Study of quench dynamics in Kondo systems using time-dependent NRG method.

T. Ślusarski, K. Wrześniewski, I. Weymann

Institute of Spintronics and Quantum Information, Faculty of Physics, A. Mickiewicz University, 61-614 Poznań, Poland

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ABSTRACT

We have studied dynamical properties of one-channel and two-channel Kondo systems after different quenches in Hamiltonian variables. Electronic structure of initial Hamiltonian (before quench) and final Hamiltonian (after quench) was calculated using density matrix numerical renormalization group method implemented using matrix product states formalism [1]. We show spectral properties and static averages of operators of impurity local variables. Quench dynamics was studied as real-time evolution of operators of interest calculated as time-dependent expectation values. We study behavior of Loschmidt echo, measuring the possibility of revival of system to its initial state after some quench.

We have considered multiple quench protocols in Kondo systems as for example: switching on/off the Kondo couplings between impurity and metallic band states, varying of J coupling to one channel while keeping constant the second one, or simultaneous quench of both coupling constants. Particularly interesting is class of quenches around non-Fermi liquid critical point in two-channel model (i.e. J1=J2). We systematically study quenches of varying strength from very small (*aka* continuous quench limit [2]) to large ones (discrete, pulse-like quenches) focusing on dependence of system response due to quench on the boundary conditions.

Furthermore we study such dynamics in the presence of applied external magnetic field of different intensities, also in the case with quenches of B field itself. We have also discussed stability of system properties with the increase of temperature. Finally we have computed conductance for most relevant examples above, showing the influence of dynamics and stability of Kondo correlated state on current properties.

BACKGROUND

- One channel Kondo model (1CK) effectively describe single impurity in bulk or connected to same leads, DMFT lattice models mapped on impurity model, adatom on surface, qubit in environment etc.
- Multichannel (two channel in our case, 2CK) Kondo model describe single impurity connected to multiple bands or many impurities connected to leads, there is mapping of 1CK models in presence of external fields to 2CK model [5]
- 1CK show Fermi liquid behaviour (with energy scale TKondo), while in 2CK there could be many energy scales [6] and non-Fermi liquid behaviour near critical point with possible quasiparticle spectrum such as Majorana modes
- Kondo model in nonequilibrium denotes open systems in presence of external fields, temperature reservoirs etc.
- Quenches are possible way to change Hamiltonian in time resulting in modified electronic structure and dynamics between initial and final state. They could be used for modelling of nonequilibrium effects in closed systems [8]

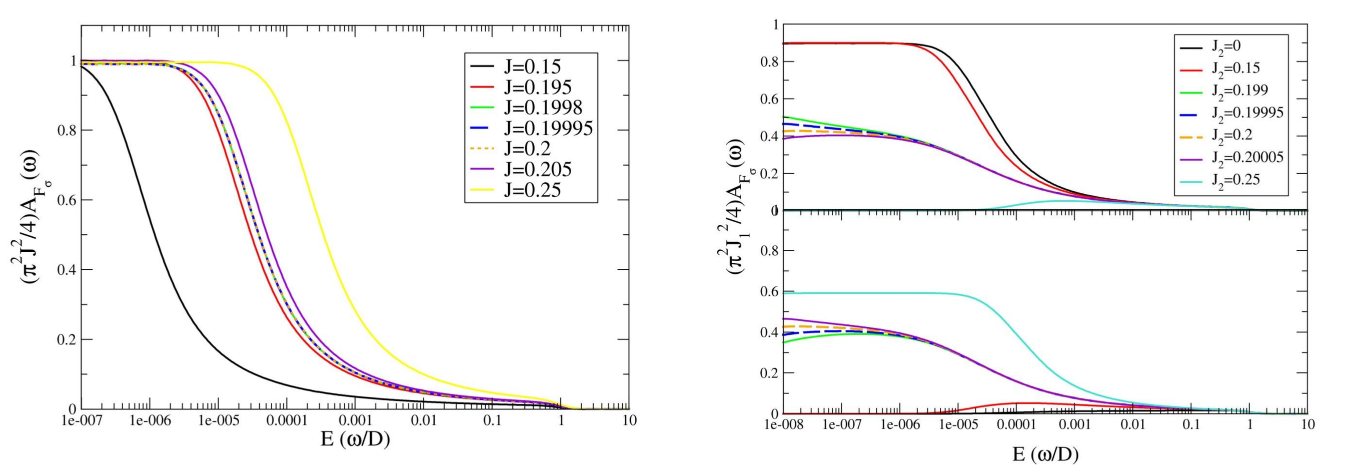
GOALS

- Finding correspondence between dynamics of 1CK and 2CK models
- Study of time evolution of relevant physical quantities
- Measuring the ability of system to return to its initial state after quenching
- Taking into account effect of magnetic field

METHOD

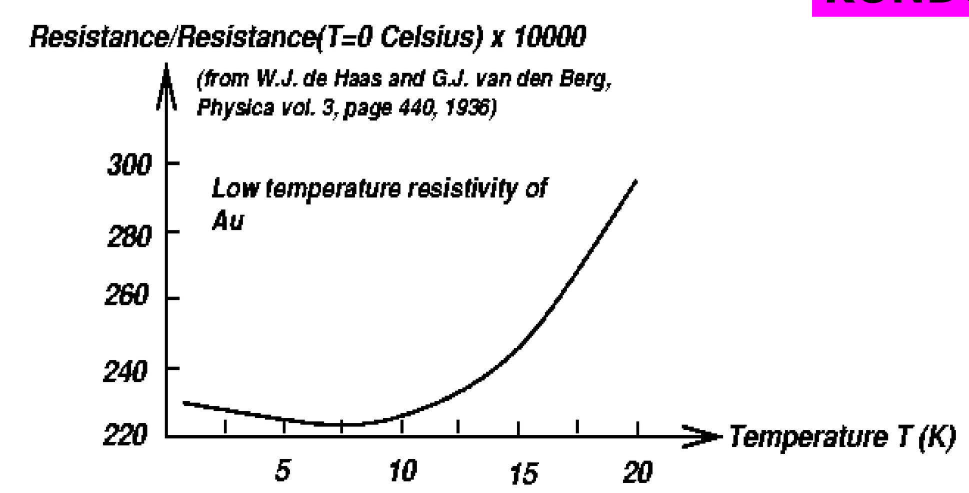
- NRG method based on Wilson idea of mapping of Kondo Hamiltonian on semi-infinite chain and solving it iteratively [9]
- Using the set of complete basis of discarded states
- Employing Denisty Matrix formalism to account for precise ground state
- Calculating spectral functions as retarded Green function
- TDNRG to calculate dynamics and time evolution of operators [1]
- Parameters of calculations: Λ=2; nr of kept states=1024 (1CK) 4096 (2CK), nr of NRG iterations=80

STATIC PROPERTIES



Normalized spectral functions of spin up composite fermion operator for 1CK (left) and 2CK (right)

KONDO EFFECT



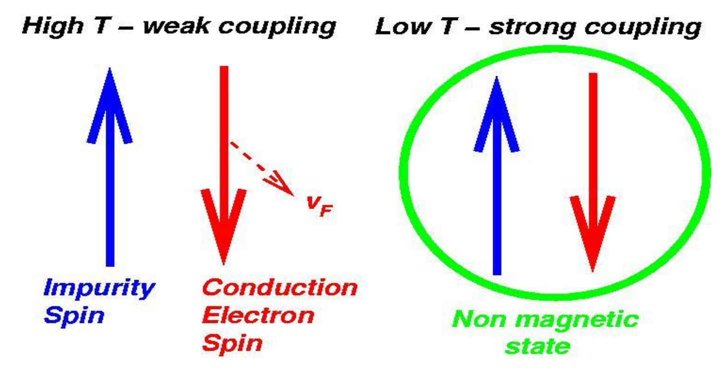


Fig. Electrical resistivity of Au metal with impurities

$$\hat{H}_{Kondo}=\frac{J}{2}\vec{S}\sum_{\sigma,\sigma'}\psi^{+}_{\sigma}\vec{\sigma}_{\sigma,\sigma'}\psi_{\sigma'}+\sum_{\vec{k}\sigma}\varepsilon_{\vec{k}}c^{+}_{\vec{k}\sigma}c_{\vec{k}\sigma}$$

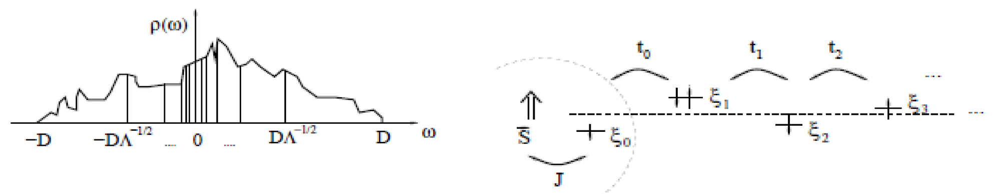


Fig. Scheme of log. discretized metallic band and Wilson chain with exponentially decaying hopping

- **discrete quantum system in presence of continuum of states (fermionic or bosonic bath)**
- **scattering of conduction electrons in a metal due to magnetic impurity (s-d scattering)**
- **perturbation theory predicts that scattering rate diverges at low temperatures**
- **asymptotic freedom – coupling becomes nonperturbatively strong at low energies and low T**
- **Renormalization group approach successfully describe low temperature limit**
- **limiting case (Schrieffer-Wolff transf.) of Anderson impurity model in strong coupling regime**

$$\hat{H}_{Wilson}=\frac{J}{2}\vec{S}\sum_{\sigma,\sigma'}f^{+}_{0,\sigma}\vec{\sigma}_{\sigma,\sigma'}f_{0,\sigma'}+\sum_{n=0}^{\infty}\sum_{\sigma}\xi_n f^{+}_{n,\sigma}f_{n,\sigma}+\sum_{n=0}^{\infty}\sum_{\sigma}t_n\left(f^{+}_{n,\sigma}f_{n+1,\sigma}+hc\right)$$

$$O(t)=Tr\{e^{-iHt}\rho e^{iHt}O\}$$

$$L(t)=\left|\langle\psi_0|e^{-iHt}|\psi_0\rangle\right|^2$$

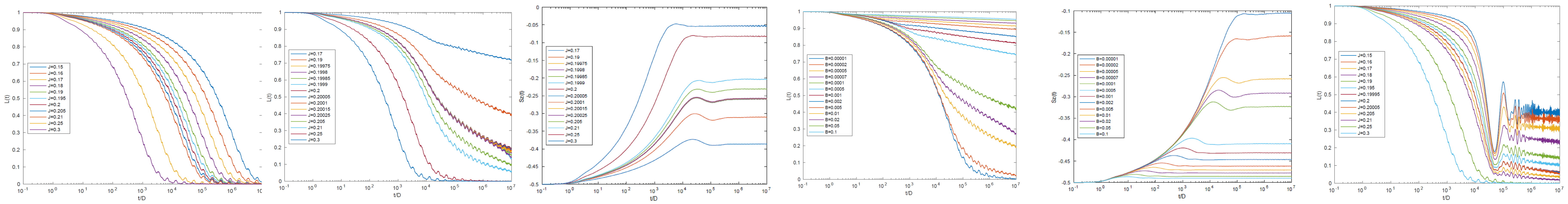
$$H(t)=\theta(-t)H_0+\theta(t)H$$

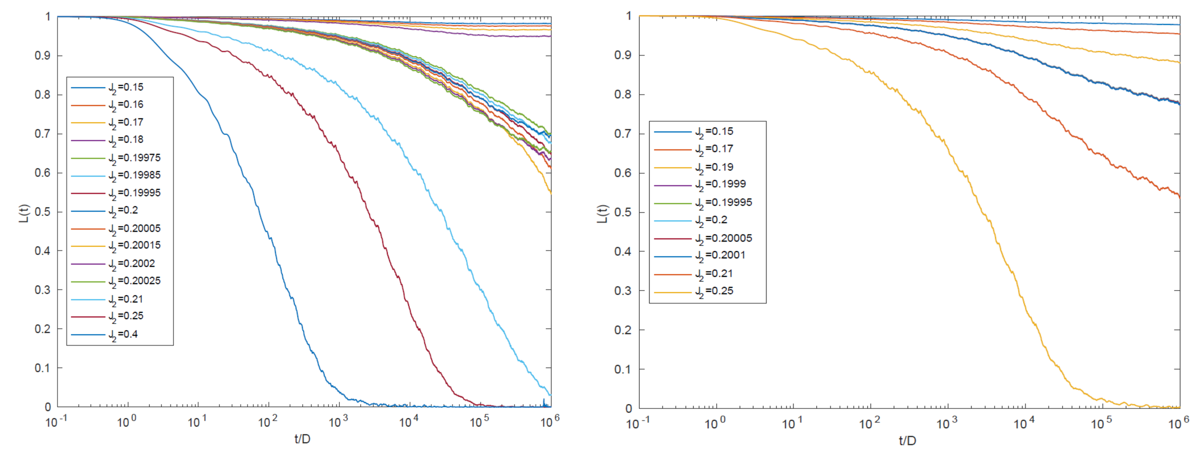
Fig. Formulas for time dependency of operator, for Loschmidt echo and for time evolution of quenched Hamiltonian

PHASE TRANSITIONS

- **classical phase transition** occurs when thermodynamic free energy exhibits nonanalyticity for some variables (derivative of free energy is discontinuous)
- such thermal phase transitions are often accompanied with classical Landau symmetry-breaking mechanism, if the system has additional topological order it could undergo **topological phase transition**
- **quantum phase transition** can't be explained by thermal fluctuations but quantum fluctuations since temperature is 0 and driving parameter is not temperature (pressure, field etc.)
- **dynamical phase transitions** occurs in real-time domain with nonanalyticities in critical times, such cusps are not generated using external parameter but rather by pure dynamics

DYNAMIC PROPERTIES





Results for 2CK (from left): echo for quench in J_2 (J_1=0.2); echo for quench in J2 (J1=0.2) for fixed B=0.00005

Results for 1CK (top from left): echo for quench in J (from 0 to value in legend); echo for quench in J with fixed B=0.00005; Sz(t) for quench in J with fixed B=0.00005; echo for constant quench in J (0 to 0.2) for various fixed B; Sz(t) for constant quench in J (0 to 0.2) for various fixed B; echo for simultaneous quench in J (from 0 to value in legend) and B (from 0 to 0.00005)

REFERENCES

[1] K. Wrześniewski, I. Weymann, Phys. Rev. B 100, 035404 (2019)
[2] H. T. M. Nghiem, T. A. Costi Phys. Rev. B 98, 155107 (2018)
[3] https://en.wikipedia.org/wiki/Kondo_effect
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[8] D. M. Fugger et al., New Jour. Of Phys. 20 013030 (2018)
[9] K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975)

CONCLUSIONS

- **In the 1CK with J-quench, the Loschmidt echo decay to 0 in appropriate time scale. The larger the quenched coupling the faster echo decays**
- **In the presence of fixed local magnetic field echo decays slower and not always to 0 at studied time scales if J-quench is small enough**
- **For values of fixed B around TK for constant quenched J, echo functions are dropping to some finite nonzero value at studied time scales, are more oscillatory and Sz(t) exhibits local extrema before saturating to some finite value**
- **Larger fixed B field results in more flat echos starting from small time scales and J-quenching is reduced**
- **For simultaneuos J and B quench, when J are smaller than B, the echos are forming local minimum pinned at one time scale**
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- **Around nonFermi liquid point (J2=J1) echo curves are grouped and behaves more like in the 1CK+fixedB case but the curve decay more monotonically, it has no inflection points in studied scale**
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Acknowledgements
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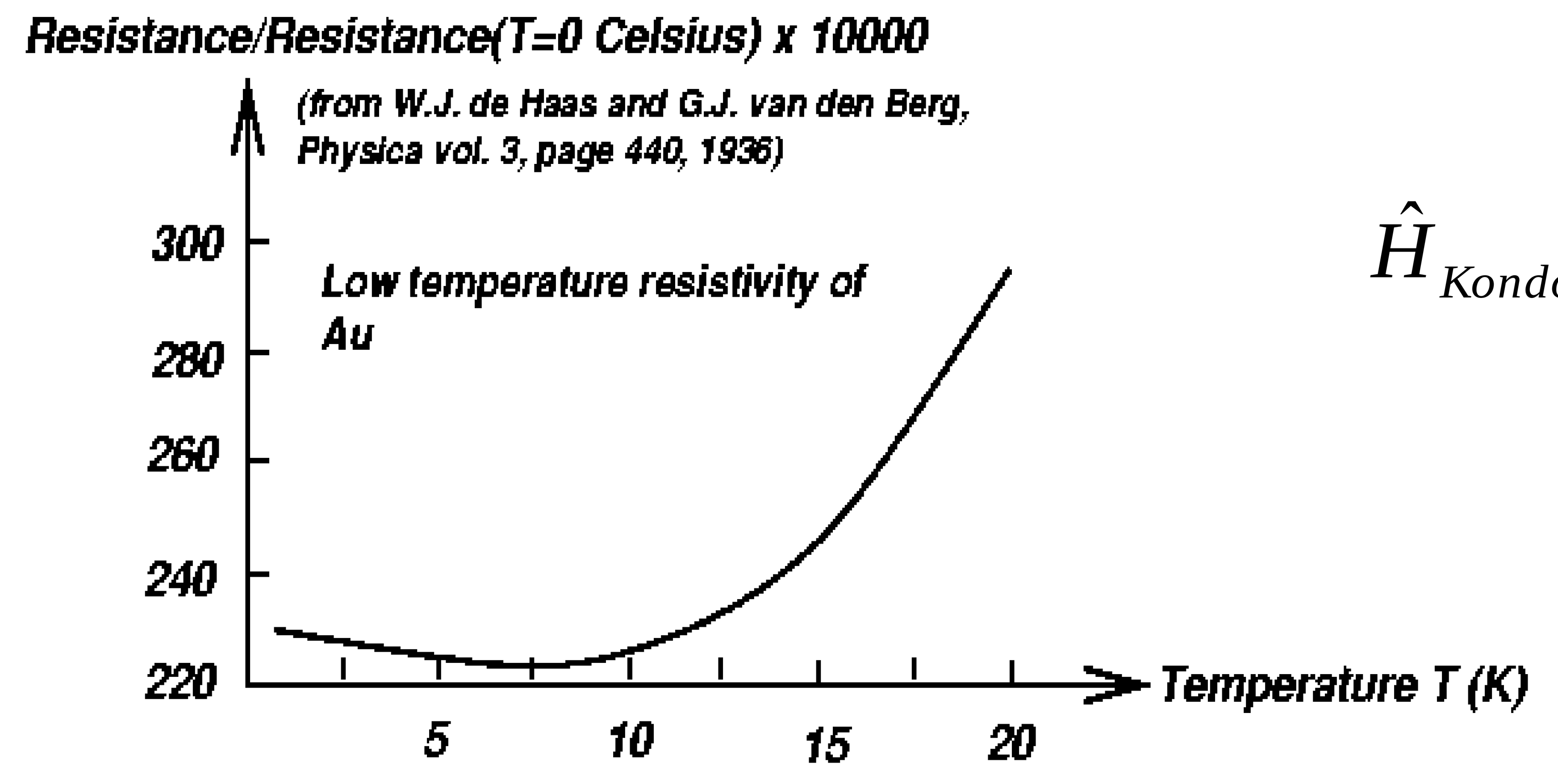

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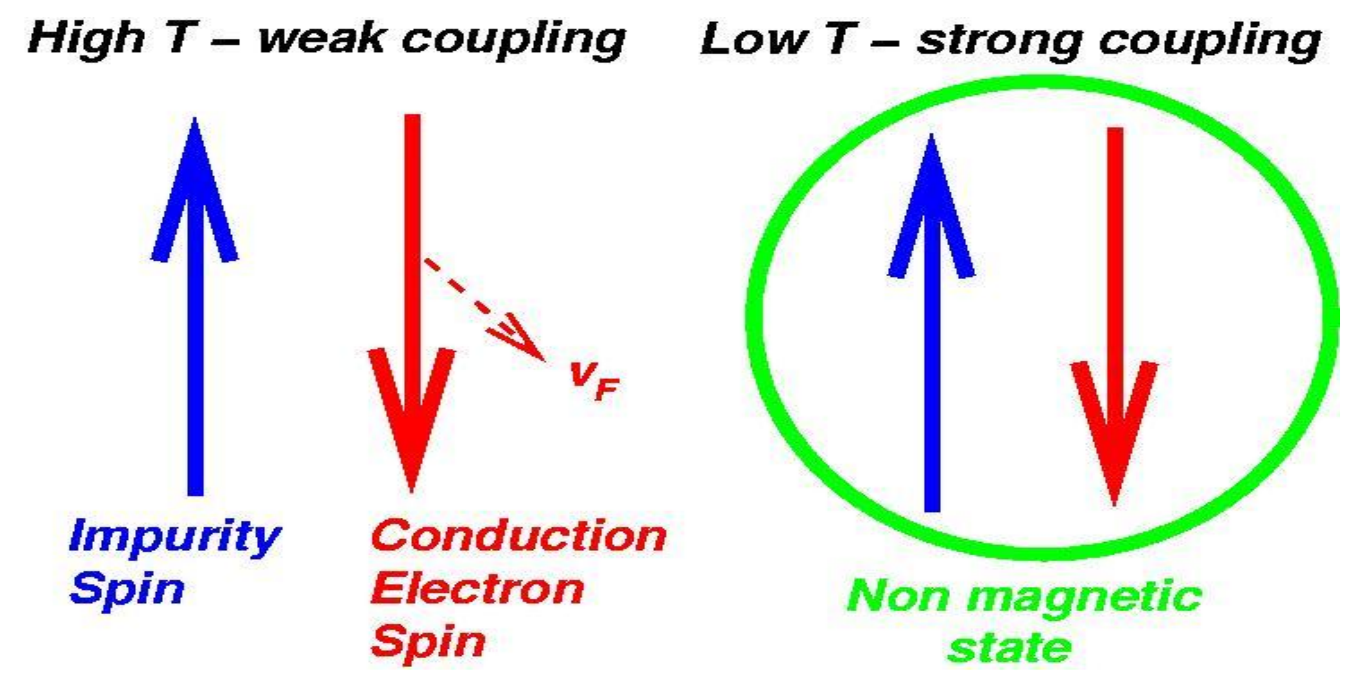

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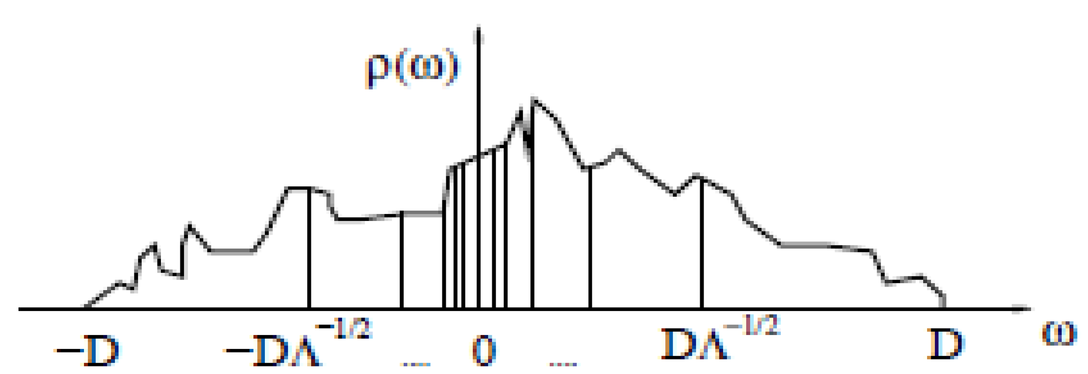

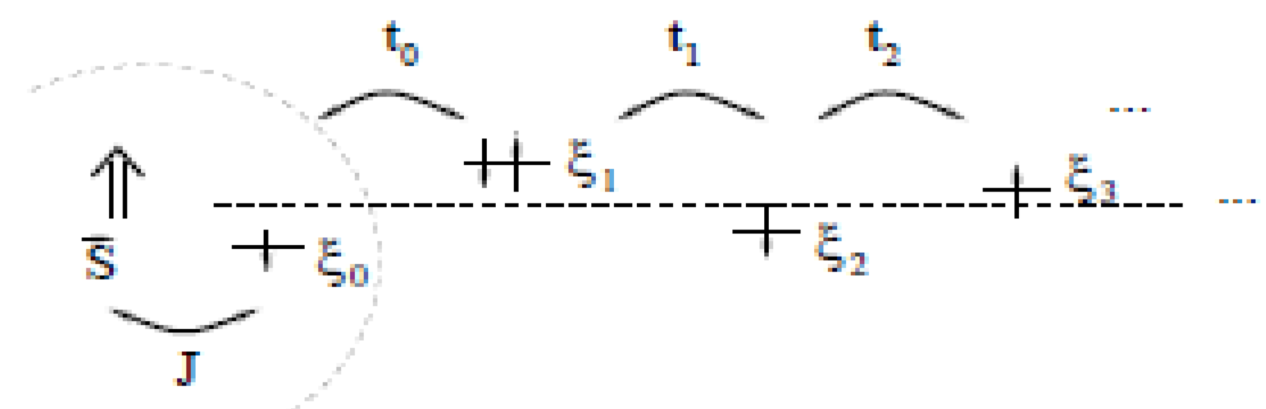

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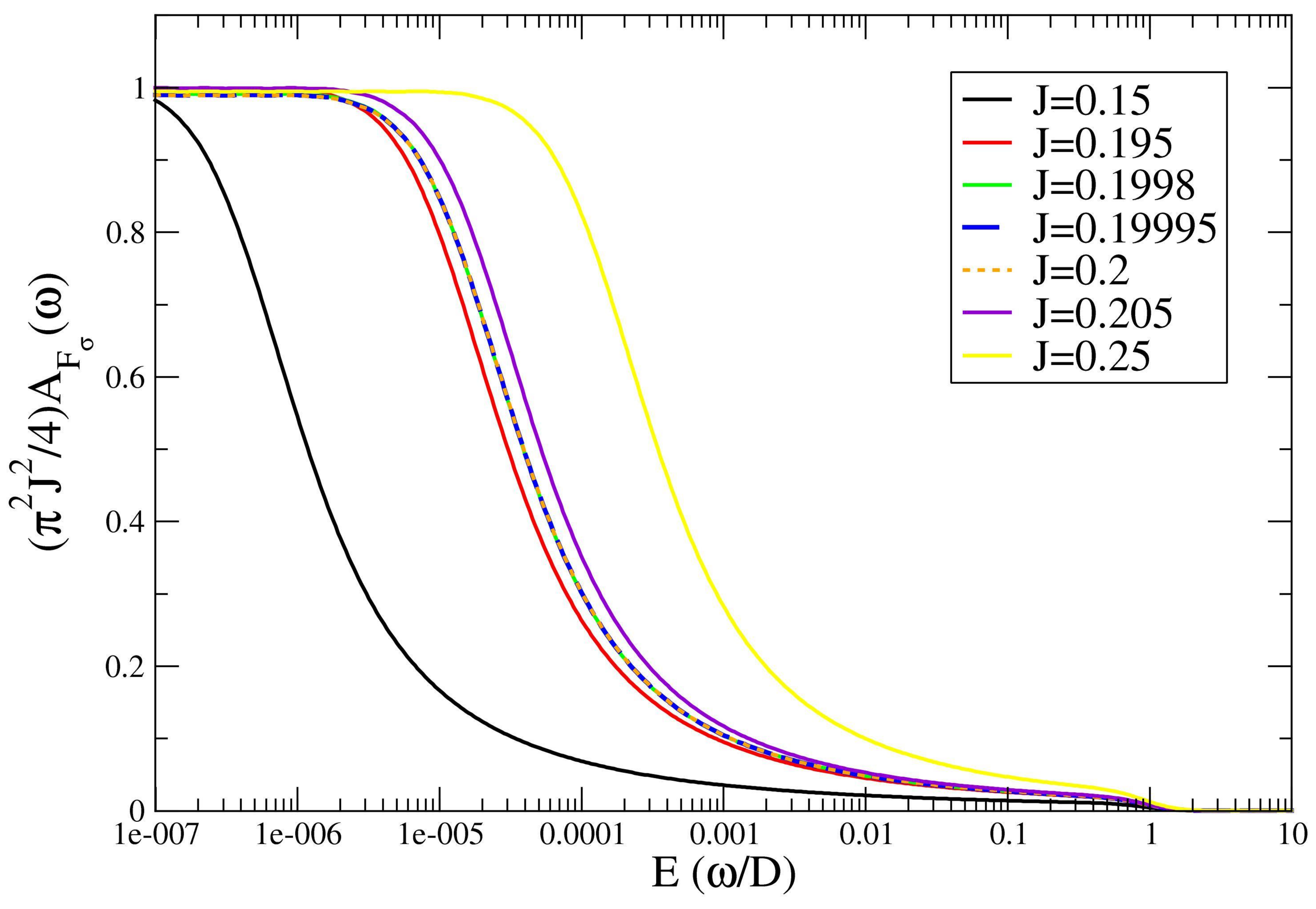
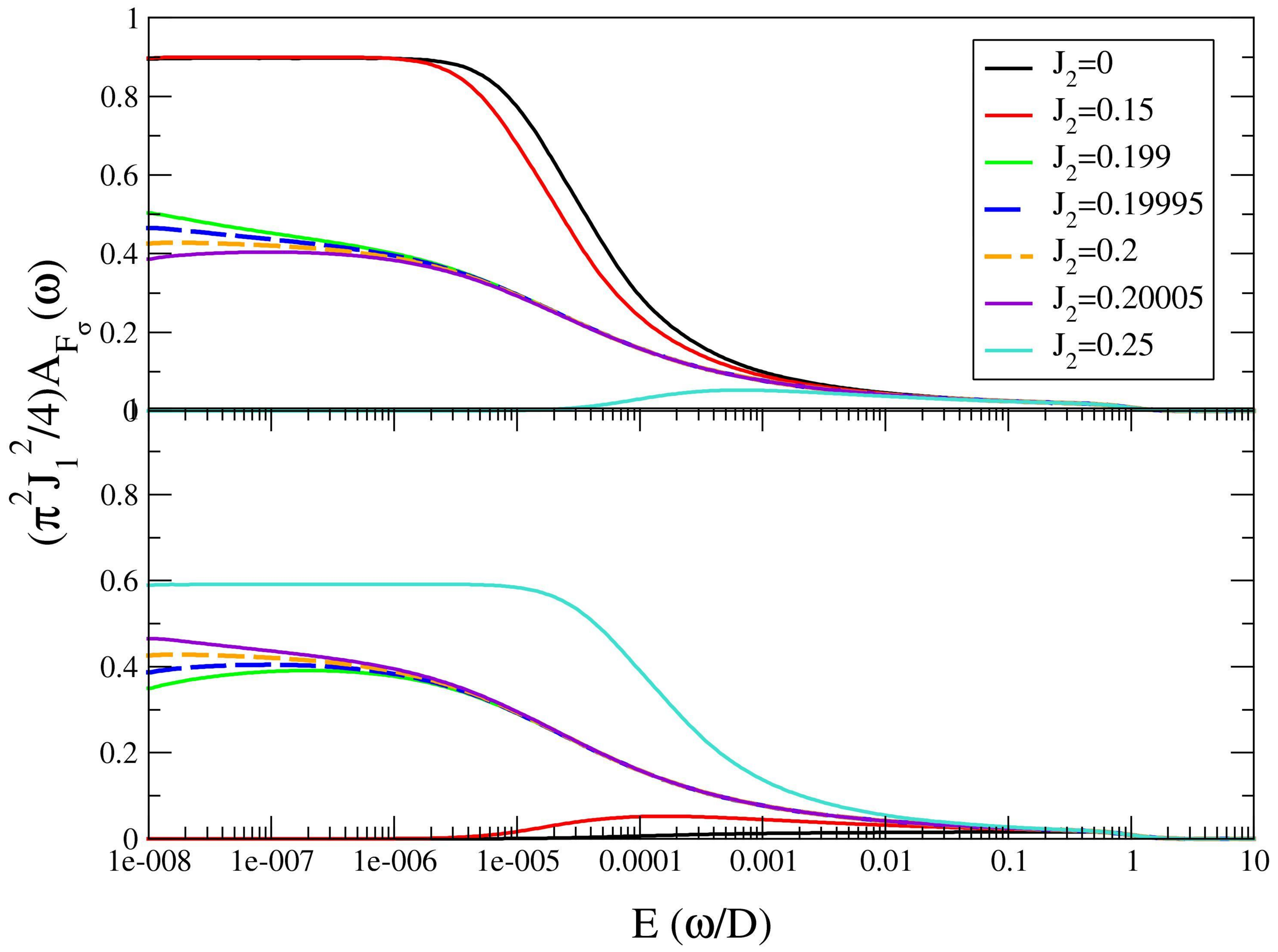
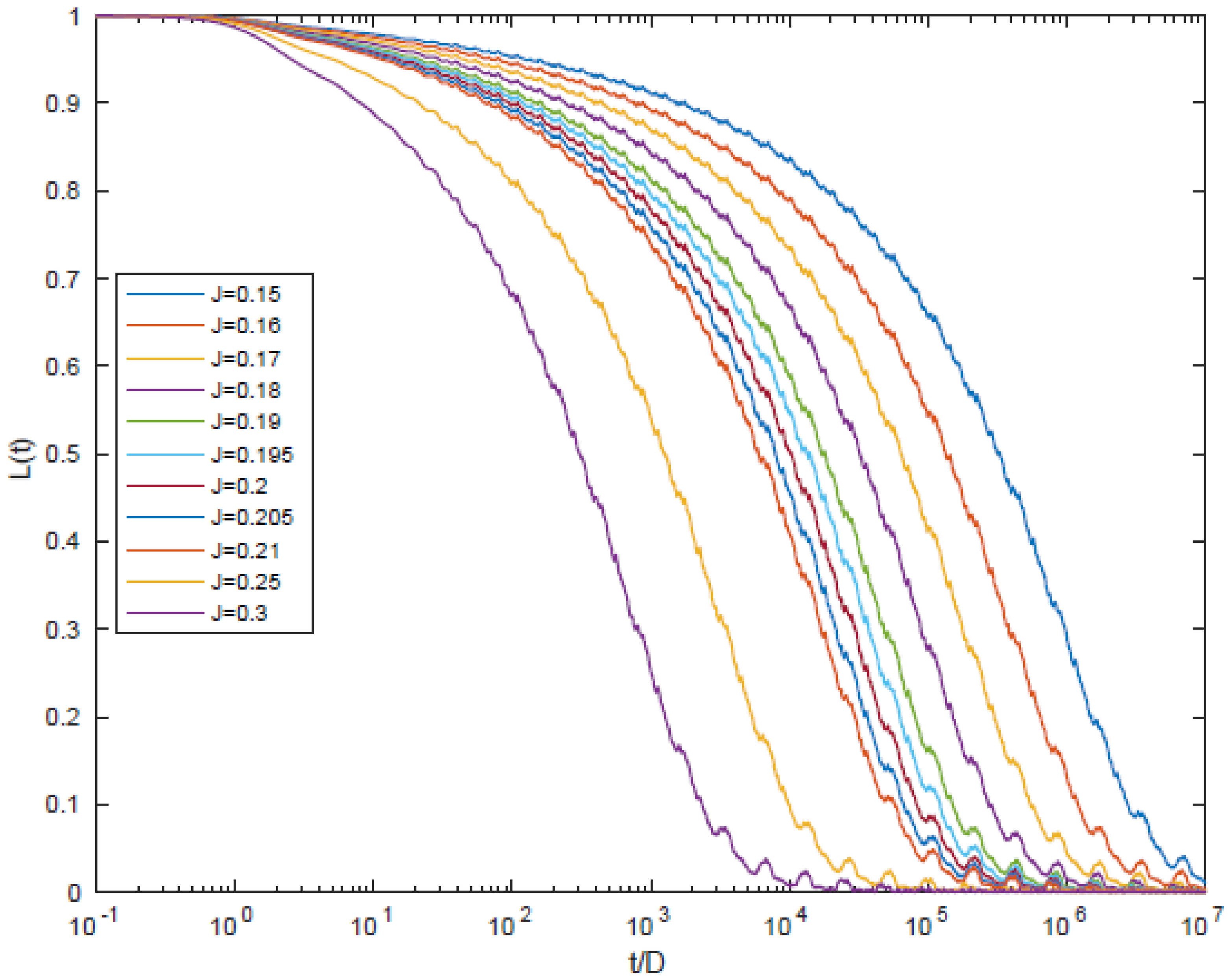
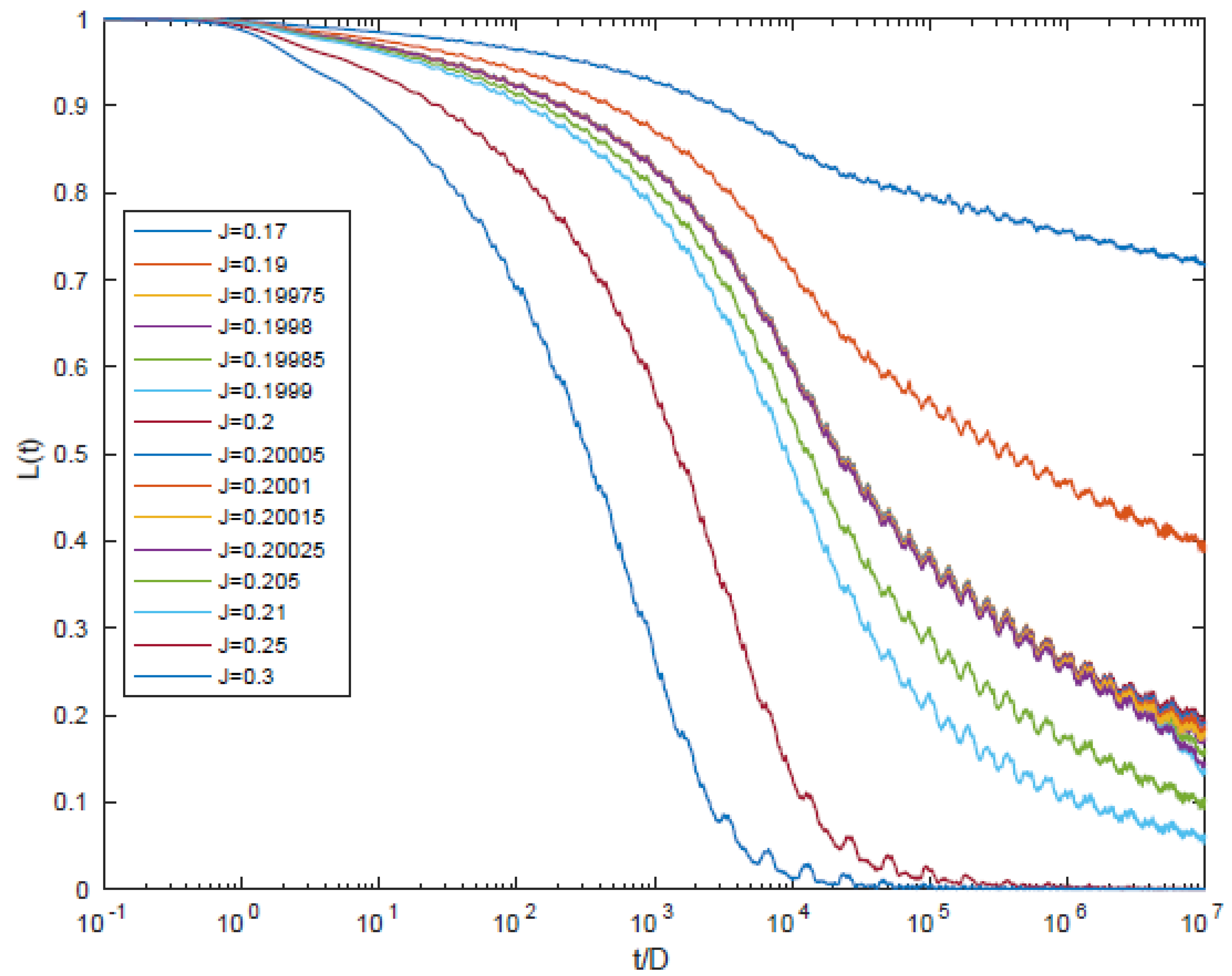


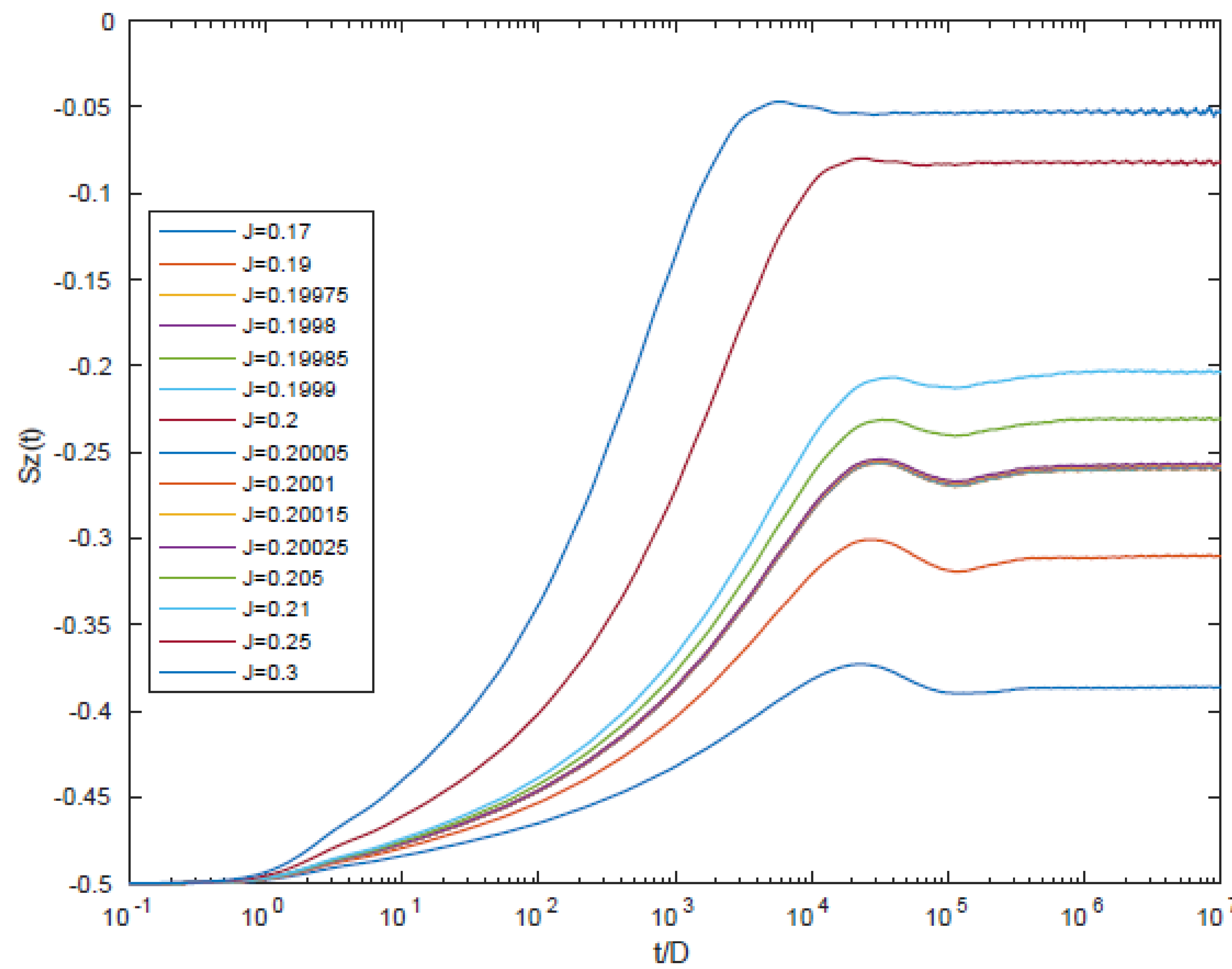


Normalized spectral functions of spin up composite fermion operator for 1CK (left) and 2CK (right, plot for two channels)

DYNAMIC PROPERTIES

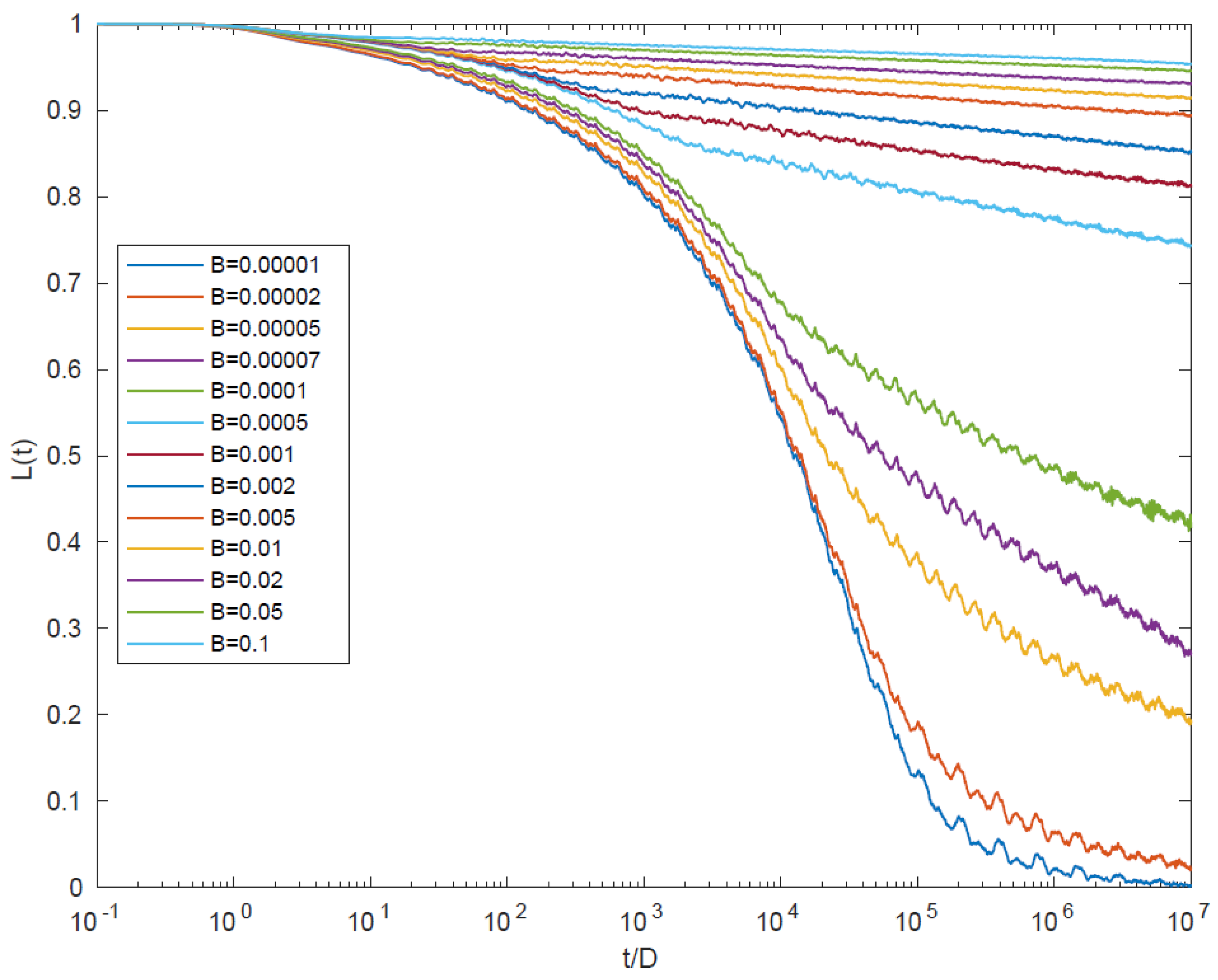


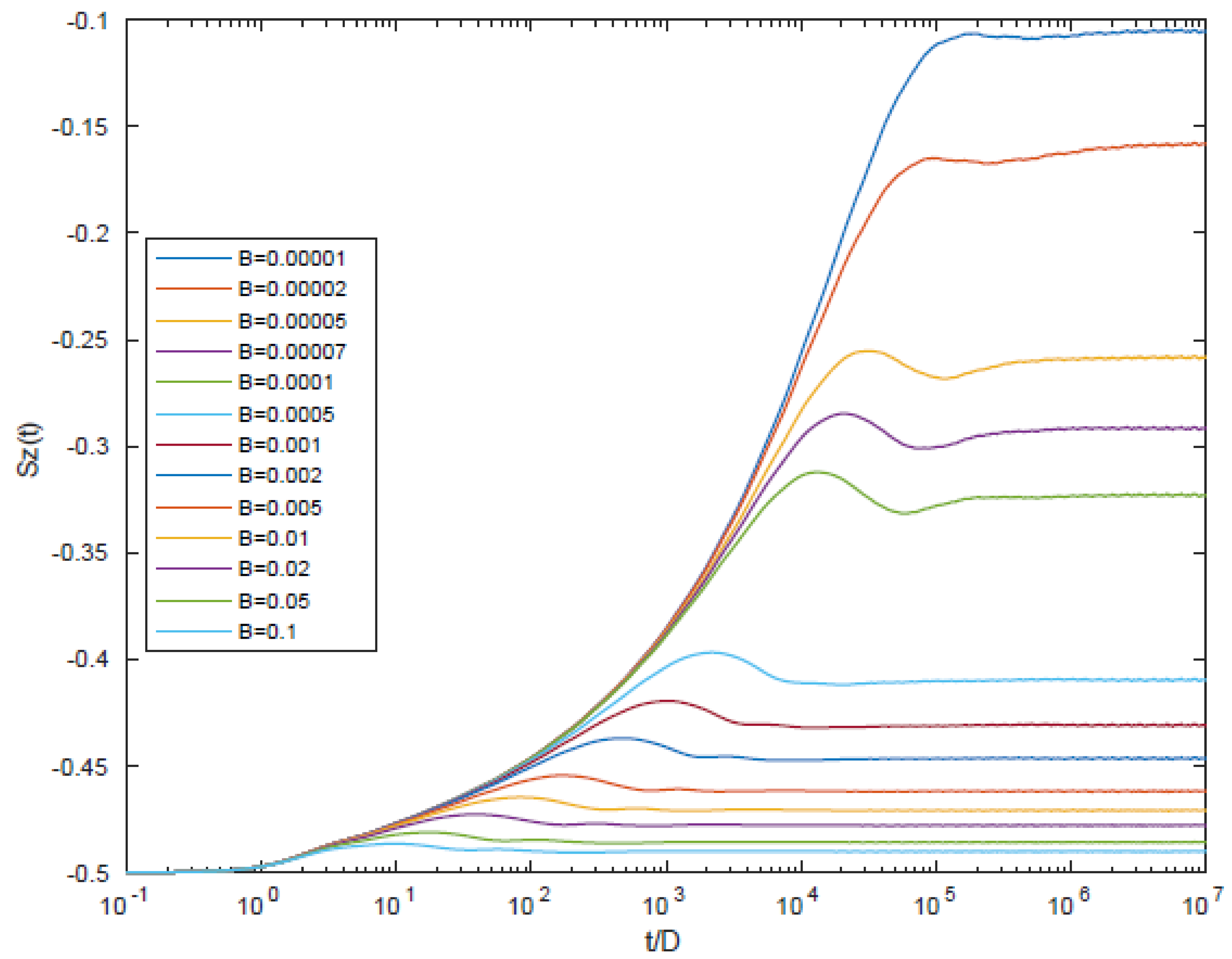


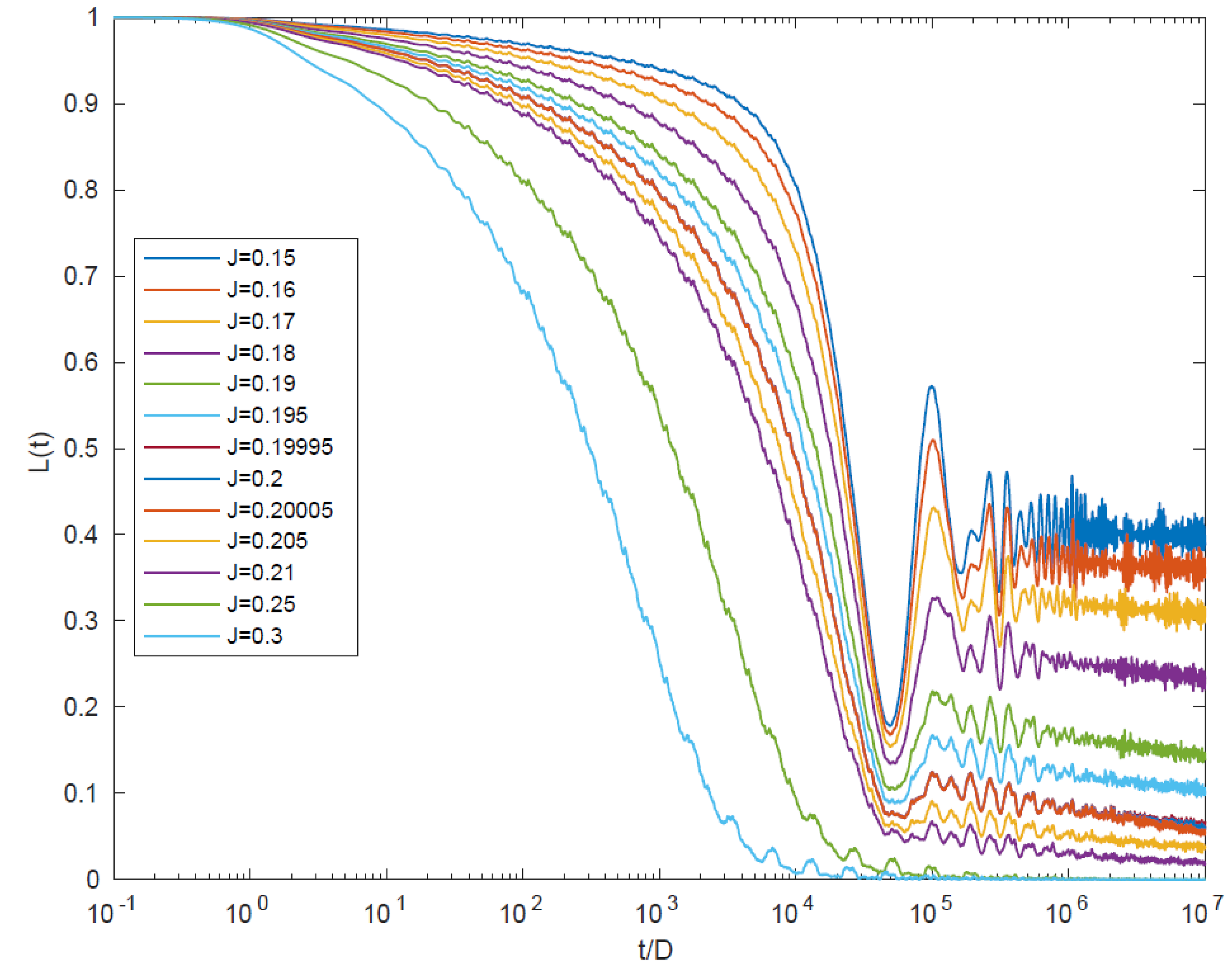


Results for 1CK (from left): echo for quench in J (from 0 to value in legend); echo for quench in J with fixed B=0.00005; Sz(t) for quench in J with fixed B=0.00005

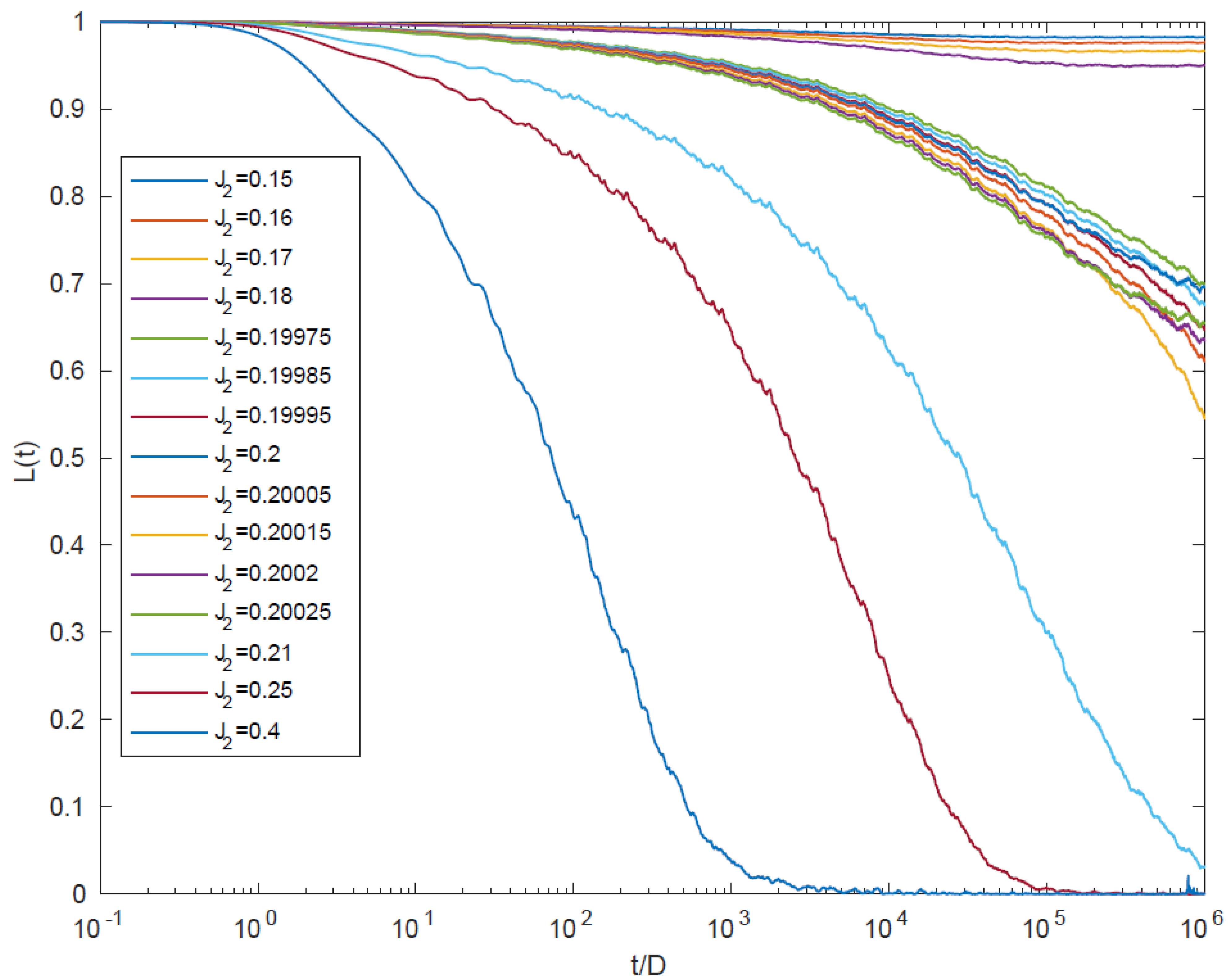
DYNAMIC PROPERTIES

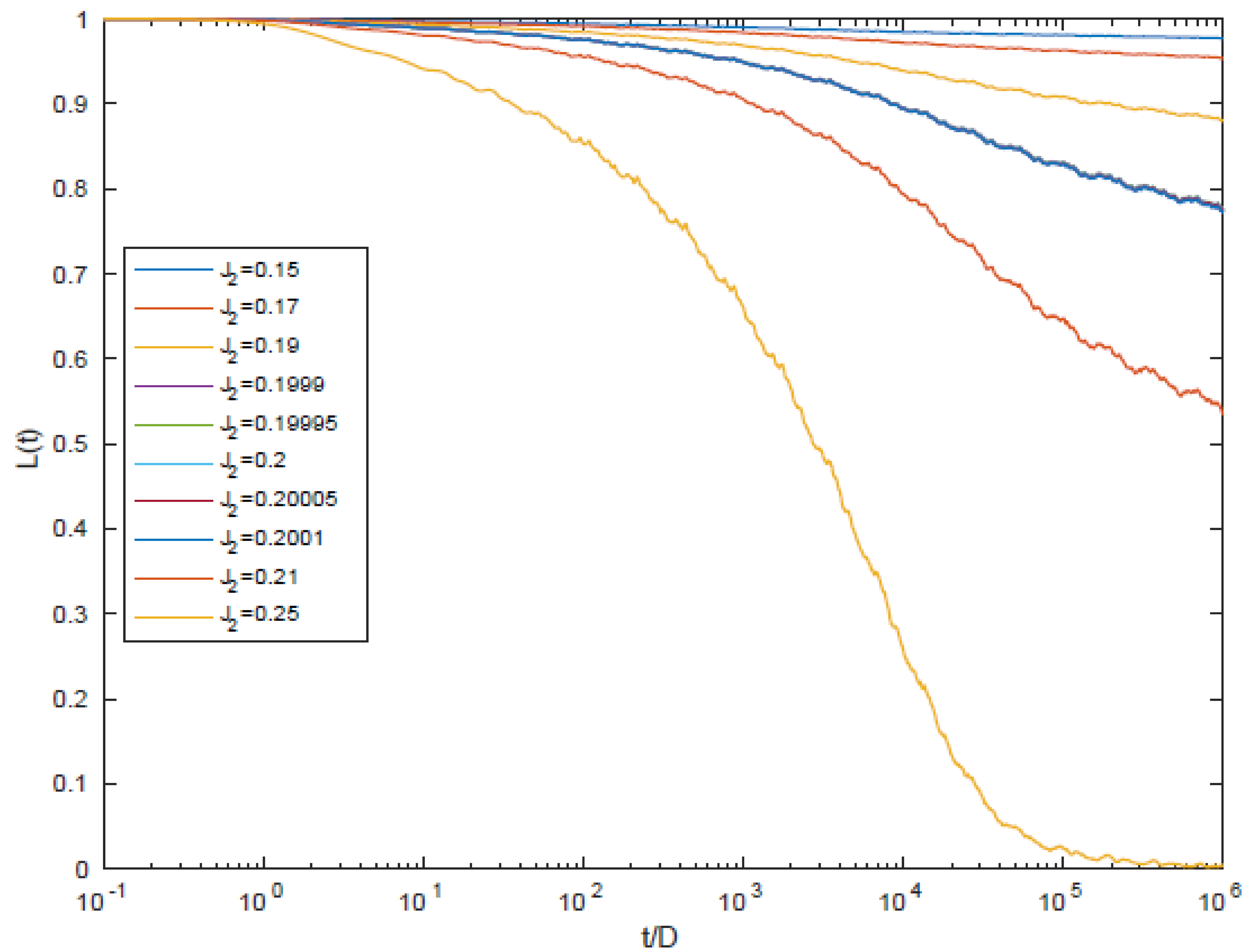






Results for 1CK (from left): echo for constant quench in J (0 to 0.2) for various fixed B; Sz(t) for constant quench in J (0 to 0.2) for various fixed B; echo for simultaneous quench in J (from 0 to value in legend) and B (from 0 to 0.00005)





Results for 2CK (from left): echo for quench in J_2 (J_1=0.2); echo for quench in J_2 (J_1=0.2) for fixed B=0.00005

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