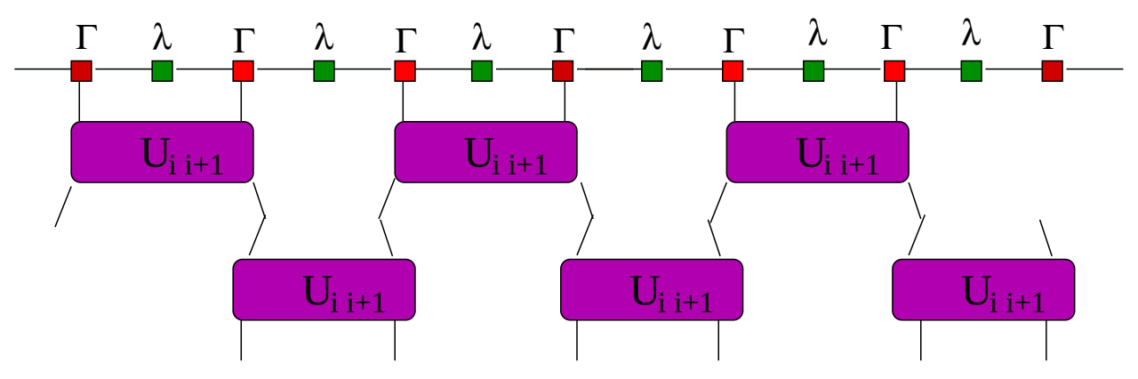
$$\Delta = \frac{J_z}{J_{xy}}, \qquad J_{xy} = -1$$

- Full diagonalization
- Time Evolving Block Decimation (TEBD)[1, 2]

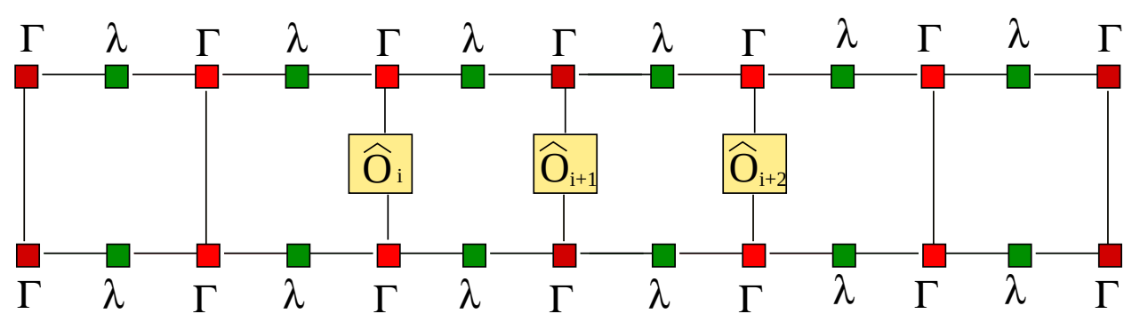
■ Matrix Product State representation of $|\psi\rangle$

■ Suzuki-Trotter expansion: $\hat{U} \approx \prod_{i=even} \hat{U}_{i,i+1} \prod_{i=odd} \hat{U}_{i,i+1}$

■ Time evolution

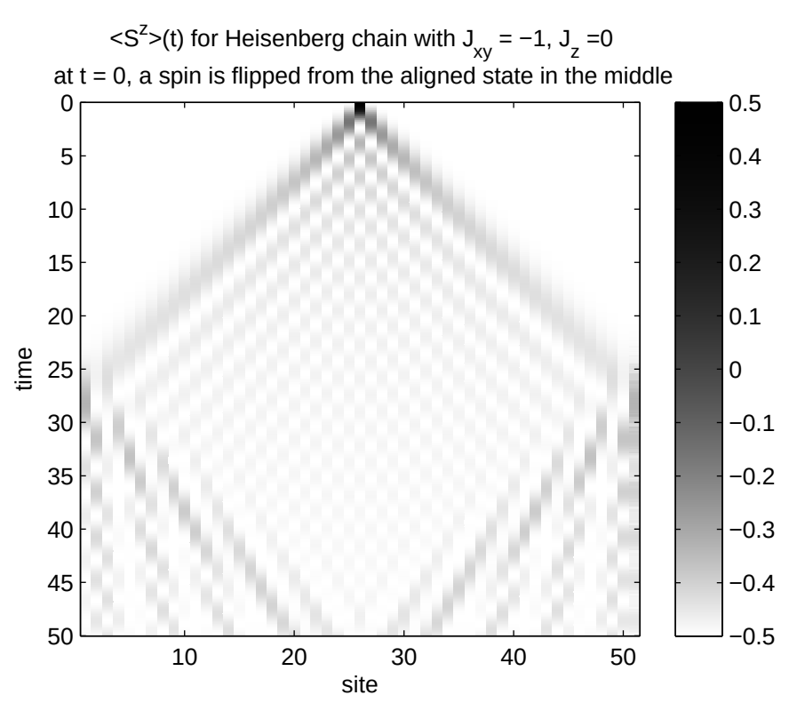


■ Observables and Correlators

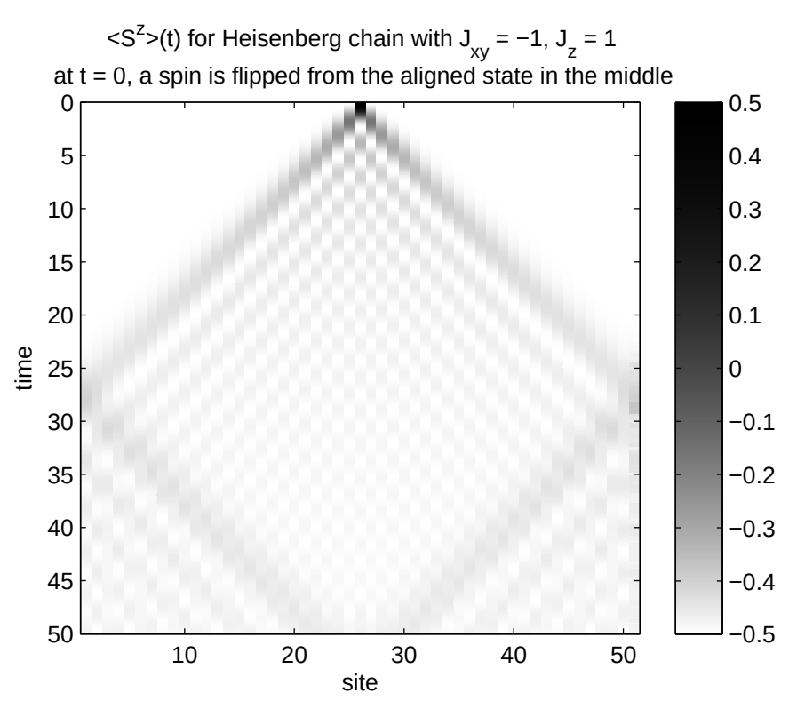


2. Evolution of excitations from FM ground state

Time evolution of single-spin excitation from ferromagnetic state ↓↓↓↓↓↓↓↓↓↑↓↓↓↓↓↓↓↓

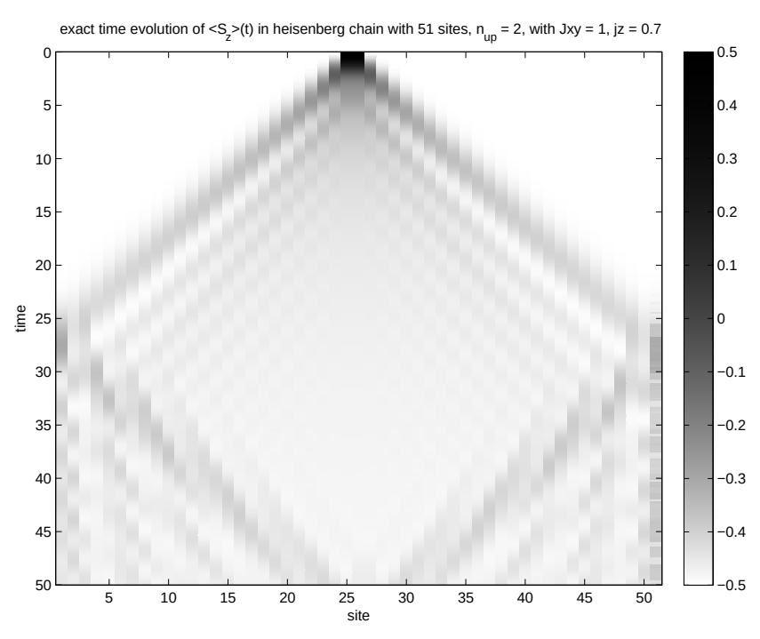


$\langle S^z\rangle$(t), $J_z = 0$

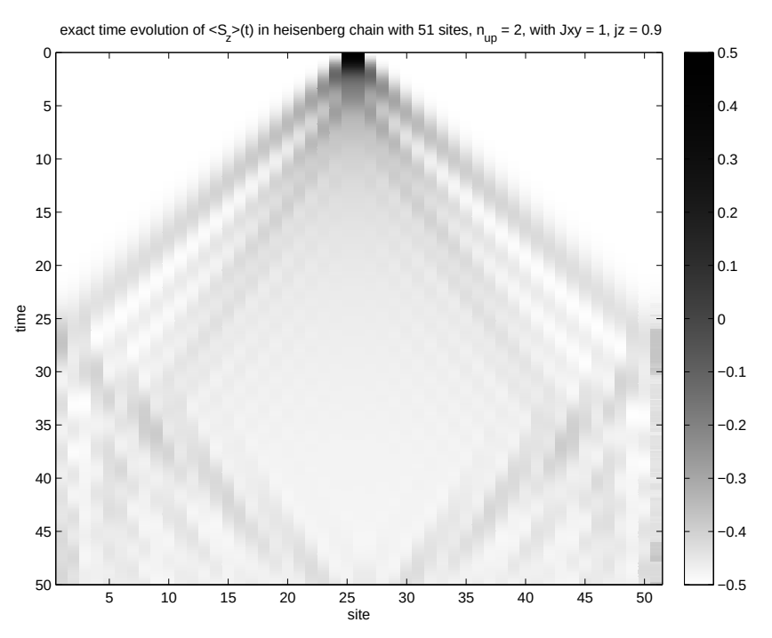


$\langle S^z\rangle$(t), $J_z = 1$

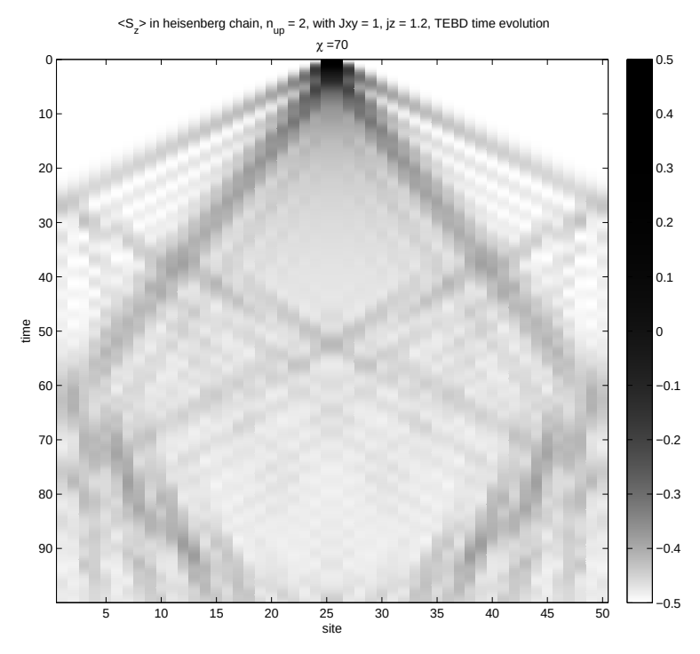
Time evolution of two-spin excitation from ferromagnetic state ↓↓↓↓↓↓↓↓↑↑↓↓↓↓↓↓↓↓



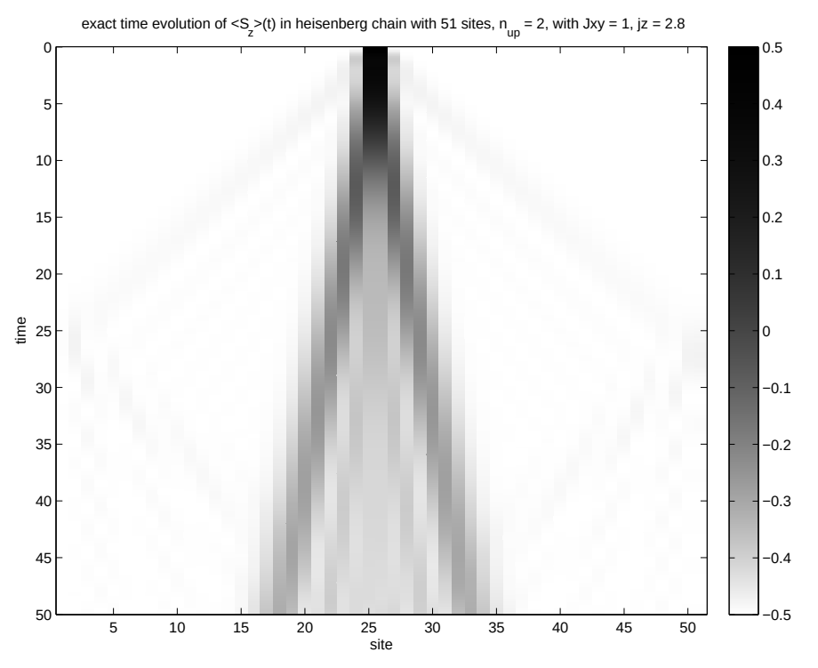
$\langle S^z\rangle$(t), J_z = 0.7



$\langle S^z\rangle$(t), J_z = 0.9

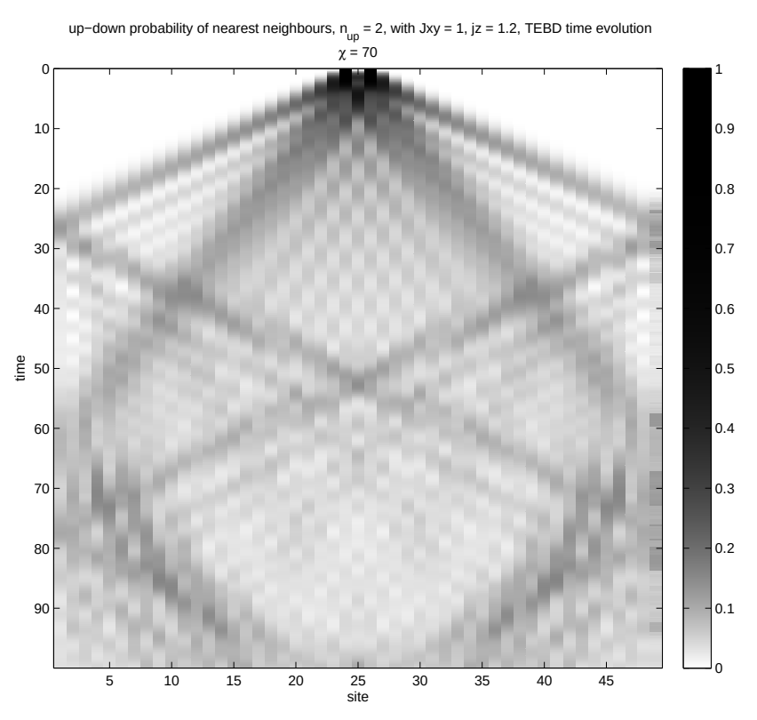


$\langle S^z\rangle$(t), J_z = 1.0

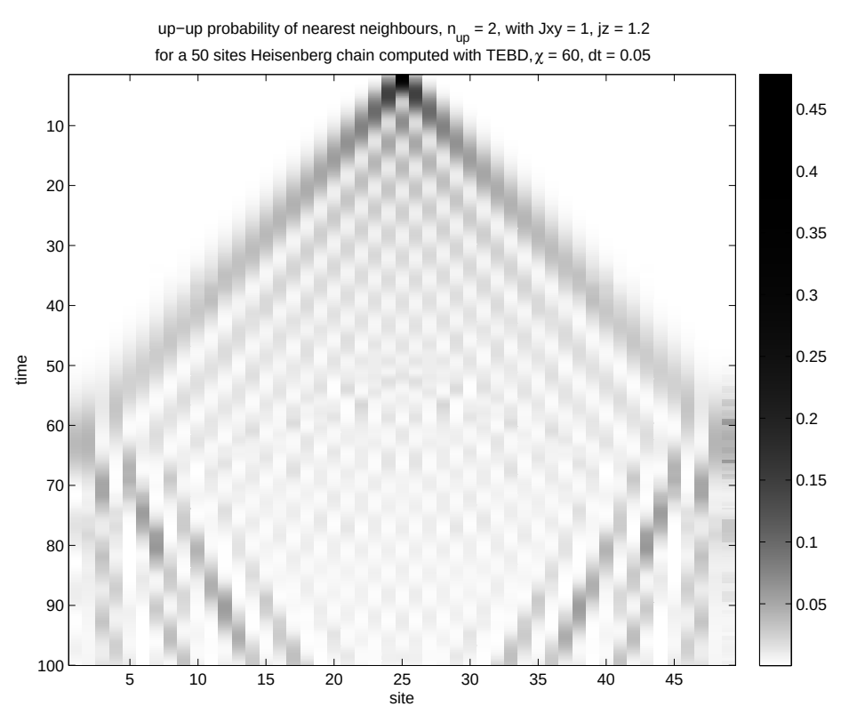


$\langle S^z\rangle$(t), J_z = 2.8

Nearest-neighbor correlations



$\mathcal{P}(|\uparrow\downarrow\rangle \text{ or } |\downarrow\uparrow\rangle)$, $J_z = 1.2$



$\mathcal{P}(|\uparrow\uparrow\rangle)$, $J_z = 1.2$

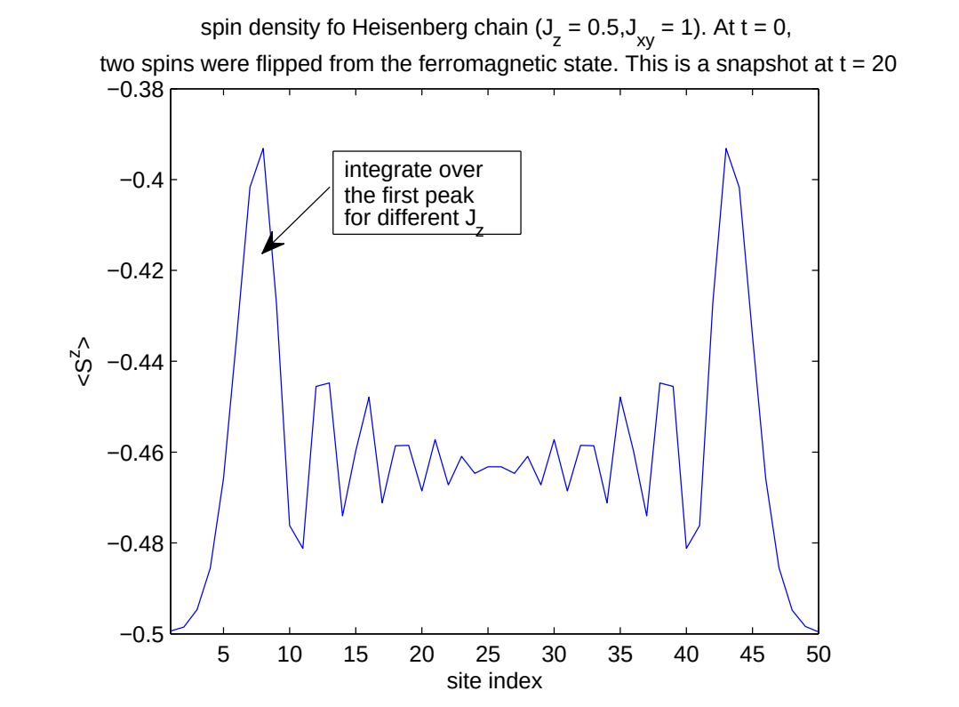
■ Two distinct propagation branches: single and two particle branches at different velocities

■ Velocity of upper branch independent of J_z

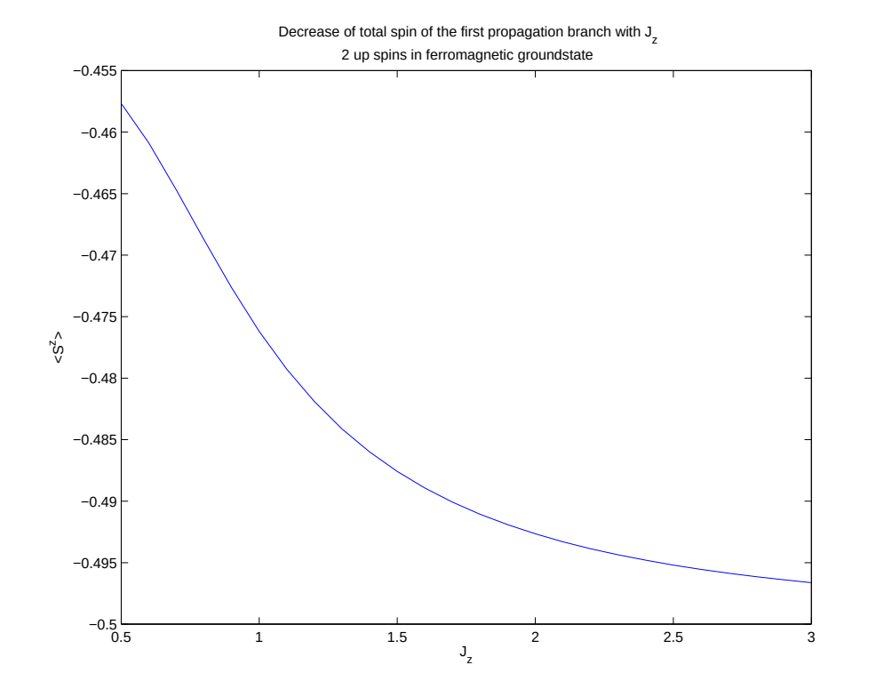
■ Velocity of lower branch decreases with increasing J_z

■ At large J_z bound states dominate

Integrated spin density of upper branch

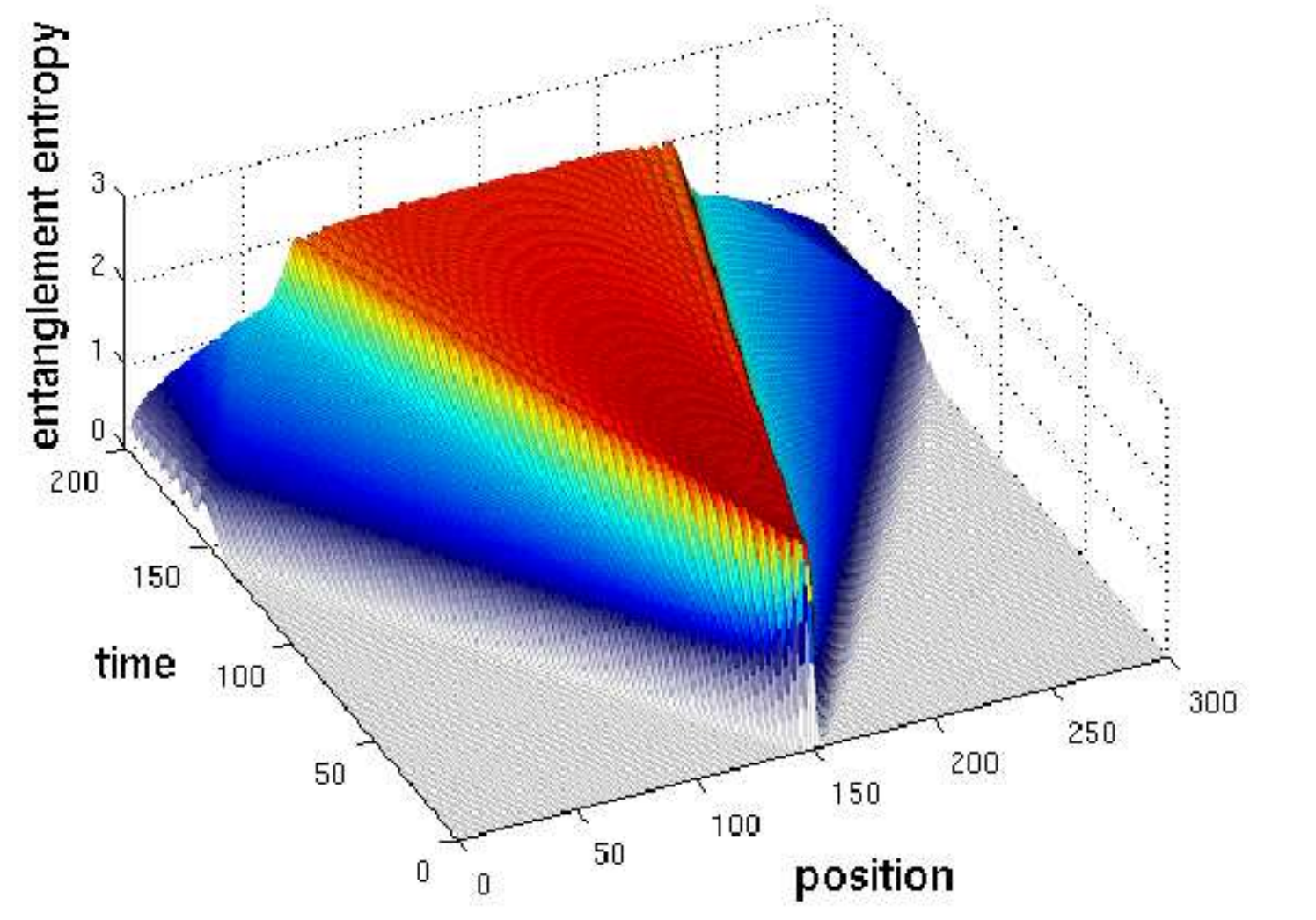


Spin density of the chain at t = 20 after two-spin excitation at t = 0



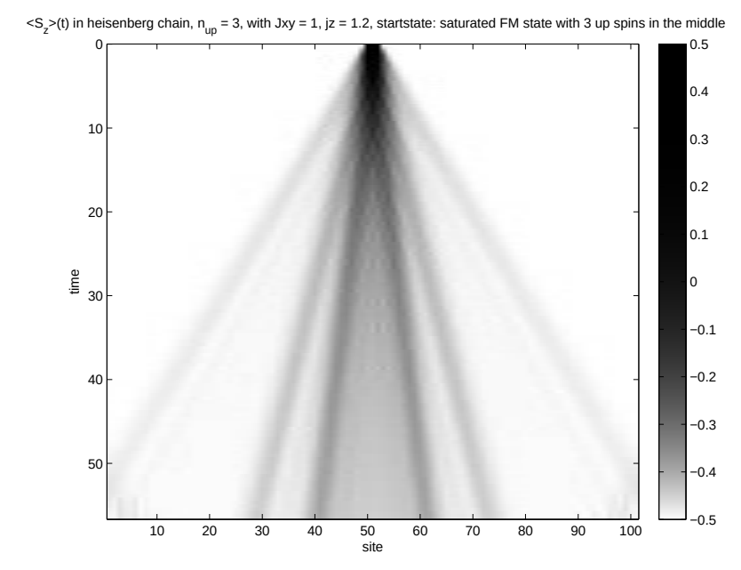
Integrated spin density of the fast propagation branch as a function of J_z

Entanglement ($J_z = 1.2$)

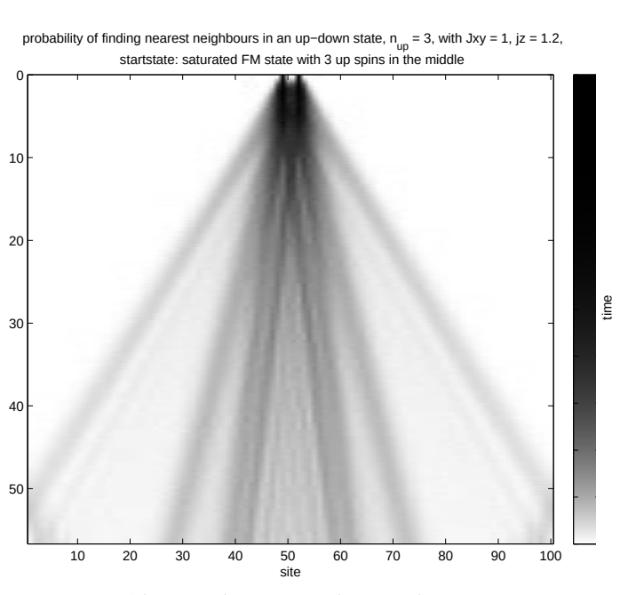


Time evolution of the entanglement entropy. Two-spin excitation, $J_z = 1.2$.

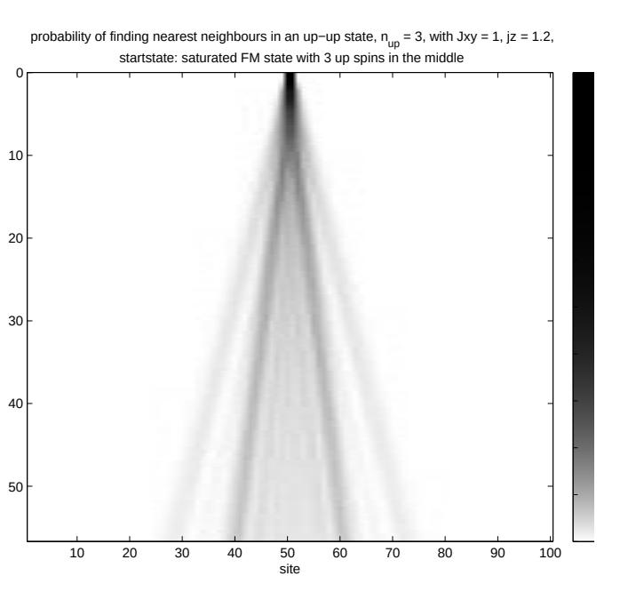
Time evolution of three-spin excitation from ferromagnetic state ↓↓↓↓↓↓↓↑↑↑↓↓↓↓↓↓↓↓



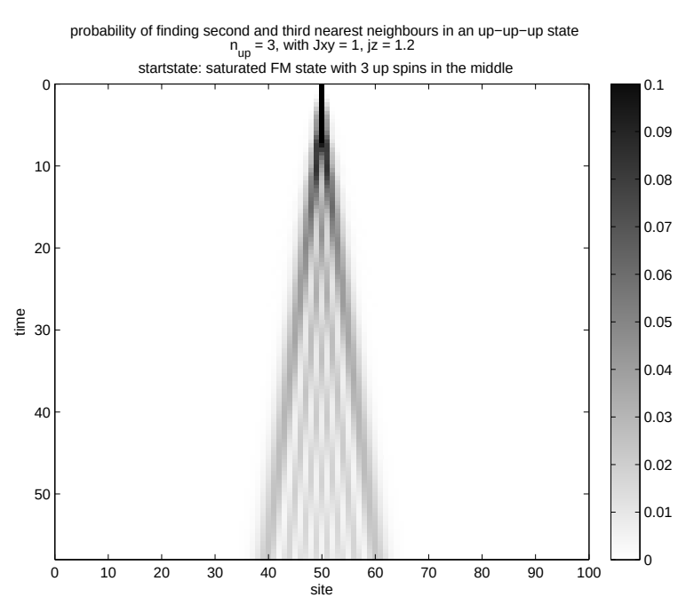
$\langle S^z\rangle$(t), $J_z = 1.2$



$\mathcal{P}(|\uparrow\downarrow\rangle \text{ or } |\downarrow\uparrow\rangle)$, $J_z = 1.2$



$\mathcal{P}(|\uparrow\uparrow\rangle)$, $J_z = 1.2$



$\mathcal{P}(|\uparrow\uparrow\uparrow\rangle)$, $J_z = 1.2$

■ Three propagation branches: single, two and three particle branches at different velocities

3. Analytical considerations

Bethe ansatz for FM excitations

■ General wave function ansatz

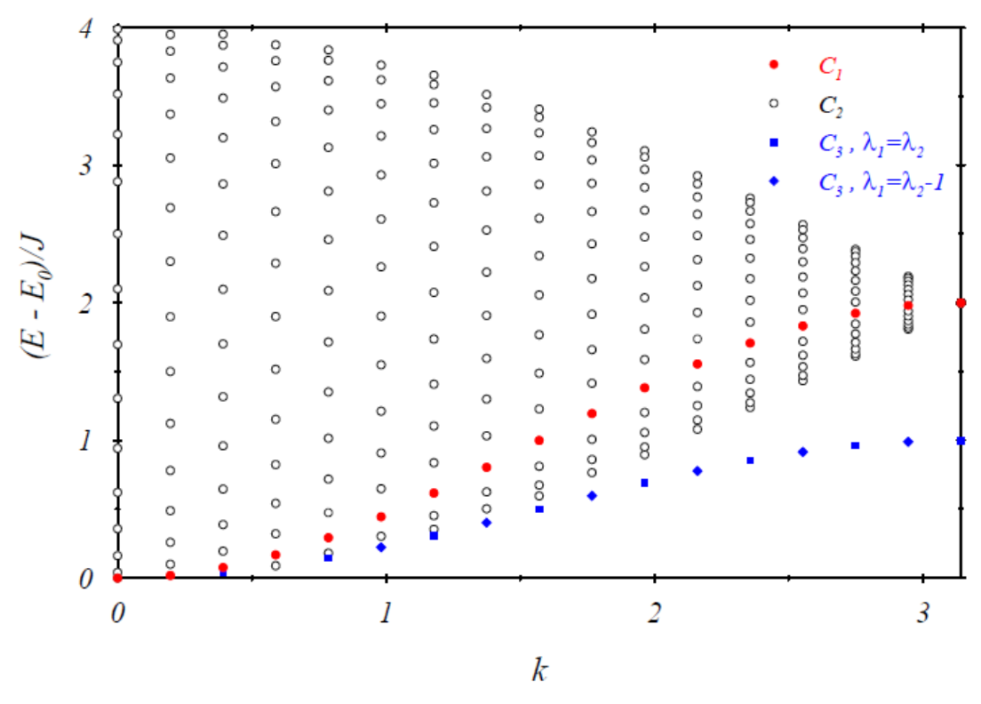
$$\psi(x_1, \dots, x_M) = \sum_{\mathcal{P}} A(\mathcal{P}) \prod_{j=1}^{M} e^{x_j k_{\mathcal{P}j}}$$

■ Single spin flip excitations: one-magnon states

$$E(k) = (\cos(k) - \Delta)$$

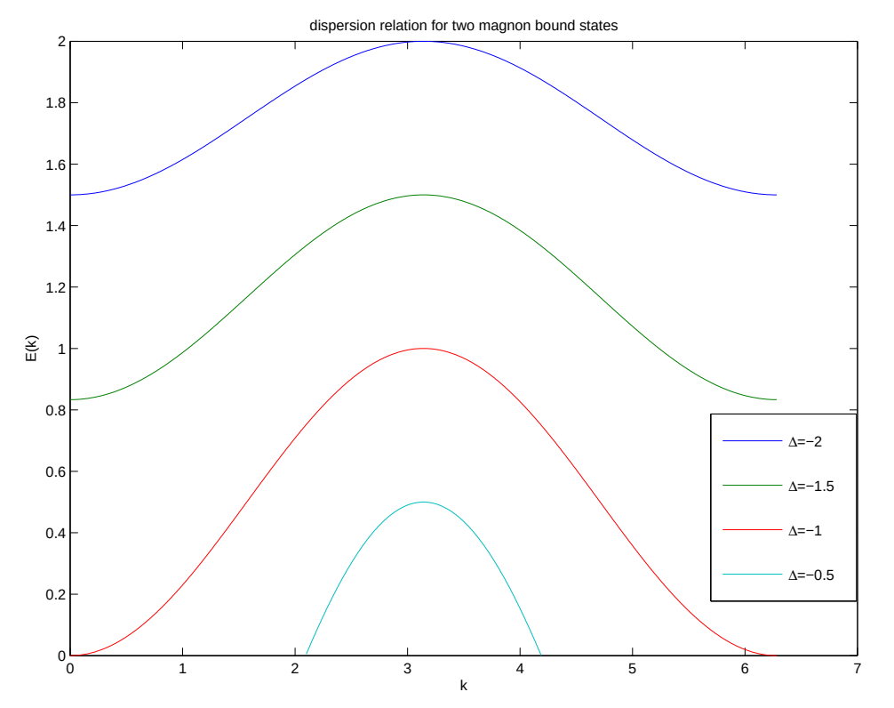
■ Two spin flip excitations: two-magnon states

■ Two spin excitation spectrum of isotropic Heisenberg chain with pbc, 36 sites [3] → two-magnon scattering states (C_1 and C_2) → two-magnon bound states (C_3)→ 2-strings



■ Dispersion relation of two-magnon bound states[4, 5]: For $\Delta < 1$: not all values of k are allowed

$$E(k) = -J_{xy}\left(\Delta - \frac{1}{2\Delta} - \frac{1}{2\Delta}\cos(k)\right)$$



References

[1] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003); 93, 040502 (2004).

[2] A.J. Daley et al., J. Stat. Mech. 2004, P04005 (2004).

[3] M. Karbach and G. Müller, Computers in Physics 11, 36 (1997), cond-mat/9809162 (1998).

[4] B. Sutherland, *Beautiful Models* (World Scientific, 2004).

[5] R. G. Pereira, S. R. White, and I. Affleck, Phys. Rev. B 79, 165113 (2009).

■ Dispersion relation for M-string excitations [4]

$$E(k) = -\frac{\sin\mu}{\sin(M\mu)}(\cos(M\mu) - (-1)^M \cos(k)), \quad \text{where} \quad \Delta \equiv -\cos(\mu)$$

Speed of propagation

■ Group velocity $v(k) = \frac{dE}{dk}$ and DOS $\rho(v) = \int \delta(v - \frac{dE}{dk})dk$

- ■ Single-magnon states

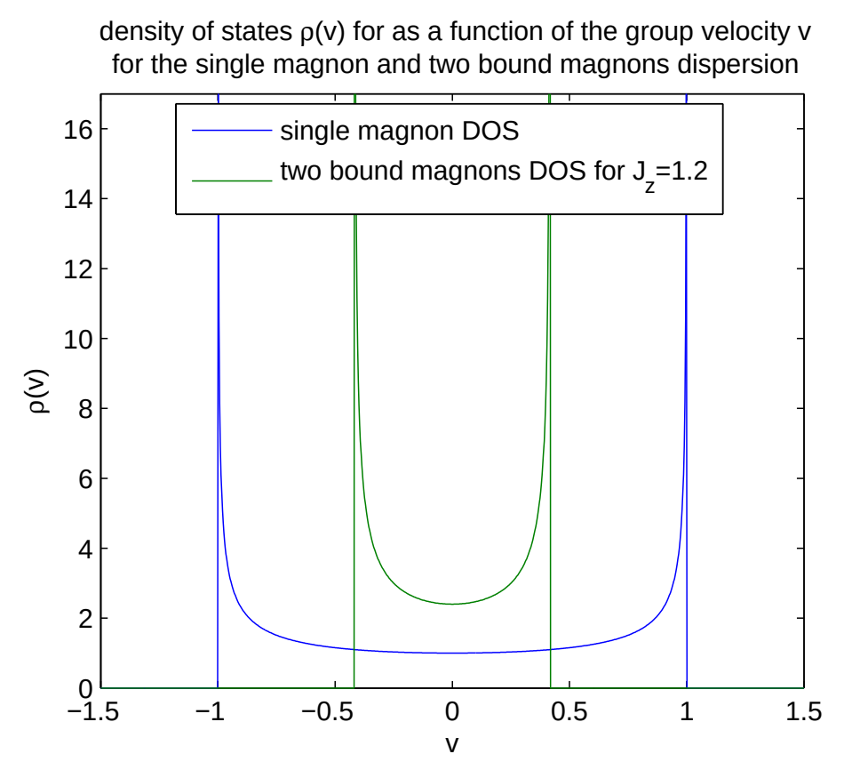
  DOS: singularities at $v = \pm 1$

$$v(k) = -\sin(k)$$
$$\rho(v) = \frac{N}{2\pi}\frac{1}{\sqrt{1-v^2}}$$

- ■ Two-magnon bound states

  DOS: for $|\Delta| < 1/\sqrt{2}$: singularities at $v = \pm\frac{1}{2\Delta}$

$$v(k) = -\frac{1}{2J_z}\sin(k)$$
$$\rho(v) = \frac{2\Delta}{\sqrt{1-(2\Delta v)^2}}$$

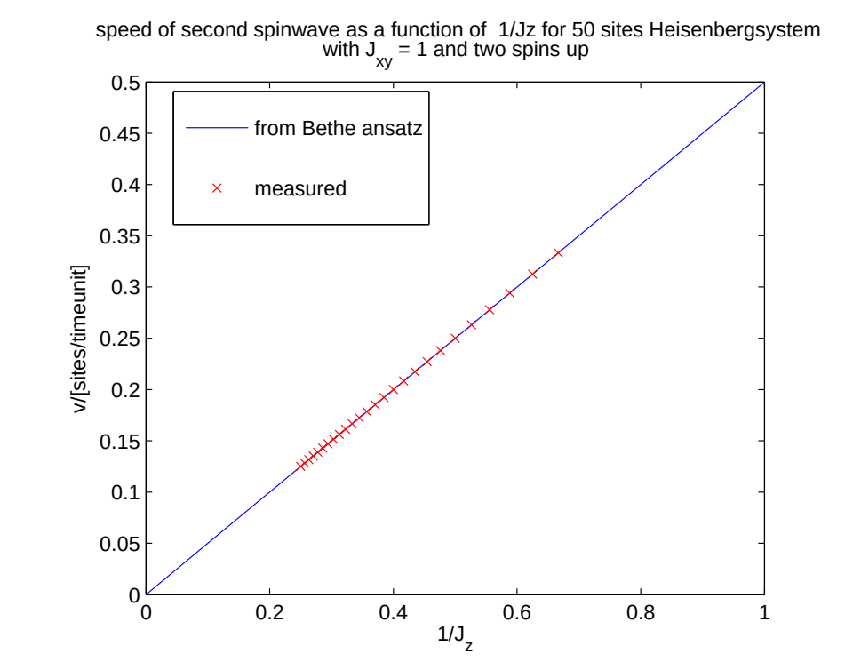


- ■ Three-magnon bound states

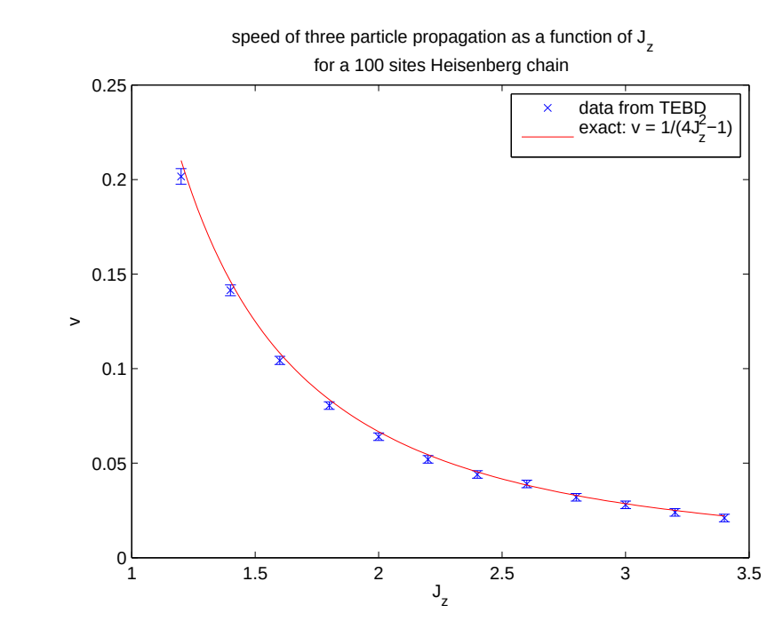
  DOS: singularities at $v = \pm\frac{1}{4J_z^2-1}$

$$v(k) = -\frac{\sin(\mu)}{\sin(3\mu)}\sin(k)$$
$$\rho(v) = \frac{\sin(\mu)}{\sin(3\mu)}\frac{1}{\sqrt{1-(\frac{\sin(3\mu)}{\sin(\mu)}v)^2}}$$

Bound state velocities vs. numerica results



Velocity of $|\uparrow\uparrow\rangle$ branch as a function of J_z, evaluated by measuring the time when the corresponding maximum arrives at the boundary of the system.



Velocity of $|\uparrow\uparrow\uparrow\rangle$ branch as a function of J_z, evaluated by measuring the time when the corresponding maximum arrives at the boundary of the system.

Identical behavior for AF and FM

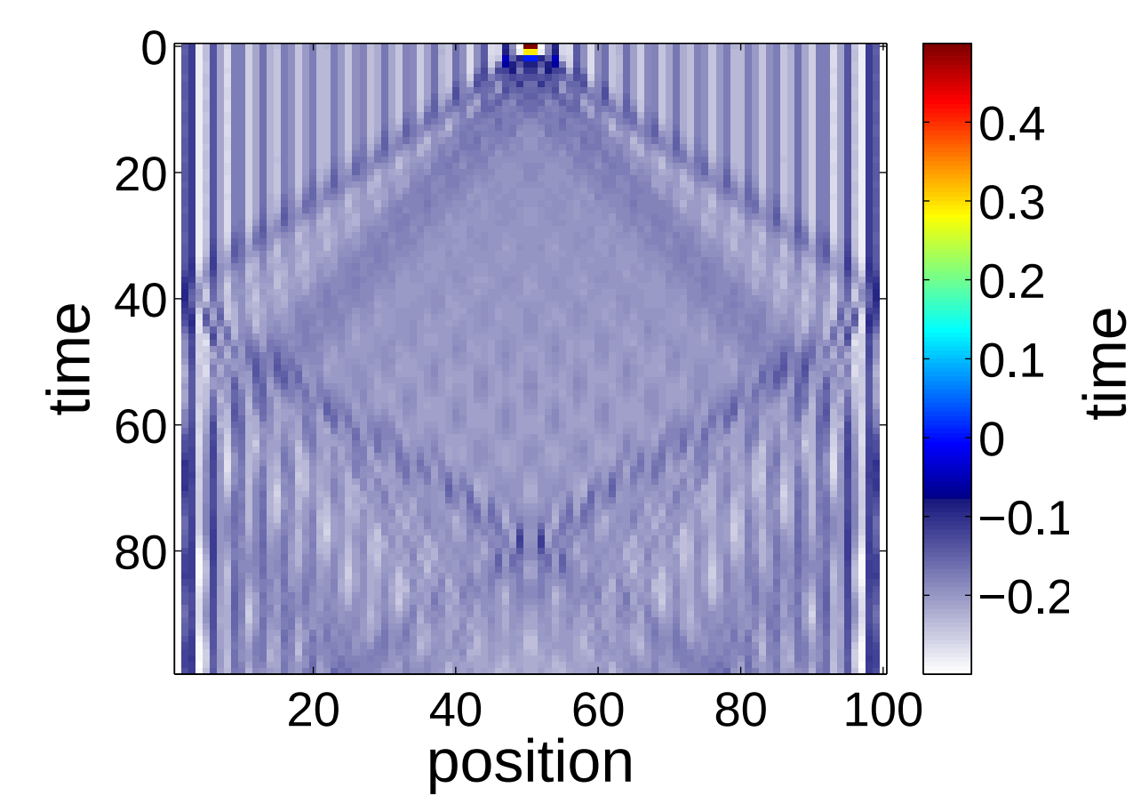
■ Same time evolution for AF and FM when starting from *same initial state* with real coefficients
- $H(\Delta) \rightarrow -H(-\Delta)$ by bipartite rotation
- H and $-H$ have same time evolution

$$\langle O(t)\rangle = \langle O(t)\rangle^* = \langle\psi|e^{iHt}Oe^{-iHt}|\psi\rangle^* = \langle\psi|e^{-iHt}Oe^{iHt}|\psi\rangle = \langle O(-t)\rangle$$

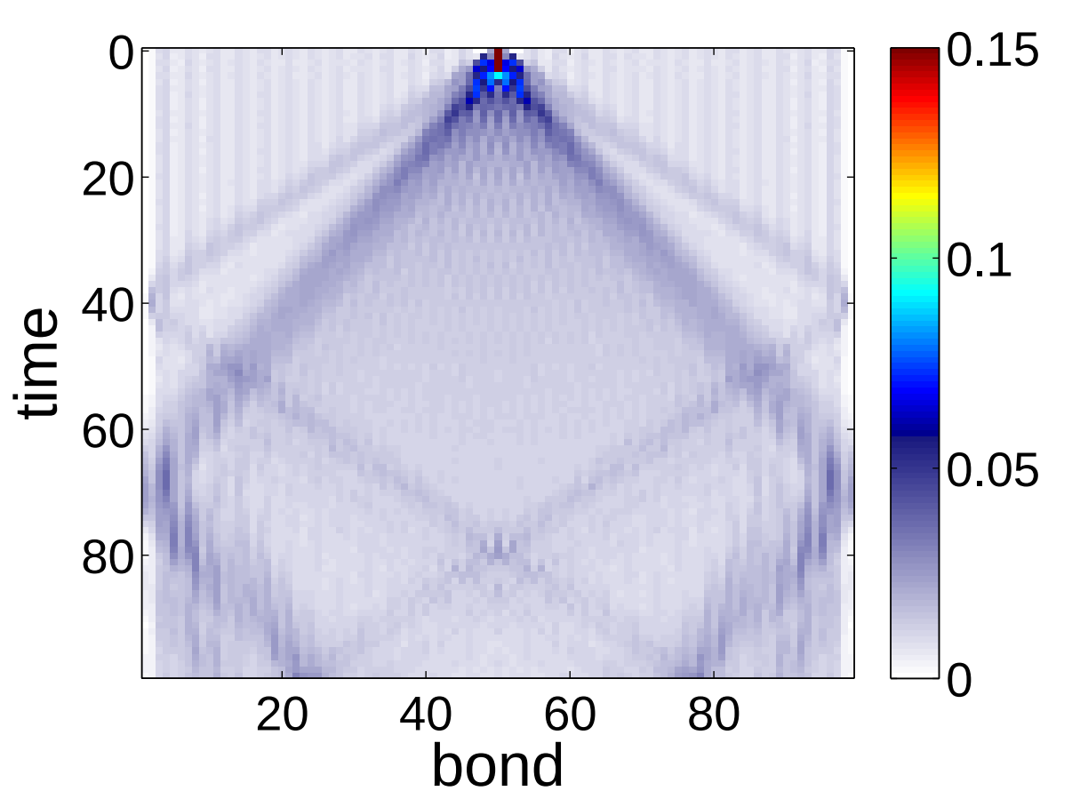
■ For $J_z > 0$: *Repulsively bound states*

4. Evolution of excitations from AF ground state at finite densities

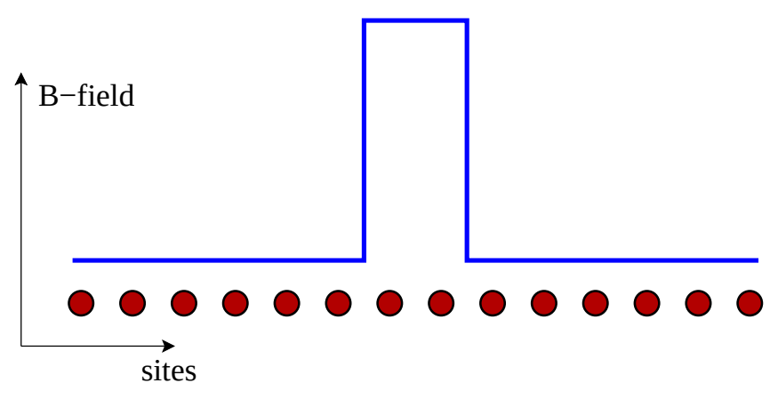
$\langle S^z\rangle$(t), J_z = 1.2



$\mathcal{P}(\uparrow\uparrow)$(t), J_z = 1.2



■ Initial state: AF ground state at filling factor $n = 0.3$ with rectangular magnetic field at two sites



■ Anti bound states stable at finite densities $n < 0.5$.

■ No distinct anti bound states seen for $n \geq 0.5$.

■ Decrease of speed of propagation with increasing n

5. Conclusions

■ Strings of M flipped spins in FM background form bound states, for both AF and FM coupling

■ Linearly propagating branches of 1,2,...M bound spins for $|\Delta|$ beyond threshold

■ Bound states dominate at large J_z

■ Velocity of the lowest propagation branch:
- Two-spin bound states: $v = 1/(2J_z)$
- Three-spin bound states: $v = 1/(4J_z^2 - 1)$

■ Bound two-spin states in AF are also stable at finite densities $n < 0.5$, speed of propagation of the two spin excitations decreases with increasing n