Thermodynamic properties of correlated fermions in lattices with spin-dependent disorder

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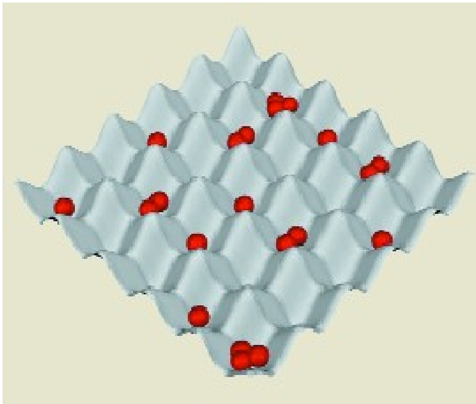
Introduction

Neutral particles in optical lattice



I. Bloch, Phys. Woṛld 17, 25 (2004)

Interacting electrons in materials

Strongly correlated materials

Hubbard model (1963):

Electron correlations in narrow energy bands

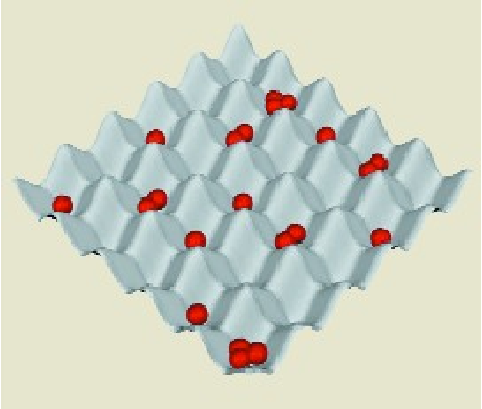
By J. Hubbard

that a possible approximation is to neglect all the integrals (8) apart from I. If this approximation, the validity of which is discussed in greater detail below, is made, then the Hamiltonian of (6) becomes

$$H = \sum_{i,j} \sum_{\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \tfrac{1}{2} I \sum_{i,\sigma} n_{i\sigma} n_{i,-\sigma} - I \sum_{i,\sigma} \nu_{ii} n_{i\sigma}, \qquad (10)$$

Introduction

Neutral particles in optical lattice



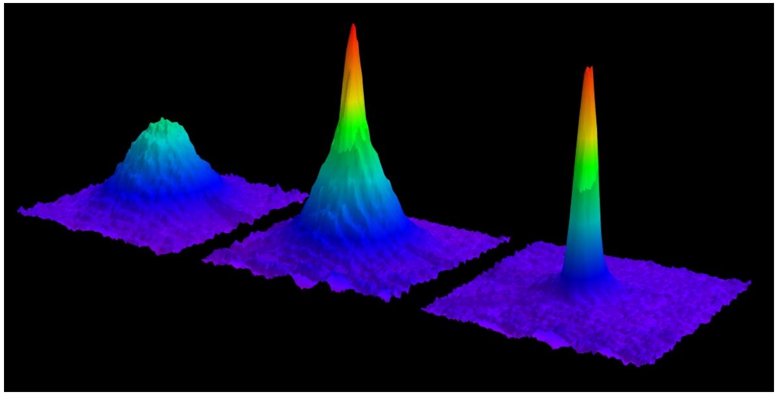
perfect crystal

very good realization of Hubbard model

Hubbard model not solved - optical lattice as quantum simulator
Searching for new quantum phases

Introduction

(1995) BEC: Eric A. Cornell, Wolfgang Ketterle, Carl E. Wieman



Introduction

Strongly correlated phase transition for the first time in optical lattice, bosons:

Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms

Markus Greiner*, Olaf Mandel*, Tilman Esslinger†, Theodor W. Hänsch* & Immanuel Bloch*

NATURE | VOL 415 | 3 JANUARY 2002 | www.nature.com

Fermions:

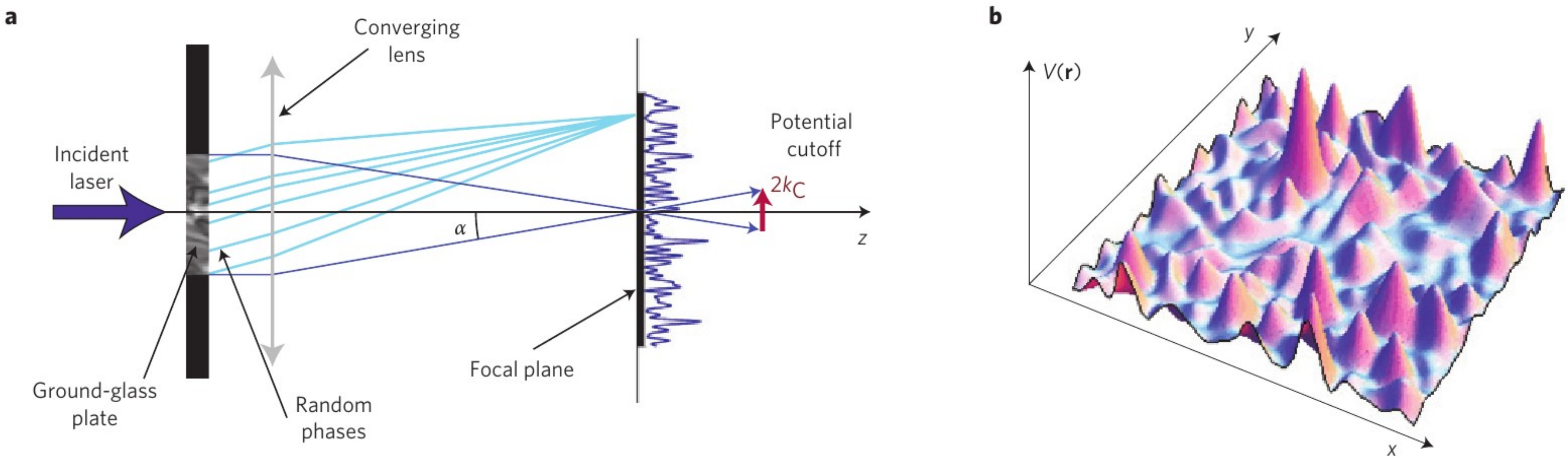
A Mott insulator of fermionic atoms in an optical lattice

Robert Jördens[1]*, Niels Strohmaier[1]*, Kenneth Günter[1,2], Henning Moritz[1] & Tilman Esslinger[1]

NATURE | Vol 455 | 11 September 2008

Introduction

Optical lattice with disorder



L. Sanchez-Palencia, M. Lewenstein, Nature Phys. 6, 87 (2010)

Motivations and aims of our work

Apart from disorder in optical lattices:

Spin-dependent lattices first proposed:

D. Jaksch, H. Briegel, J. Cirac, C. Gardiner, and P. Zoller, Phys. Rev. Lett. 82, 1975 (1999)

Spin-dependent lattices first implemented:

O. Mandel, M. Greiner, A. Widera, T. Rom, T. Hänsch, and I. Bloch, Nature (London) 425, 937 (2003)

P. Soltan-Panahi, J. Struck, P. Hauke, A. Bick, W. Plenkers, G. Meineke, C. Becker, P. Windpassinger, M. Lewenstein, and K. Sengstock, Nat. Phys. 7, 434 (2011)

- disorder in lattice realized
- spin-dependent lattice realized

Spin-dependent disorder in optical lattice possible to realize
(beyond standard solid state physics)

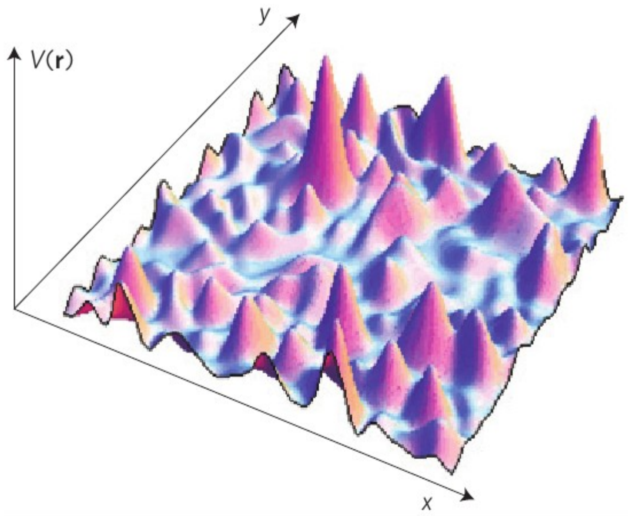
Comprehensive thermodynamics?

Hubbard model with spin-dependent disorder

$$H = t\sum_{(i,j)}\sum_{\sigma=\uparrow,\downarrow}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i}\sum_{\sigma=\uparrow,\downarrow}\epsilon_{i\sigma}\hat{n}_{i\sigma} + \sum_{i} U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

$$\hat{n}_{i\sigma} \equiv \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$$

Disorder in the model:
- comes through diagonal terms
- quenched disorder



Similar model: *R. Nanguneri, M. Jiang, T. Cary, G.G. Batrouni, and R.T. Scalettar, Phys. Rev. B 85, 134506 (2012)*

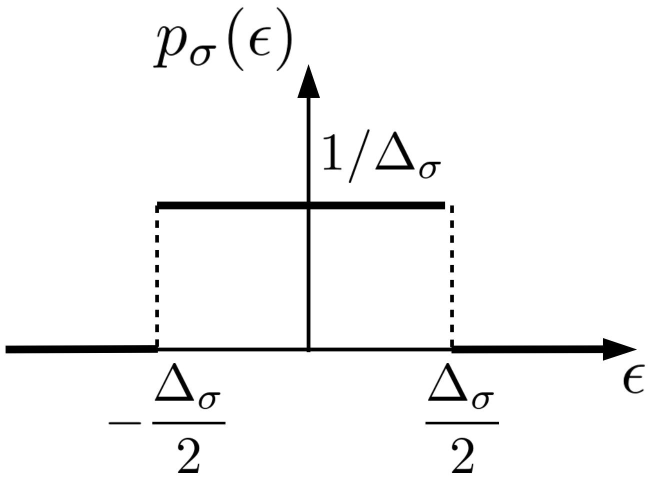
but: U<0, Bogolubov de Gennes mean field theory

More about disorder in the model

$$H = \ldots + \sum_i \sum_{\sigma=\uparrow,\downarrow} \epsilon_{i\sigma} \hat{n}_{i\sigma} + \ldots$$

We assume uncorrelated rectangular probability distribution function:

$$P(\epsilon_{1\uparrow}, \epsilon_{1\downarrow}, \ldots) = \prod_i p_\uparrow(\epsilon_{i\uparrow}) p_\downarrow(\epsilon_{i\downarrow})$$



Two cases compared:

Spin-dependent disorder:	$p_\uparrow(\epsilon) \neq p_\downarrow(\epsilon)$	$\Delta_\uparrow = 0; \quad \Delta_\downarrow \equiv \Delta$
Spin-independent disorder:	$p_\uparrow(\epsilon) = p_\downarrow(\epsilon)$	$\Delta_\uparrow = \Delta_\downarrow \equiv \Delta$

Thermodynamic properties

Magnetization:

$$m \equiv \lim_{N_L \to \infty} \langle\langle \sum_i \hat{m}_i \rangle\rangle_{\text{dis}} / N_L$$

Double occupation:

$$d \equiv \lim_{N_L \to \infty} \langle\langle \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle\rangle_{\text{dis}} / N_L$$

Charge susceptibility:

$$\chi_c = \left(\frac{\partial n}{\partial \mu} \right)_T$$

Magnetic susceptibility:

$$\chi = \left(\frac{\partial m}{\partial h} \right)_T$$

Also others: $N_\sigma(\mu), \ldots$

Green function

Grand canonical potential (thermodynamics):

$$\Xi = \sum_{N,\gamma_N} \langle \gamma_N | e^{-\beta(H-\mu\hat{N})} | \gamma_N \rangle$$

$\vec{R}_i$ lattice site

α

spin

One-particle Green function:

$$G_{\alpha\beta}(\tau,\tau') = -\langle\langle T_\tau \hat{a}_\alpha(\tau)\hat{a}^\dagger_\beta(\tau')\rangle\rangle_{\text{dis}}$$

$$\langle \ldots \rangle = \frac{1}{\Xi} \sum_{N,\gamma_N} \langle \gamma_N | e^{-\beta(H-\mu\hat{N})} \ldots | \gamma_N \rangle$$

“time” ordering

$$T_\tau \hat{a}_\alpha(\tau)\hat{a}^\dagger_\alpha(\tau') = \begin{cases} \hat{a}_\alpha(\tau)\hat{a}^\dagger_\alpha(\tau') & \text{dla} \quad \tau > \tau' \\ -\hat{a}^\dagger_\alpha(\tau')\hat{a}_\alpha(\tau) & \text{dla} \quad \tau < \tau' \end{cases}$$

Operator in modified Heisenberg picture

$$\hat{a}_\alpha(\tau) = e^{\tau(H-\mu N)}\hat{a}_\alpha e^{-\tau(H-\mu N)}$$

Method: dynamical mean field theory

- *W. Metzner, D. Vollhardt, Phys. Rev. Lett. 59, 121 (1987)*
- *A. Georges, G. Kotliar, W. Krauth, M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)*
- *M. Ulmke, V. Janis, D. Vollhardt, Phys. Rev. B 51, 10411 (1995)*

Semi elliptic DOS

Dyson equation:

$$G_{00}(i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{i\omega_n - \epsilon - \Sigma(i\omega_n) + \mu}$$

Consequences of high dimension limit (local problem):

$$G_{00}(\tau,\tau') = -\langle\langle c_{0\sigma}(\tau) c^*_{0\sigma}(\tau')\rangle_{S_{\mathrm{eff}}[\mathcal{G}_0]}\rangle_{dis}$$

QMC Hirsch-Fye

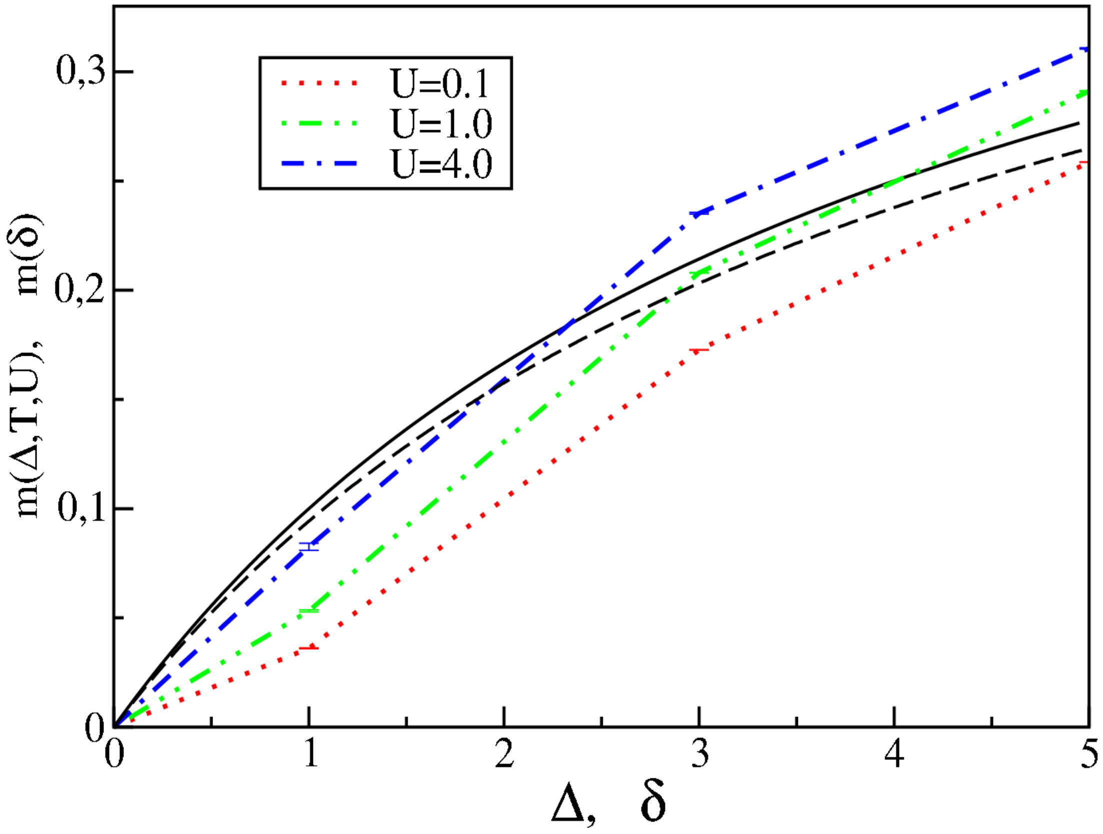
$$G_{00} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma G_{00}$$

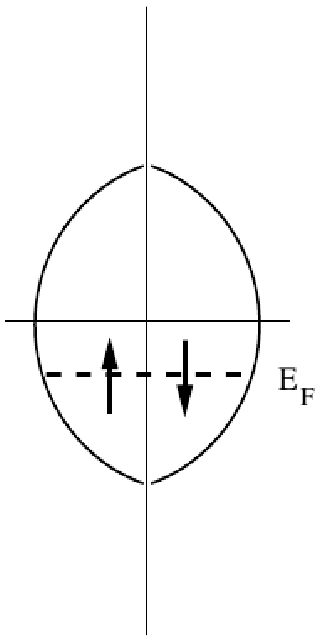
$$S_{\mathrm{eff}} \approx \int_0^\beta d\tau \int_0^\beta d\tau' c^*_{0\sigma}(\tau)(\mathcal{G}_0^{-1}(\tau,\tau') - \epsilon) c_{0\sigma}(\tau') + \int_0^\beta d\tau U n_{0\downarrow}(\tau) n_{0\uparrow}(\tau)$$

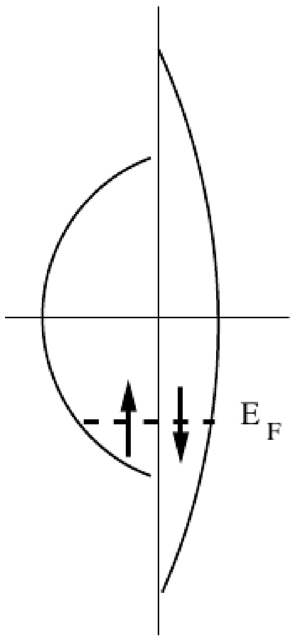
Results - magnetization

Spin-independent disorder: $m = 0$

Spin-dependent disorder: $m \neq 0$



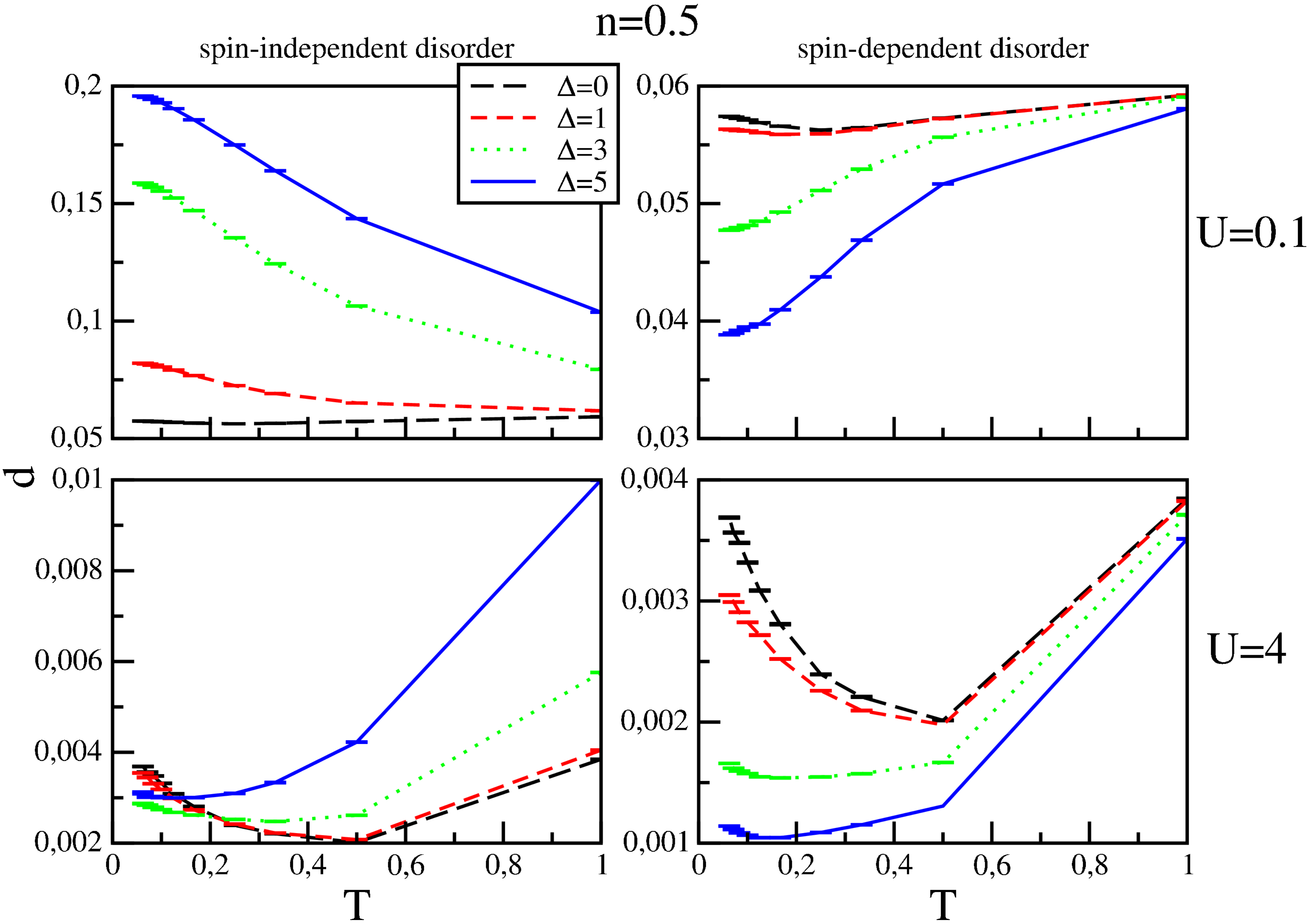




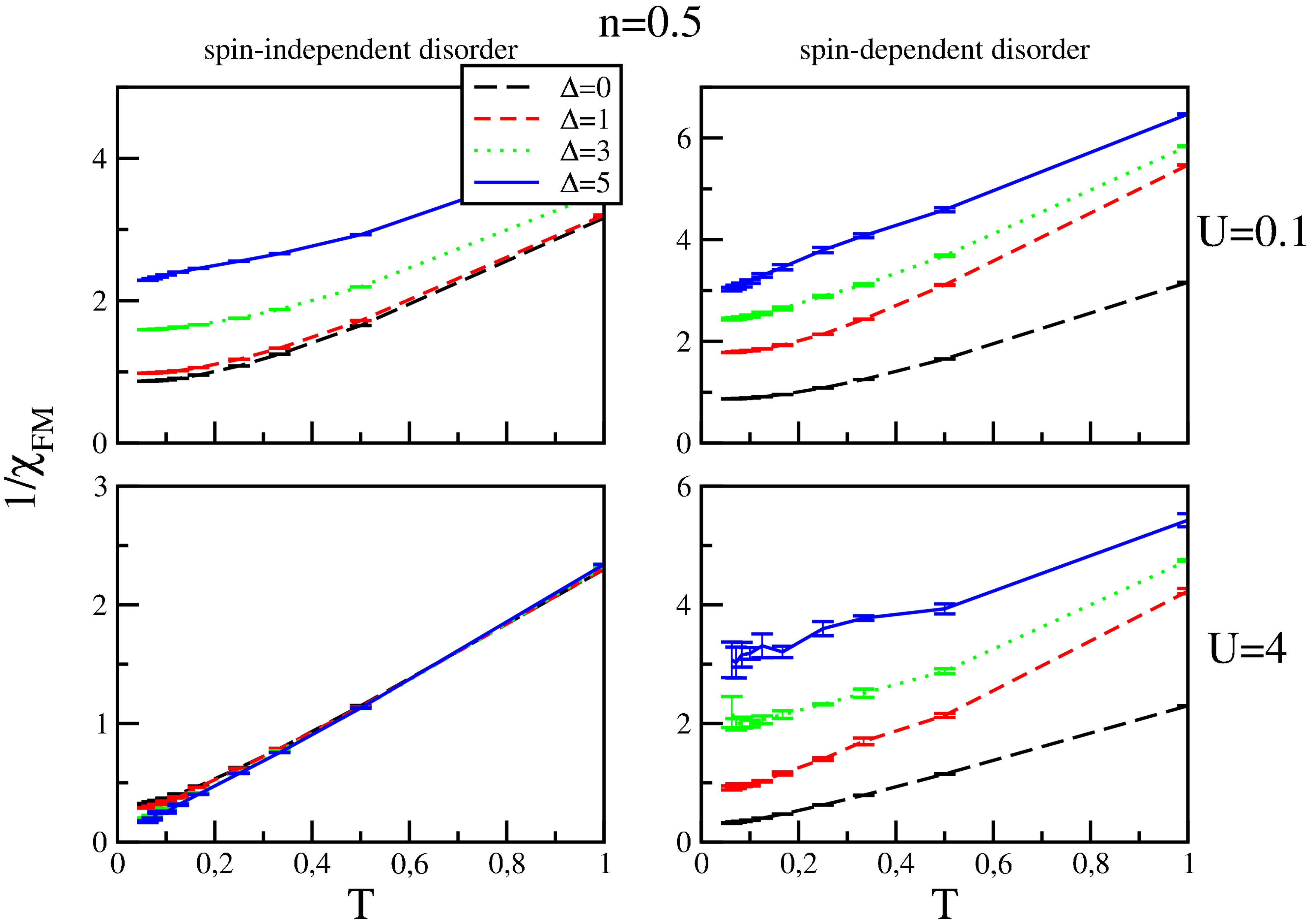
n=0.5 ; T=1/16

not so significant U dependence
- magnetization by noninteracting system

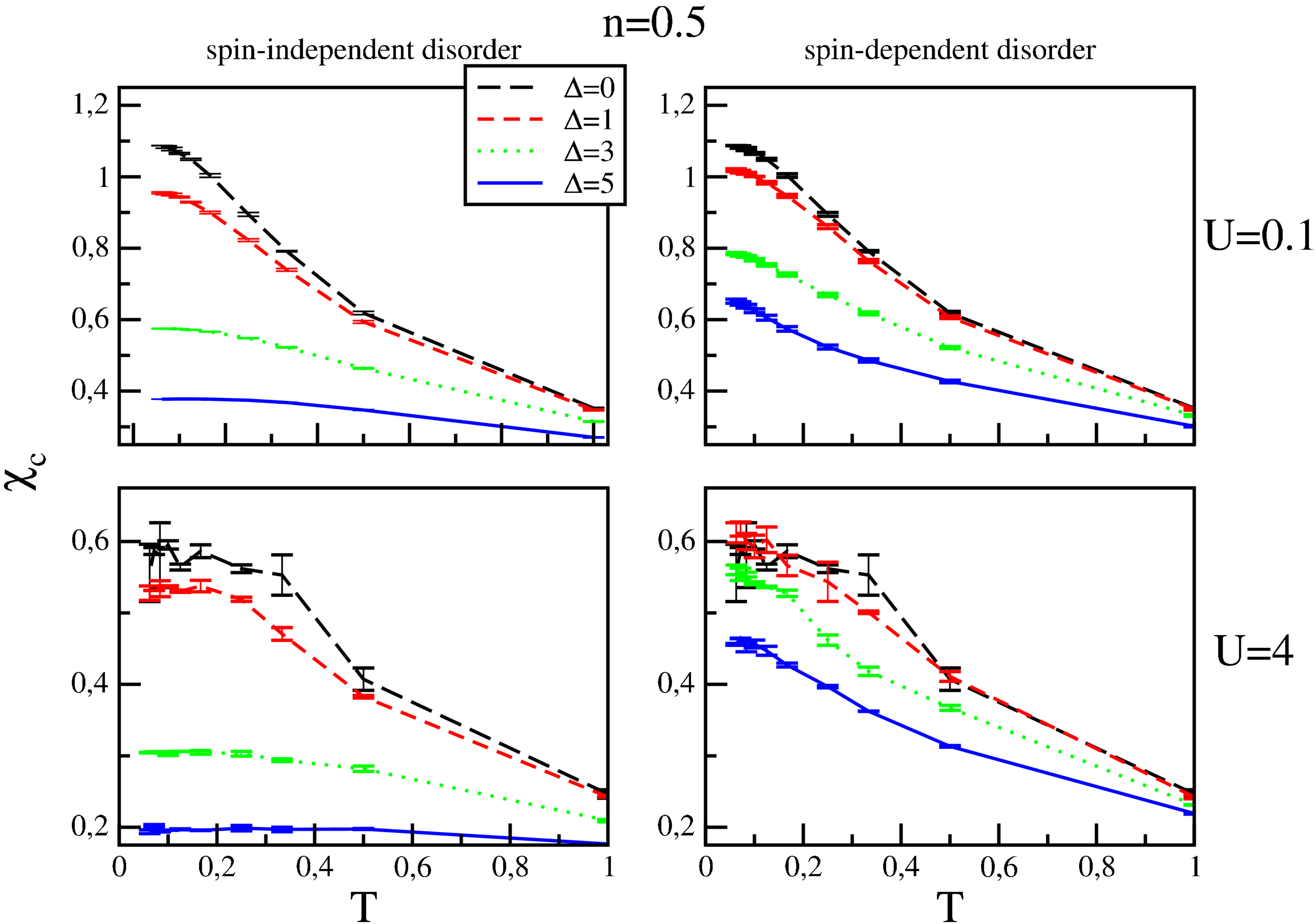
Results – double occupation



Results – ferromagnetic susceptibility



Results – charge susceptibility



Hubbard model with spin-dependent disorder

Spin imbalanced system

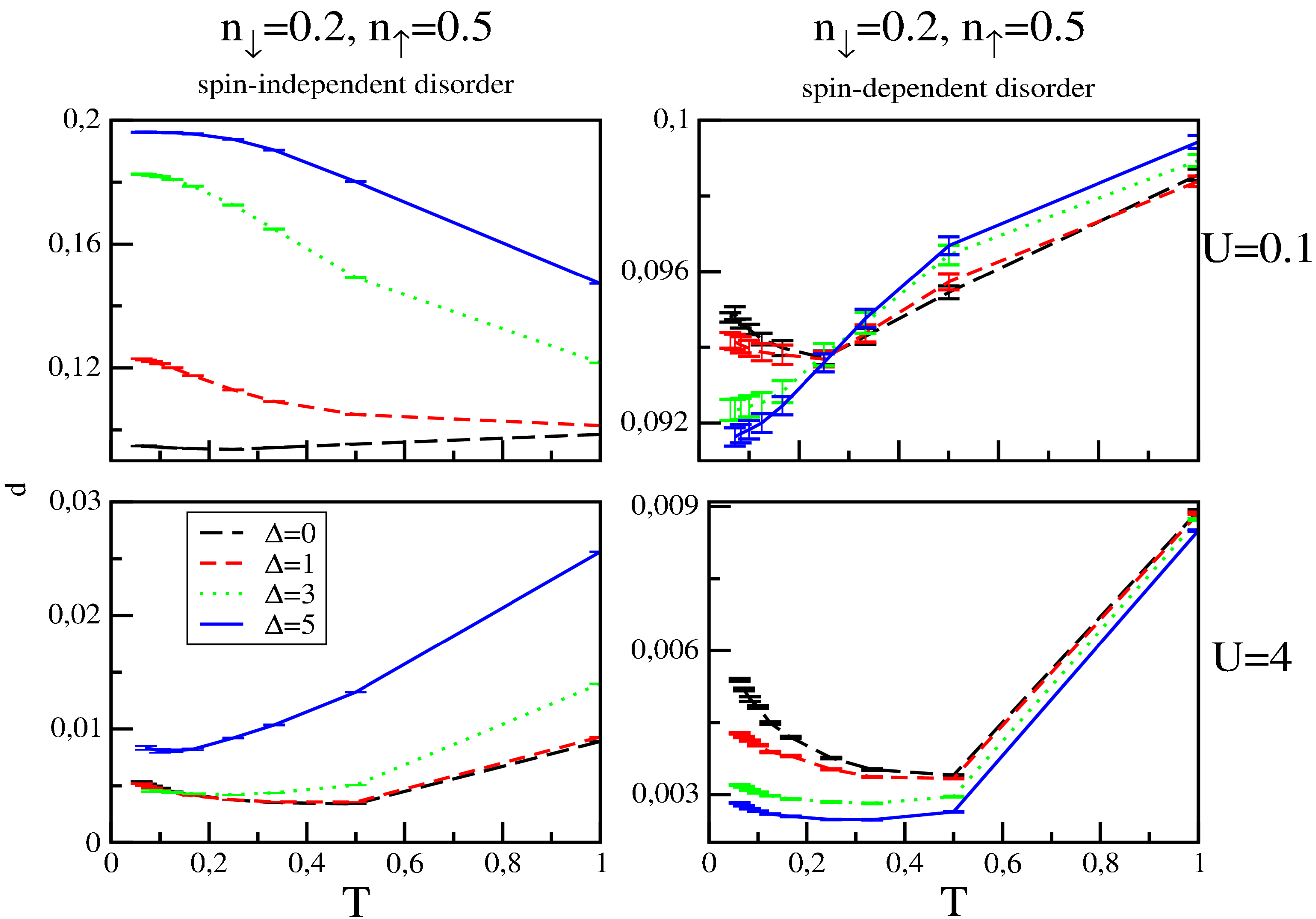
Spin-imbalanced system - fixed $n_\uparrow, n_\downarrow$

Grand canonical Hamiltonian for spin-imbalanced system:

$$H = t \sum_{(i,j)} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \sum_i \sum_{\sigma=\uparrow,\downarrow} \epsilon_{i\sigma} \hat{n}_{i\sigma} + \sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu_\uparrow \sum_i \hat{n}_{i\uparrow} - \mu_\downarrow \sum_i \hat{n}_{i\downarrow}$$

Densities fixed → constant magnetization

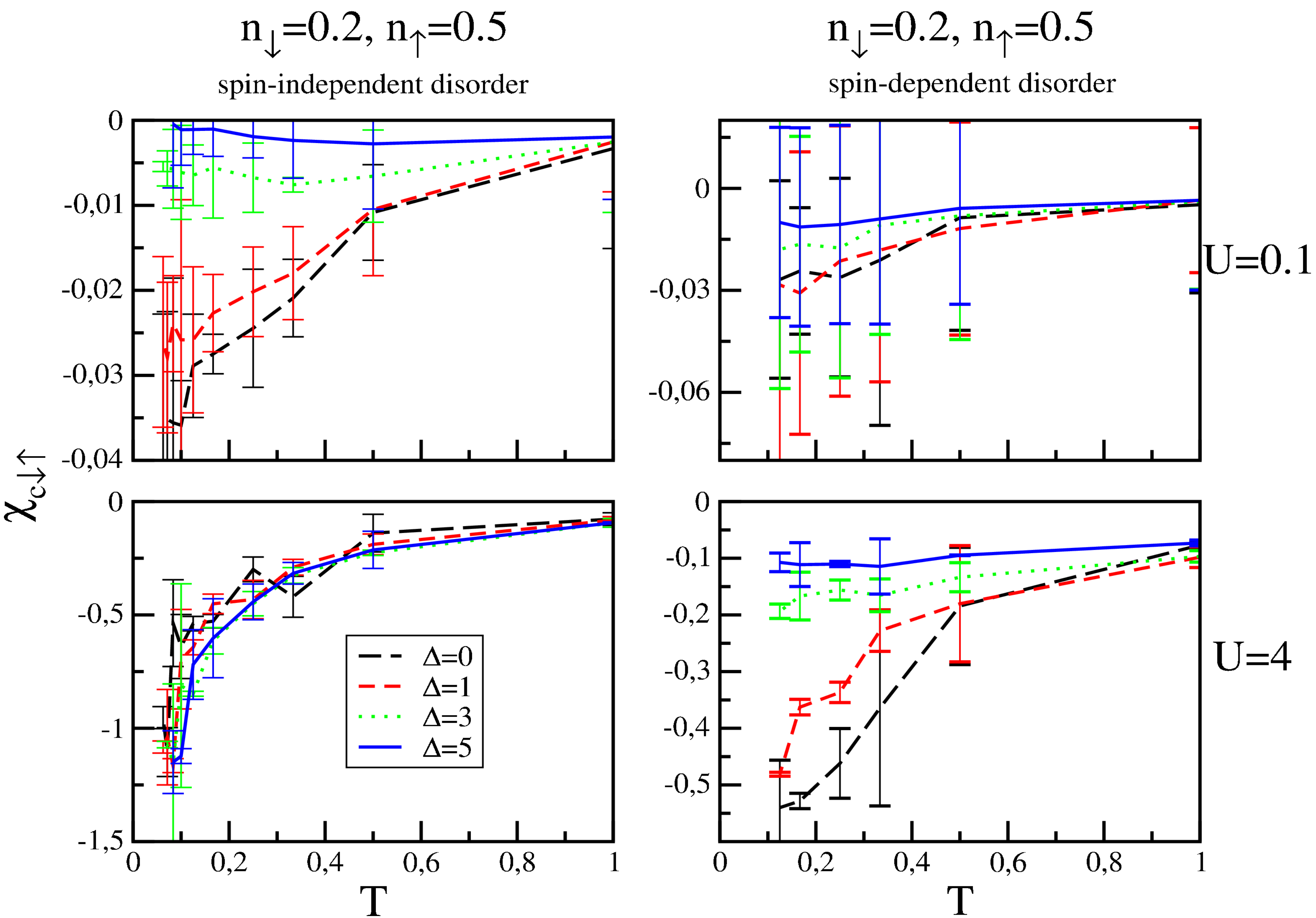
Results – double occupation



Off-diagonal compressibility

$$\chi_{c\sigma\sigma'} = \left(\frac{\partial n_\sigma(\mu_\uparrow, \mu_\downarrow, T)}{\partial \mu_{\sigma'}} \right)_T = \beta \langle \langle \hat{n}_\sigma \hat{n}_{\sigma'} \rangle - \langle \hat{n}_\sigma \rangle \langle \hat{n}_{\sigma'} \rangle \rangle_{\mathrm{dis}} / N_L$$

Results - off-diagonal compressibility



Results – other physical properties

Other thermodynamical properties can be found in:

K. M, J. Skolimowski, P. B. Chakraborty, K. Byczuk, D. Vollhardt, 2013, arXiv:1302.3395