

Real-time broadening of nonequilibrium density profiles and the role of the specific initial-state realization

R. Steinigeweg¹, F. Jin², D. Schmidtke¹, H. De Raedt³, K. Michielsen^{2,4}, J. Gemmer¹

¹ Department of Physics, University of Osnabrück, D-49069 Osnabrück, Germany

² Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany

³ Zernike Institute for Advanced Materials, University of Groningen, NL-9747AG Groningen, The Netherlands

⁴ RWTH Aachen University, D-52056 Aachen, Germany

Introduction

In strictly isolated systems, any coupling to heat baths or particle reservoirs and any driving by external forces is absent. In such systems, the only possibility to induce a nonequilibrium process is the preparation of a proper initial state. We investigate the spin transport of the anisotropic XXZ spin-1/2 chain starting from a class of pure initial states. These initial states feature identical density profiles, where a maximum δ peak is located in the middle of the chain and lies on top of a homogeneous background, but lead to totally different dynamics to the chain.

Model and observables

The Hamiltonian of the XXZ spin-1/2 chain with periodic boundary conditions reads

$$H = -J \sum_{r=1}^L S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z,$$

where $S_r^{x,y,z}$ are spin-1/2 operators at site r , L is the number of the sites, $J < 0$ is the antiferromagnetic exchange coupling constant, and Δ is the anisotropy. We are interested in the nonequilibrium dynamics of the local occupation numbers $n_r = S_r^z + 1/2$. Specifically, we consider the expectation values

$$p_r(t) = \text{Tr} n_r \rho(t),$$

for the density matrix $\rho(t)$ at time t . The spatial variance can be defined by

$$\sigma(t)^2 = \sum_{r=1}^L r^2 \delta p_r(t) - \left[\sum_{r=1}^L r \delta p_r(t) \right]^2,$$

where $\delta p_r(t) = 2[p_r(t) - p_{eq}]$ and $\sum_{r=1}^L \delta p_r(t) = 1$.

Initial states

Let $|\varphi_k\rangle$ be the common eigenbasis of all n_r , i.e., the Ising basis, the initial state reads

$$|\psi(0)\rangle \propto n_L |\Phi\rangle, \quad |\Phi\rangle = \sum_{k=1}^{2^L} c_k |\varphi_k\rangle,$$

where c_k are complex coefficients and $n_L/2$ projects onto Ising states with a particle in the middle of the chain. By construction, $p_L(0) = 1$ is maximum.

Two special classes of states are prepared according to the choices of the coefficients:

1) c_k are the same;

2) c_k are drawn at random according to the unitary invariant Haar measure.

The first class of states is a product state and the second is the so-called typical state.

These two classes of states share the same density profiles, namely $p_{r \neq L/2} = p_{eq} = 1/2$ and $p_{L/2} = 1$.

For the second class of initial states, we find the **exact** relation

$$p_r(t) - p_{eq} = 2 \langle (n_{L/2} - p_{eq})(n_r(t) - p_{eq}) \rangle,$$

where $\langle \cdot \rangle = \text{Tr}[\cdot]/2^L$. Furthermore, the spatial variance satisfies the following equation

$$\frac{d}{dt} \sigma(t)^2 = 2D(t), \quad D(t) = \frac{4}{L} \int_0^t dt' \langle j(t')j \rangle,$$

where $j = \sum_{r=1}^L S_r^x S_{r+1}^y - S_r^y S_{r+1}^x$ is the spin current. Therefore the nonequilibrium dynamics for the typical state (class 2) is directly connected to the Kubo formula.

Numerical method and results

The time evolution of a pure state $|\psi(t)\rangle$ can be calculated by the method of full exact diagonalization. But this method is restricted to $L \sim 20$ sites, even if symmetries such as translation invariance of the Hamiltonian are taken into account. Thus, we proceed differently and rely on a forward propagation of $|\psi(t)\rangle$ in real time. Such a propagation can be done by the use of fourth-order Runge-Kutta [1] or more sophisticated schemes such as Trotter decompositions [2] or Chebyshev polynomials [3]. Here we use a massively parallelized implementation of a Chebyshev polynomial algorithm. In this way, we can treat system sizes as large as $L = 36$.

The numerical results for the density profile $p_r(t)$ are shown in Fig. 1 for two different classes of initial states. The results for the typical initial state (class 2) clearly shows that the initial δ peak monotonously broadens as a function of time and the nonequilibrium density profiles have the irreversible tendency to equilibrate. For $\Delta = 0.5$, it is clear that the width of the density profile increases linearly as a function of time, which indicates a ballistic dynamics. For $\Delta = 1.5$, Fig. 2 clearly shows a Gaussian expansion of the density profile with the width $\sigma(t) \propto \sqrt{t}$, which indicates a clean dynamics for diffusion. For $\Delta = 1.0$, Fig. 3 points to a dynamics of superdiffusion.

The nonequilibrium dynamics for the product state (class 1) is completely different from the case with the typical state, as shown in Fig. 1.

Conclusions

We have investigated the real-time broadening of nonequilibrium density profiles in the XXZ spin-1/2 chain. We have shown for a subclass with internal randomness that the resulting nonequilibrium dynamics clearly demonstrates the existence of diffusion for large exchange anisotropies. Entirely different behavior emerges for the initial states without any randomness involved. More results and discussions can be found in Ref. [4,5].

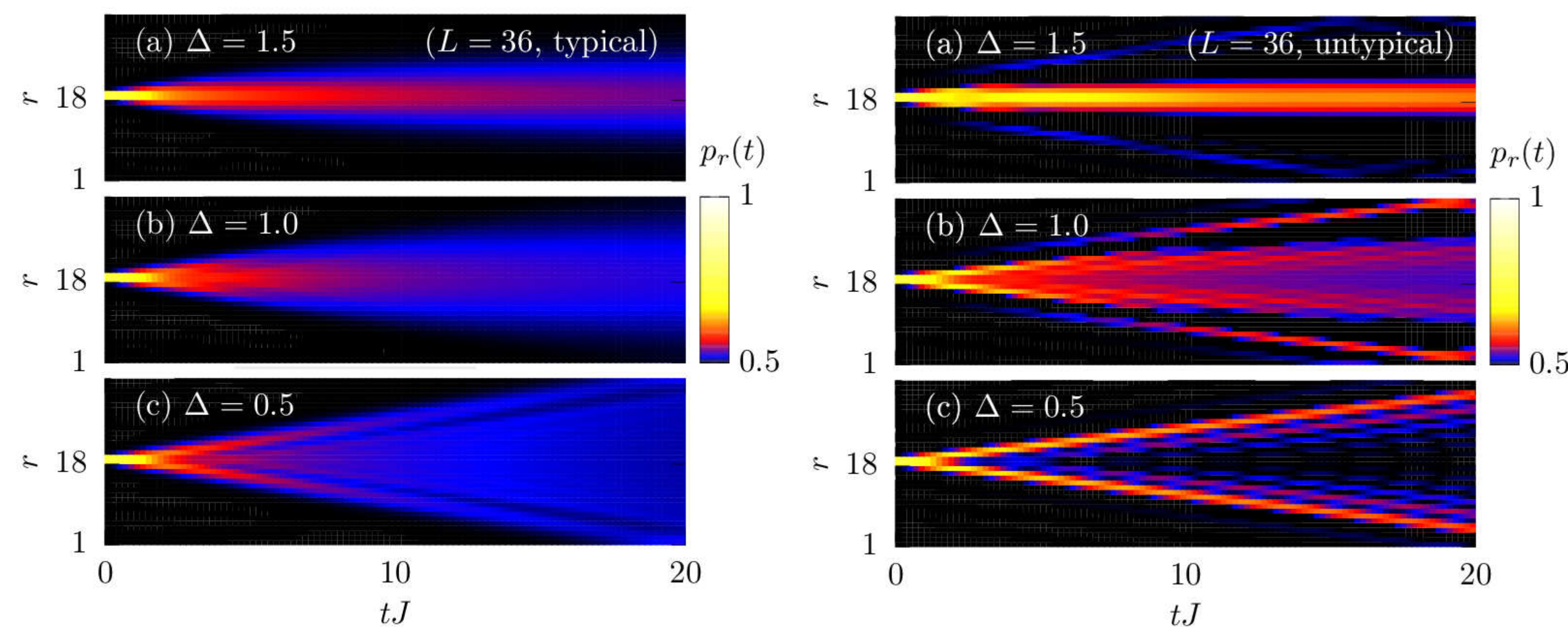


Fig. 1. Time-space density plot of occupation numbers $p_r(t)$ for a typical initial state (left) and product state (right).

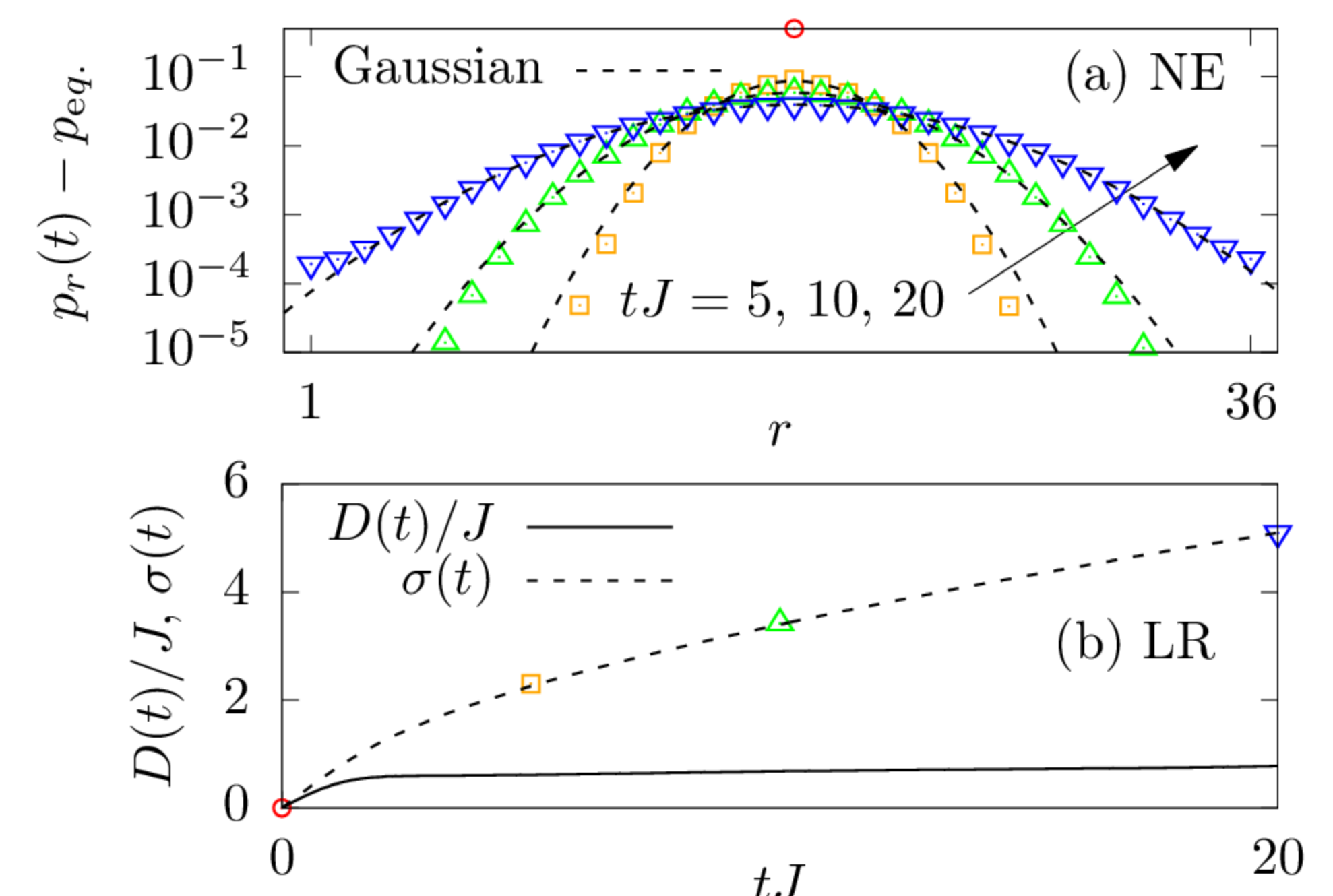


Fig. 2. (a) Density profile $p_r(t)$ at times $tJ = 0, 5, 10, 20$ for a single anisotropy $\Delta = 1.5$ for a typical initial state; (b) Time dependence of diffusion coefficient $D(t)$ and profile width $\sigma(t)$ according to the linear response theory.

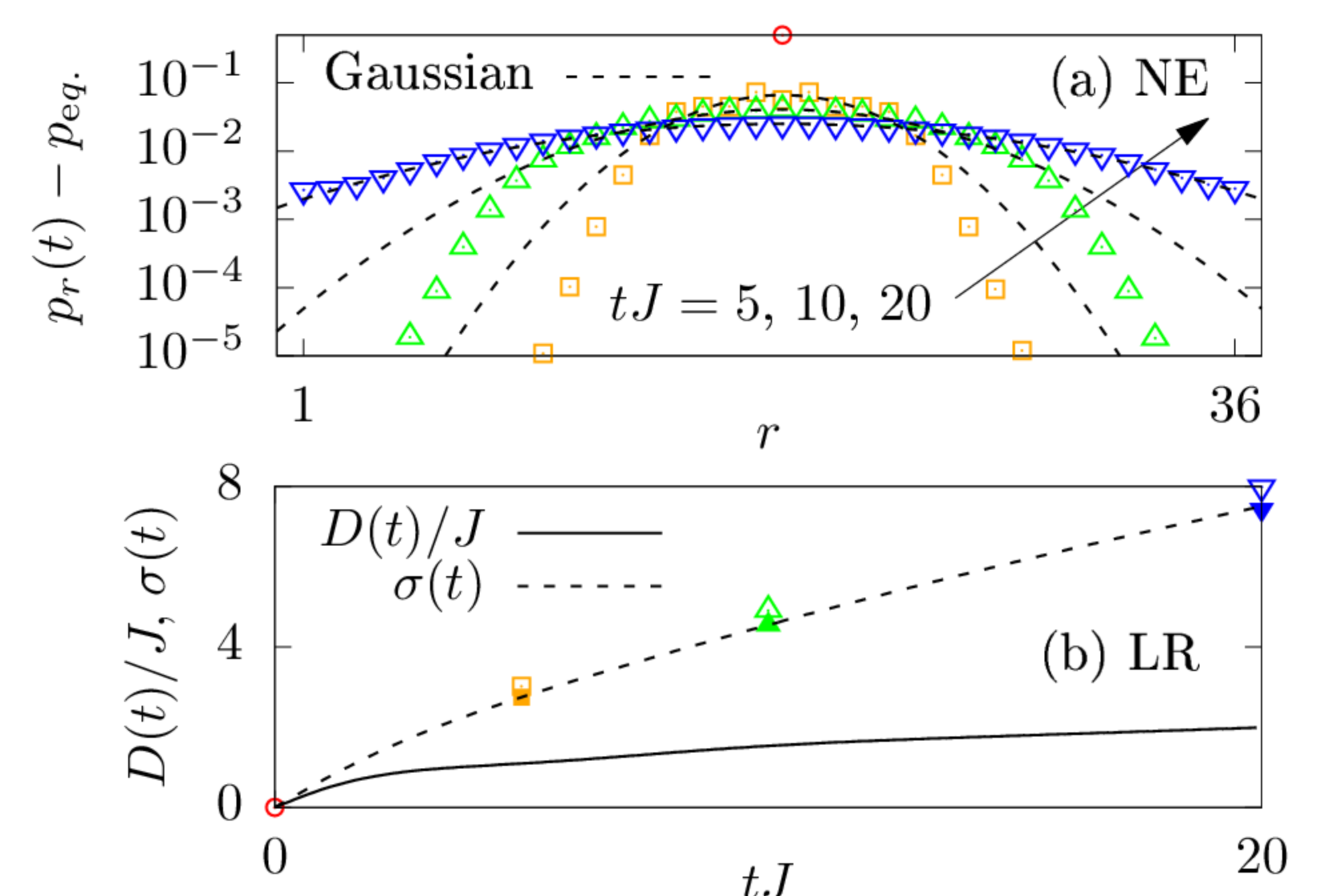


Fig. 3. The same as Fig. 2 except for anisotropy $\Delta = 1.0$.

References

- [1] R. Steinigeweg, J. Gemmer, and W. Brenig, Phys. Rev. Lett. **112**, 120601 (2014).
- [2] H. De Raedt, Comp. Phys. Rep. **7**, 1 (1987).
- [3] V.V. Dobrovitski, and H. De Raedt, Phys. Rev. E **67**, 056702 (2003).
- [4] R. Steinigeweg, F. Jin, D. Schmidtke, H. De Raedt, K. Michielsen, and J. Gemmer, Phys. Rev. B **95**, 035155 (2017).
- [5] R. Steinigeweg, F. Jin, H. De Raedt, K. Michielsen, and J. Gemmer, Phys. Rev. E **96**, 020105 (2017).