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

Karol Makuch

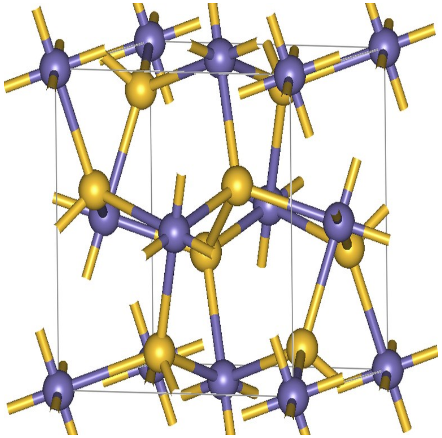
WYDZIAŁ FIZYKI UNIWERSYTET WARSZAWSKI

J. Skolimowski, K. Byczuk (University of Warsaw)
P. B. Chakraborty (Indian Statistical Institute, Chennai Centre)
D. Vollhardt (University of Augsburg)

Lublin, 01.04.2014

INNOVATIVE ECONOMY NATIONAL COHESION STRATEGY
FNP Foundation for Polish Science
EUROPEAN UNION EUROPEAN REGIONAL DEVELOPMENT FUND

Introduction



Electrons in crystal play a key role in such phenomena as e.g.:
-magnetism
-conductivity

Electrons in crystal

Hamiltonian for electrons in crystalline potential

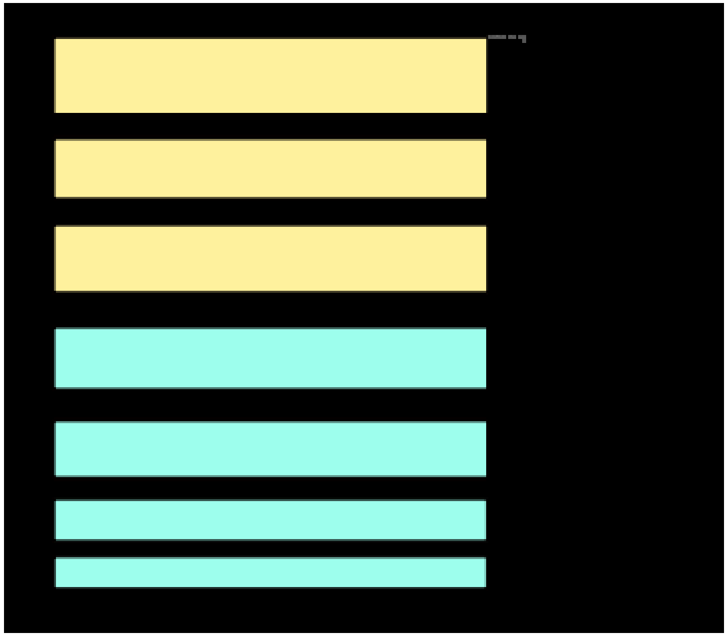
$$H = \sum_{i=1}^{N} \frac{(-i\hbar\nabla_i)^2}{2m} + \sum_{i=1}^{N} V_{ions}(\vec{r}_i) + \sum_{i=1}^{N}\sum_{j<i}^{N} U_{Coulomb}(\vec{r}_i - \vec{r}_j)$$

Kinetic energy

Periodic potential
from ions

Coulomb interactions
between electrons

Band structure



Noninteracting electrons:

Bloch's wave functions (single particle):

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{n\vec{k}}(\vec{r})$$

$$n = 0, 1, \ldots$$

Possible amount of $\vec{k}$ the same as number of lattice sites

Electrons in crystal - complicated

$$H = \sum_{i=1}^{N} \frac{(-i\hbar\nabla_i)^2}{2m} + \sum_{i=1}^{N} V_{ions}(\vec{r}_i) + \sum_{i=1}^{N}\sum_{j<i}^{N} U_{Coulomb}(\vec{r}_i - \vec{r}_j)$$

Wannier functions (localized):

$$W_{n\vec{R}_i}(\vec{r}) = \sum_{\vec{k}} e^{i\vec{k}\vec{R}_i}\psi_{n\vec{k}}(\vec{r})$$

Hamiltonian (second quantization)

$$H = \sum_{\alpha\beta} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \sum_{\alpha\beta} V_{\alpha\beta} a_\alpha^\dagger a_\beta + \sum_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger U_{\alpha\beta\gamma\delta} a_\delta a_\gamma$$

spin

$\vec{R}_i$ lattice site

$$n = 0, 1, \ldots$$

Hubbard model

$$H = \sum_{\alpha\beta} t_{\alpha\beta} a^\dagger_\alpha a_\beta + \sum_{\alpha\beta} V_{\alpha\beta} a^\dagger_\alpha a_\beta + \sum_{\alpha\beta\gamma\delta} a^\dagger_\alpha a^\dagger_\beta U_{\alpha\beta\gamma\delta} a_\delta a_\gamma$$

-single energy band
-interactions only on the same lattice site

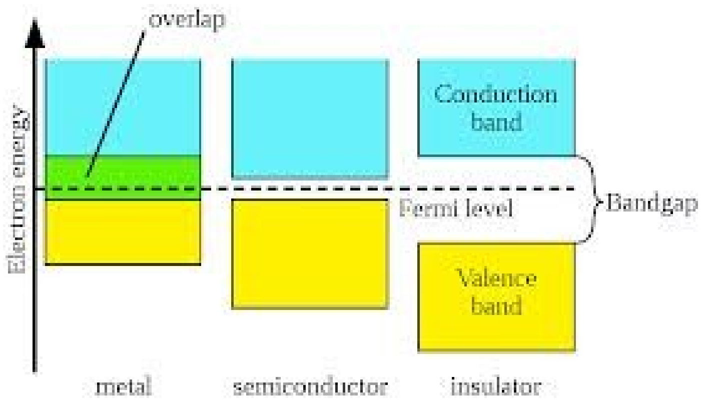
Electron correlations in narrow energy bands

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

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

Examples of types of insulators



Band insulators

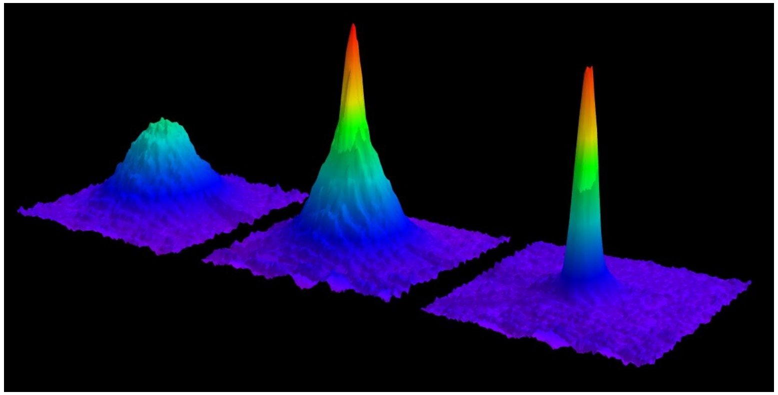
Mott insulators (by Coulomb interactions)

Anderson insulators (disorder)

Optical lattices

1997 Nobel prize to Steven Chu, Claude Cohen-Tannoudji and William D. Phillips "for development of methods to cool and trap atoms with laser light"

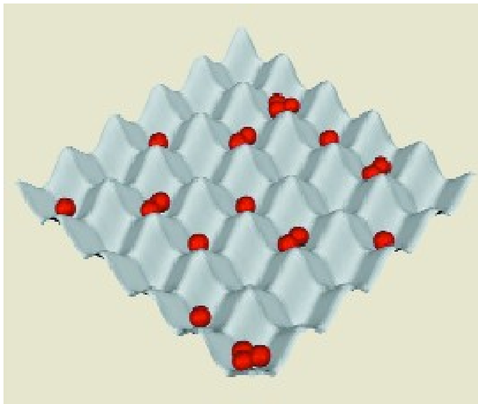
(1995) BEC: Eric A. Cornell, Wolfgang Ketterle, Carl E. Wieman



2001 Nobel prize, “for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"

Optical lattices

Neutral particles in optical lattice



I. Bloch, Phys. World 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

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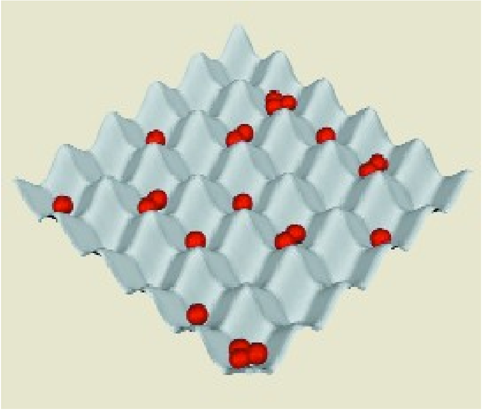
Optical lattices

Neutral particles in optical lattice



perfect crystal

very good realization of Hubbard model

Hubbard model not solved - optical lattice as quantum simulator

Optical lattices

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:

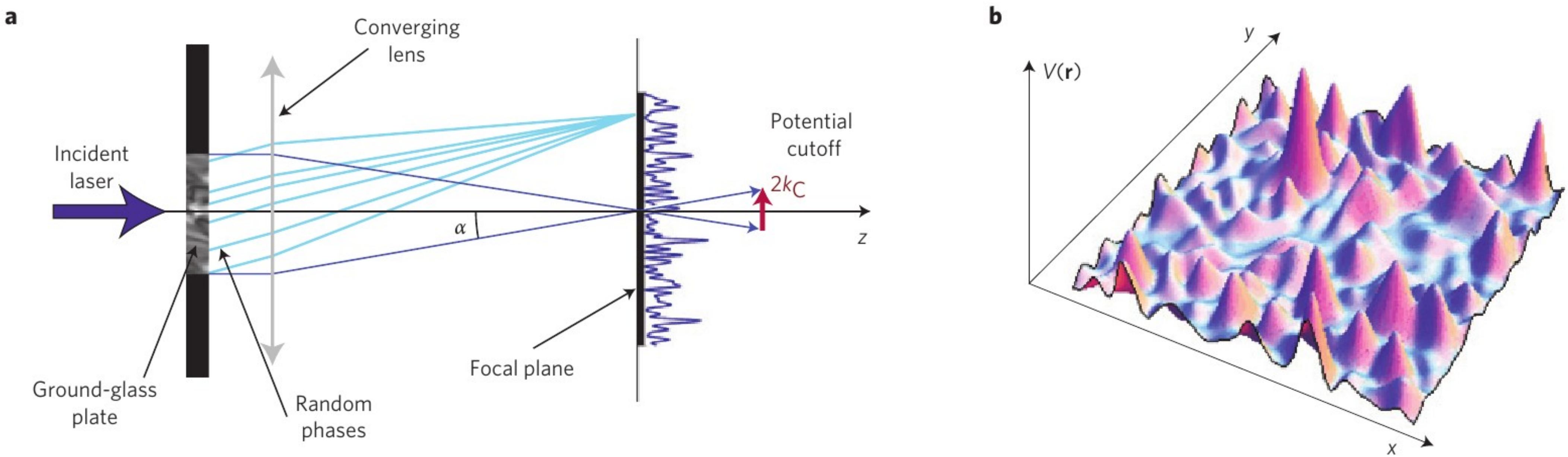
A Mott insulator of fermionic atoms in an optical lattice

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

NATURE | Vol 455 | 11 September 2008

Optical lattices – disorder

Optical lattice with disorder



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

2011:

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)

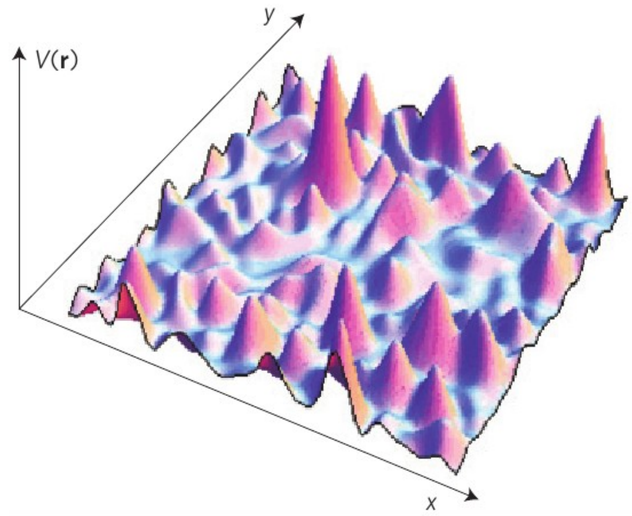
Comprehensive thermodynamics?

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)*

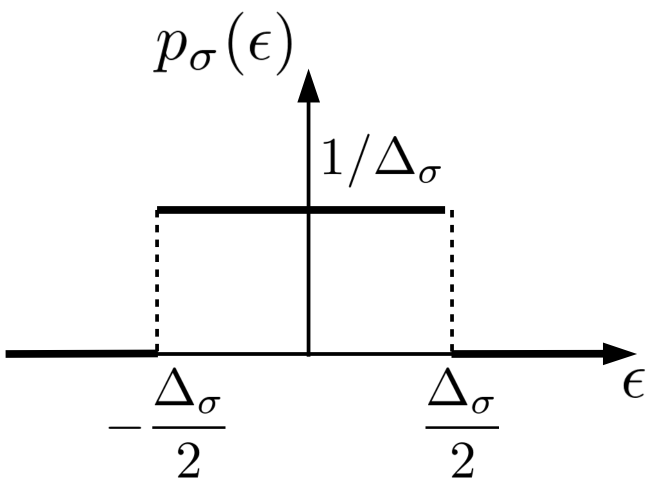
but: U<0, Bogolubov de Gennes mean field theory

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:

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

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

“time” ordering

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

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

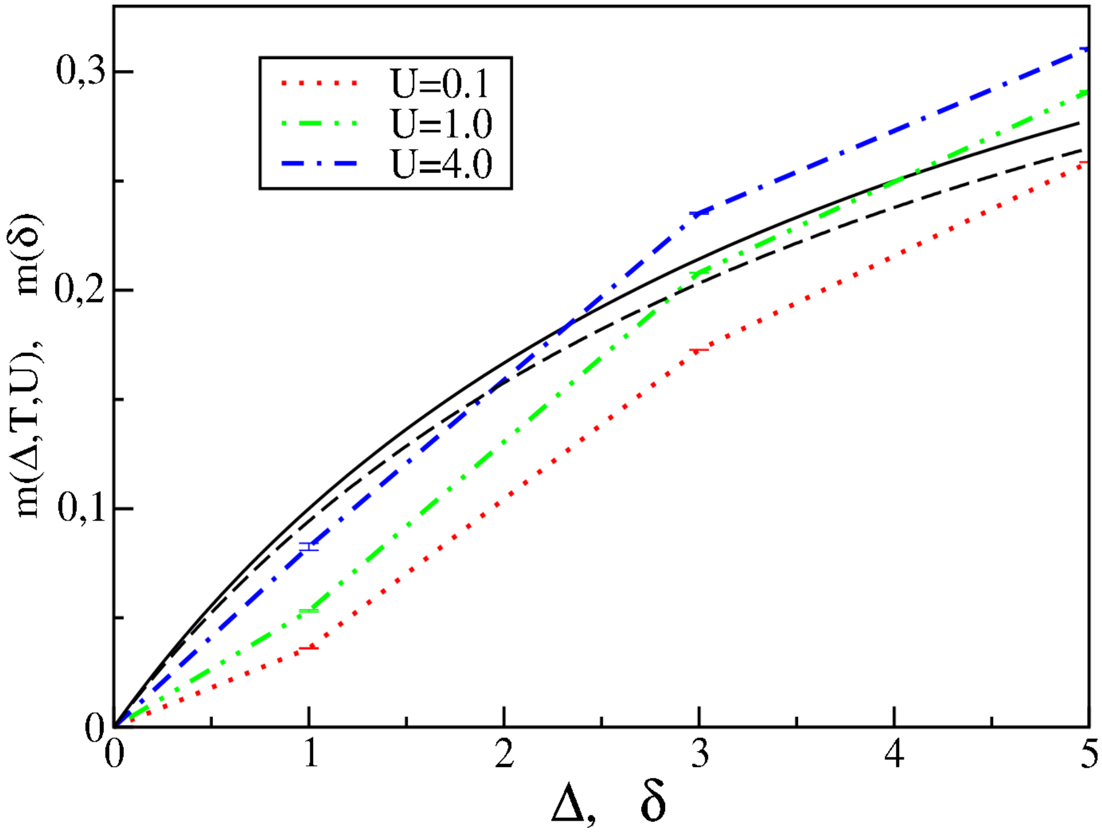
$$G_{00} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma G_{00}$$

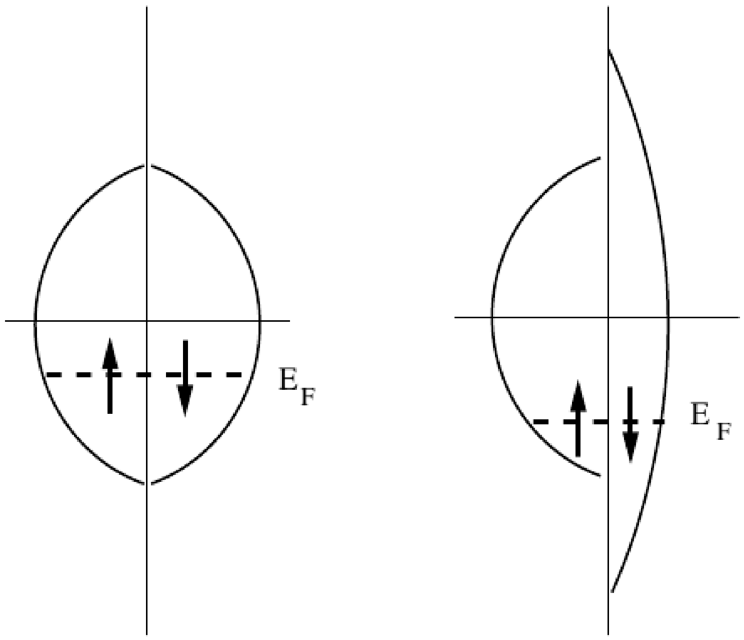
$$S_{\mathrm{eff}} \approx \int_0^\beta d\tau \int_0^\beta d\tau' c^*_{0\sigma}(\tau)(\mathcal{G}_0^{-1}(\tau,\tau') - \epsilon) c_{0\sigma}(\tau') + \int_0^\beta d\tau U n_{0\downarrow}(\tau) n_{0\uparrow}(\tau)$$

Results - magnetization

Spin-independent disorder: $m = 0$

Spin-dependent disorder: $m \neq 0$

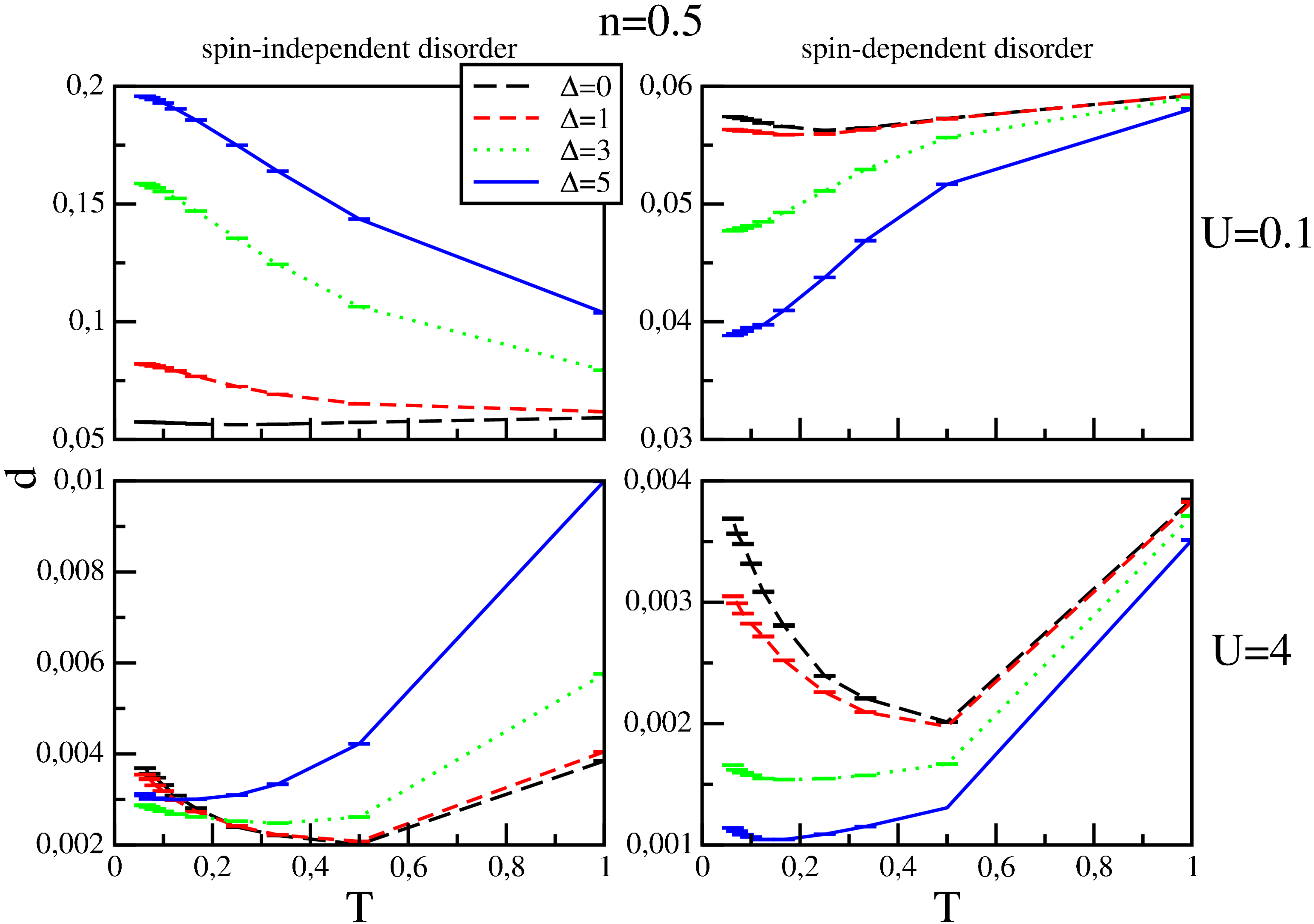




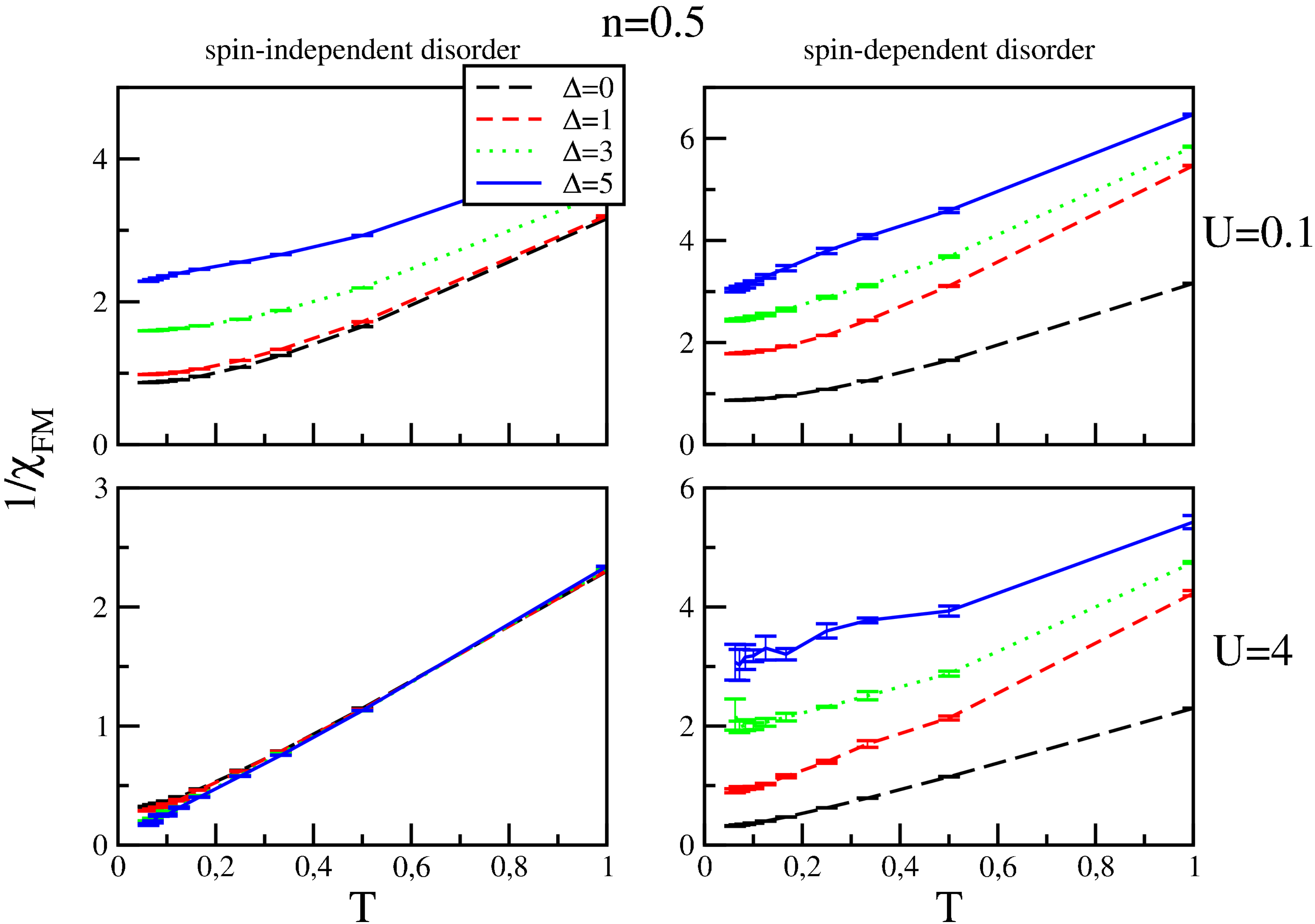
n=0.5 ; T=1/16

not so significant U dependence
- magnetization by noninteracting system

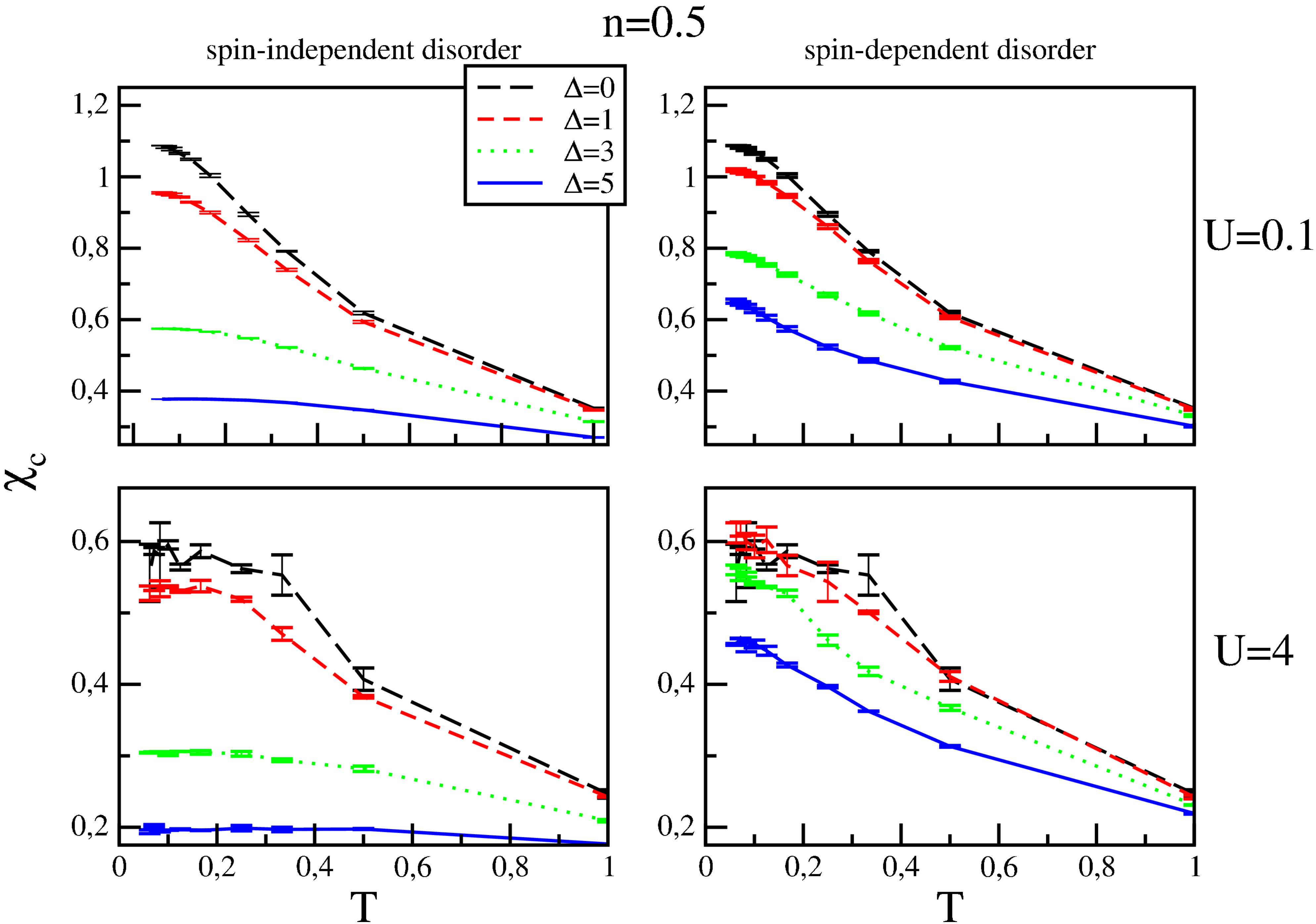
Results – double occupation



Results – ferromagnetic susceptibility



Results – charge susceptibility



Hubbard model with spin-dependent disorder

Spin imbalanced system

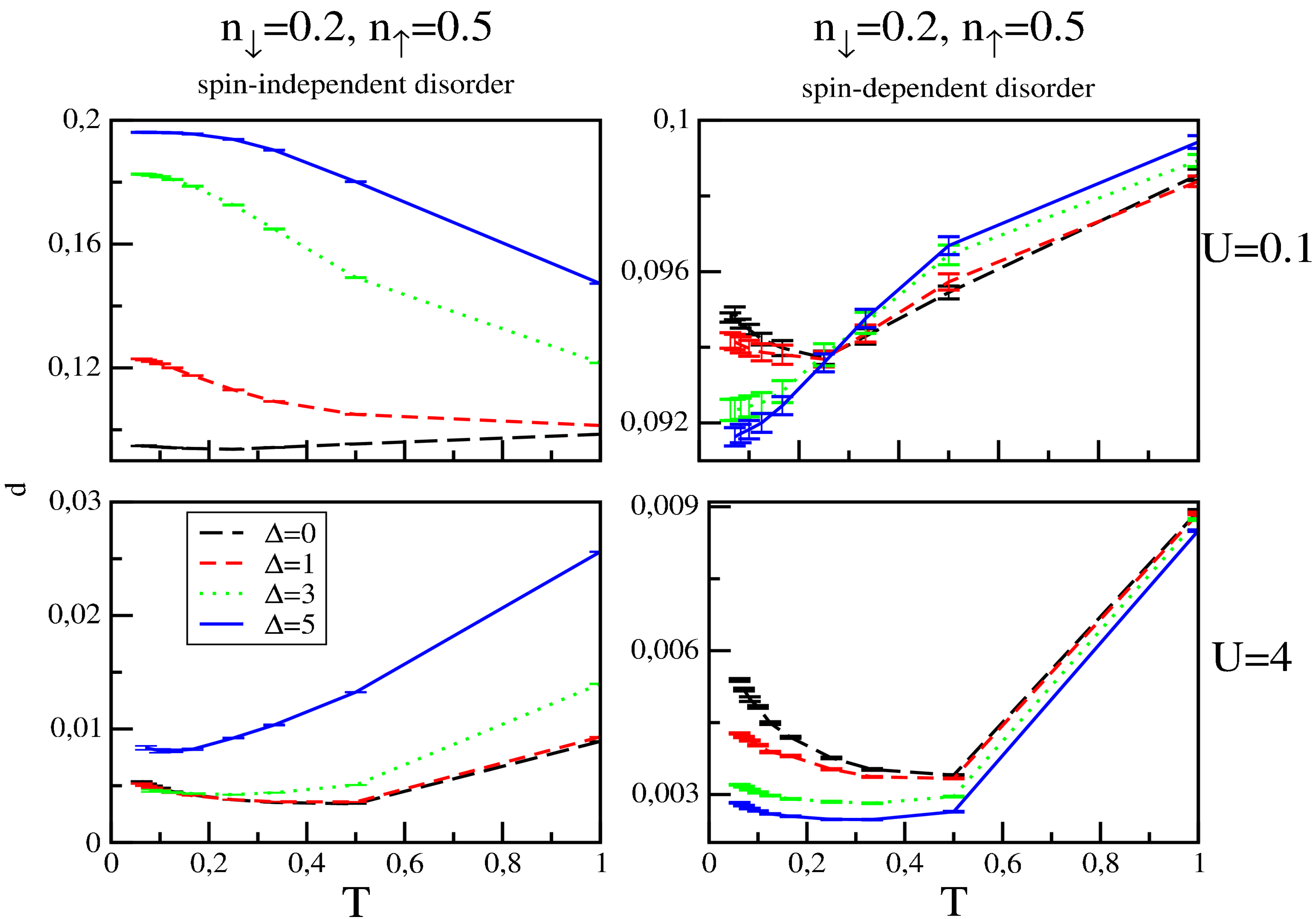
Spin-imbalanced system - fixed $n_\uparrow, n_\downarrow$

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

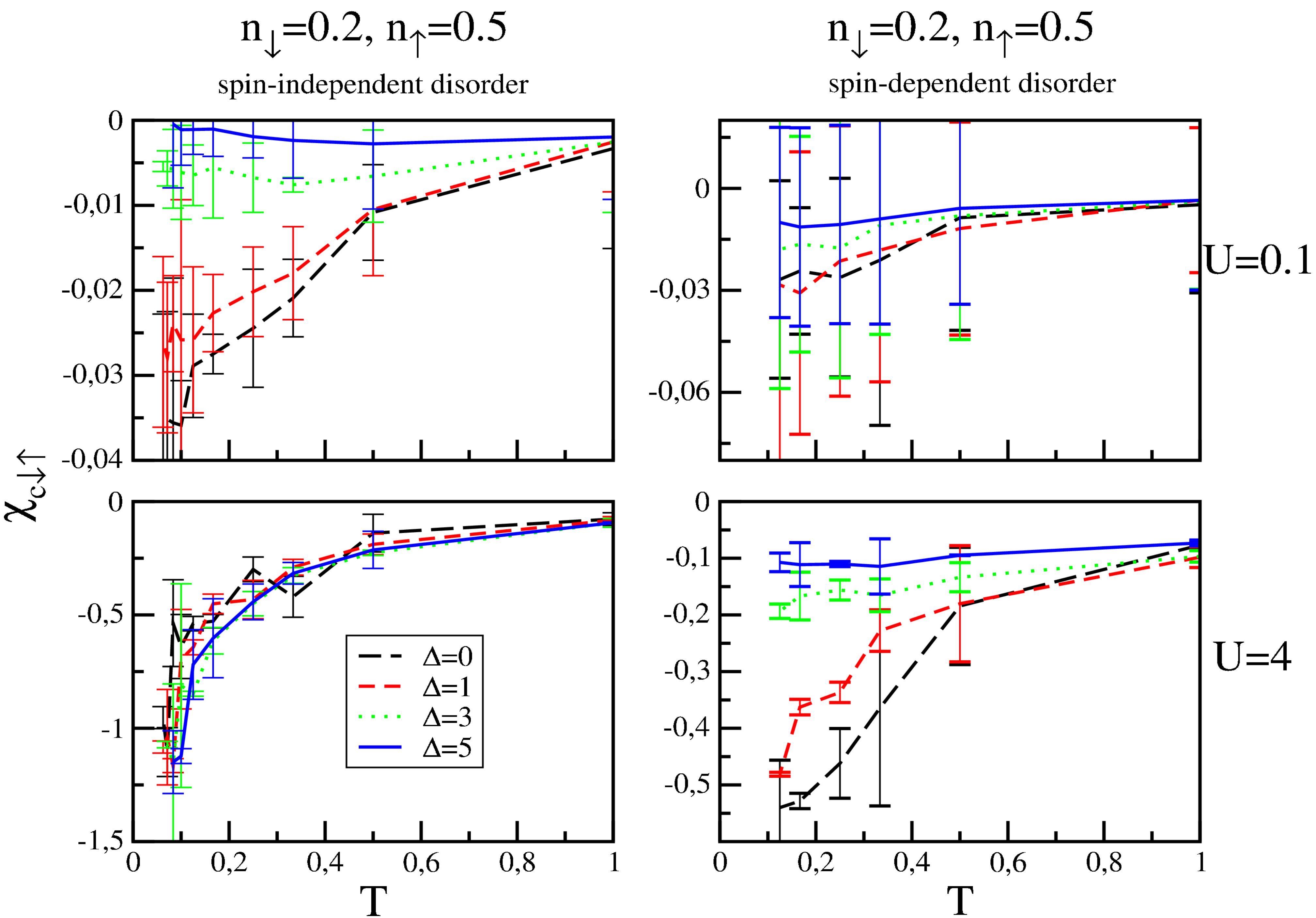
Results – double occupation



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, New J. Phys. 15, 045031 (2013)

Further work:
-lower temperatures, investigation of localization, single impurity problem by Numerical Renormalization Group