1 Spin structure factor

Our experiment measures the bulk spin structure factor $\bar{S}_{\boldsymbol{Q}}$ for an inhomogeneous realization of the Hubbard model. Theoretical approaches such as QMC and NLCE consider a homogenous system with a finite number of lattice sites L^3 and calculate the structure factor

$$S_{\boldsymbol{Q}} = \frac{4}{L^3} \sum_{i,j} e^{i\boldsymbol{Q}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} \langle \sigma_{zi} \sigma_{zj} \rangle \tag{1}$$

In the local density approximation we can think of every point $\boldsymbol{r}$ of our lattice site as a homogeneous system for which $S_{\boldsymbol{Q}}(\boldsymbol{r})$ can be obtained. We can relate the measured bulk spin structure factor $\bar{S}_{\boldsymbol{Q}}$ to the local $S_{\boldsymbol{Q}}(\boldsymbol{r})$ as

$$\bar{S}_{\boldsymbol{Q}} = \frac{1}{N} \int S_{\boldsymbol{Q}}(\boldsymbol{r}) \, \mathrm{d}^3\boldsymbol{r} \tag{2}$$

The NLCE data provided by Ehsan gives $S_{\boldsymbol{Q}}$ directly whereas the QMC data provided by Thereza gives $S_{\boldsymbol{Q}}/n$. To compare with experiment we have decided to use $S_{\boldsymbol{Q}}/n$ such that

$$\bar{S}_{\boldsymbol{Q}} = \frac{1}{N} \int \left[\frac{S_{\boldsymbol{Q}}}{n} \right]_{\boldsymbol{r}} n(\boldsymbol{r}) \, \mathrm{d}^3\boldsymbol{r} \tag{3}$$

Also, in our LDA calculations we have assumed that there is spherical symmetry in the system so

$$\bar{S}_{\boldsymbol{Q}} = \frac{4\pi}{N} \int \left[\frac{S_{\boldsymbol{Q}}}{n} \right]_{r_d} n(r_d) \; r_d^2 \, \mathrm{d}r_d \tag{4}$$

where r_d is the distance from the origin along a 111 body diagonal of the lattice. This last point can generate significant discussion since away from the diagonal the lattice depths are different along the x, y, z directions and an anisotropic Hubbard model should be used. However, for simplicity this is how we decided to treat the system.

2 NLCE data

Ehsan has provided us with exact NLCE (numerical linked-cluster expansion) data down to $T/t = 1.6$. Below this temperature he can do a resummation to obtain the thermodynamic quatities. At values of the temperature around $T/t = 0.4$ the results start getting very noisy, however we can recover a useable data set by applying a low pass filter to the data[1]. The original data and the filtered data are shown in Fig. 1. Larger T/t values are less noisy, but the filter is still used up to $T/t = 1.4$ to remove some spurious points that show up in the data. At $T/t > 1.6$ the data is exact and it has no spurious points.

We can use the NLCE data to see that the density as a function of chemical potential is pretty much frozen for $T/t < 1.0$, see Fig. 2. The high temperature series expansion (HTSE) that I was using before to calculate density profiles works down to about $T/t \approx 1.6$, so I was unable to capture the "Mottness" of the density profile as we see it in the experiment.

The data for S_π/n provided by NLCE is shown in Fig. 3. Notice that to avoid errors when dividing by a small value of n we have decided to force all data to 1 for densities less than a density cutoff. The density cutoff is adjusted for each value of U/t.

[1]The type of filter used is the Savitzky-Golay filter `http://www.wire.tu-bs.de/OLDWEB/mameyer/cmr/savgol.pdf`

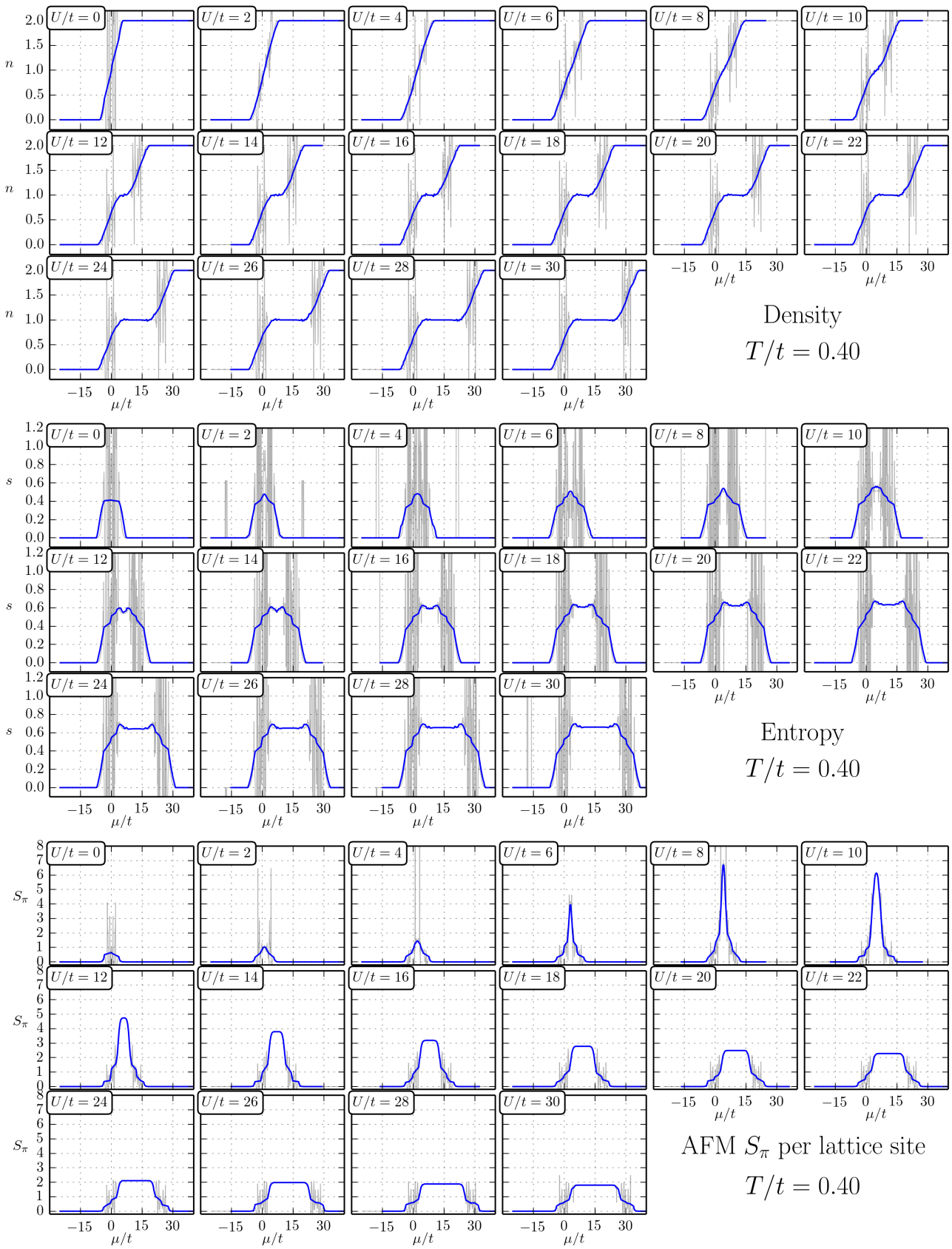

Figure 1: Lowest temperature data accessible to the NLCE by extrapolation, $T/t = 0.4$. The original data provided by Ehsan is shown in gray and the data after filtering is shown in blue.

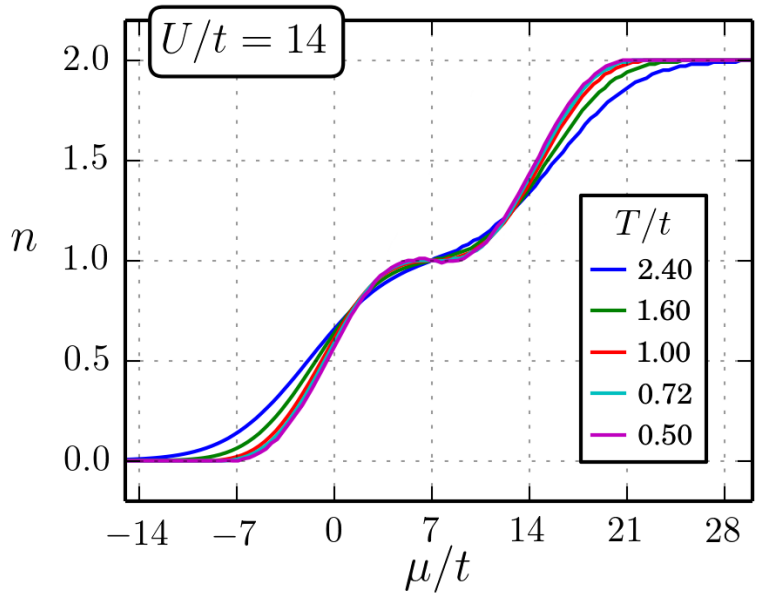

Figure 2: NLCE data at $U/t = 14$. For $T/t \leq 1$ the density does not shown much variation.

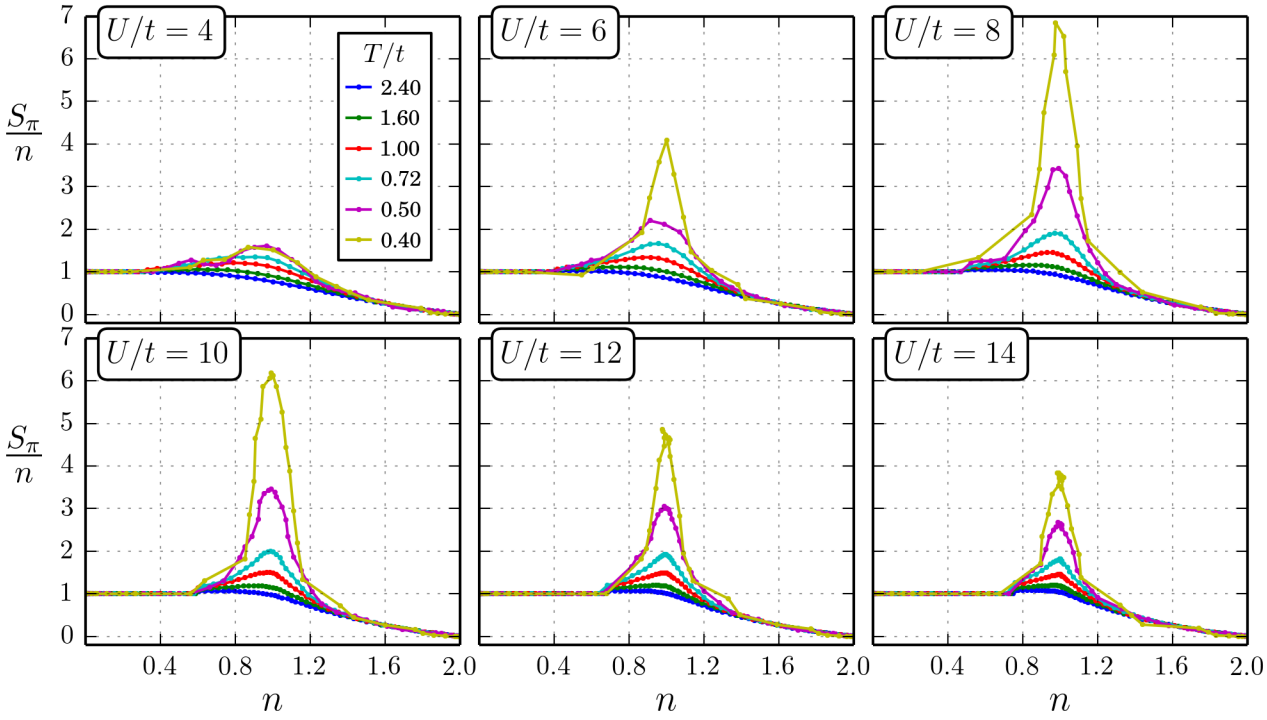

Figure 3: NLCE S_π/n data for various interactions and tempeatures.

3 QMC data

The QMC data does not suffer from noise problems for small values of T/t, however there is much less of it available. Fig. 4 shows the available U/t and T/t values. The entropy and double occupancy, not shown in the Figure are also available from Thereza's dataset, as well as the structure factor in the $\boldsymbol{\theta}$ direction.

4 NLCE data and QMC data comparison

In Fig. 5 we show QMC and NLCE datasets side on the same plot. A direct comparison is possible at $U/t = 6$, and then the QMC data at $U/t = 7$ is compared with NLCE at $U/t = 8$ which reveals that the NLCE structure factor is perhaps too broad as a function of n. It is clear from this plots that the density is frozen for $T/t < 1.0$ and that both QMC and NLCE have very good agreement on the density.

5 Comparison of experimental data with theory

The way we will proceed is as follows:

1. Set up a trap geometry based on our experimental calibration. The trap geometry determines the local chemical potential, the local U/t and the local T/t.
2. Use the NLCE data to calculate a density profile with the above parameters. The temperature used needs to be $T/t < 1.0$, since $n(\mu)$ is frozen below this temperature, the obtained density profile is good for all $T/t < 1$.
3. Set a value of $[T/t]_0$, this is the local value of T/t at the center of the trap. Use the local n (from 2) along with the local U/t and T/t to calculate the local S_π/n.
4. Integrate the local S_π/n over the trap to obtain the bulk spin structure factor $\bar{S}_\pi$.
5. Repeat 3 and 4 for different valus of $[T/t]_0$ until the resulting $\bar{S}_\pi$ agrees with the experimental measurement.

From the discussion in the previous section we have established that the density is very well characterized by either the NLCE or the QMC data. On the other hand, S_π/n is not so good from NLCE at low temperatures and is not availabe for many U/t and T/t from QMC. For comparing with theory we have put together a combined QMC + NLCE data set and for step 3 in the prescription we interpolate linearly between the available points in the data set in order to get S_π/n at arbitrary values of n, U/t and T/t.

5.1 Density profiles with NLCE data

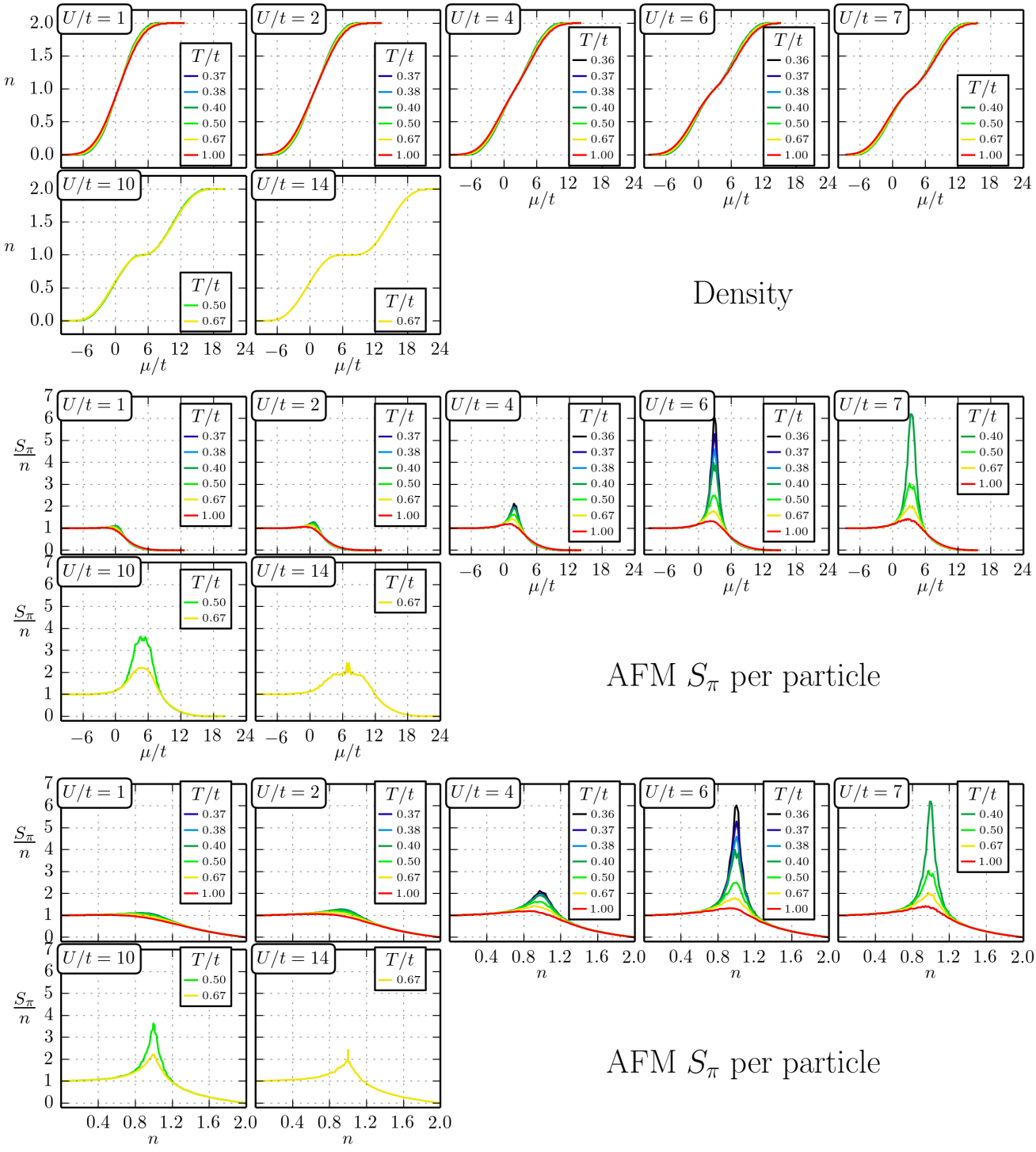

Figure 4: All available QMC data. Entropy, double occupancy and S_θ/n not shown.

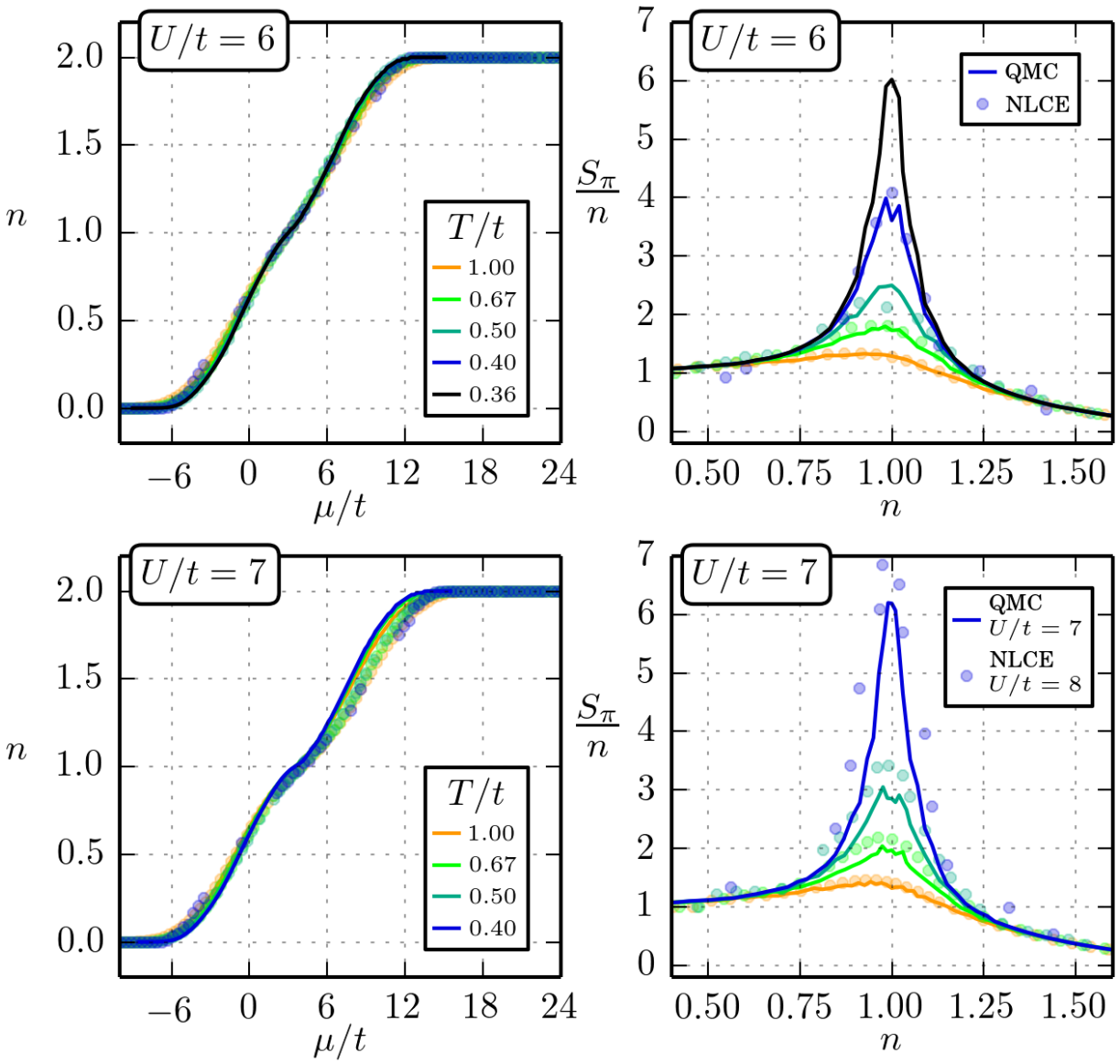

Figure 5: Comparison between QMC and NLCE data. At $U/t = 6$ both methods have data available whereas the QMC data at $U/t = 7$ is compared with the NLCE data at $U/t = 8$.