t-J Model: DQMC with Infinite U approach

- Project in collaboration with Richard Fye and Richard Scalettar

- Determinant Quantum Monte Carlo
- Infinite U in Hubbard and t-J models
- Approach 1: $U \to \infty$
- Approach 2: $U = \infty$
- Making DQMC code
- Checks of code
- Sign Problem
- Summary and Next

Determinant Quantum Monte Carlo

- Stochastic

- Can treat large systems

- Can not treat t-J model - can not handle subspace with no doubly occupied sites.

Determinant Quantum Monte Carlo

$$\hat{H} = \hat{K} + \hat{V}$$

$$\hat{K} = -t \sum_{<ij>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) - \mu \sum_{i\sigma} n_{i\sigma}$$

$$\hat{V} = U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right)$$

Trotter: $Z = Tr(e^{-\beta H}) \approx Tr(e^{-\Delta\tau V} e^{-\Delta\tau K})^L$, $\Delta\tau = \beta/L$.
$\hat{K}$ - quadratic form.
$\hat{V}$ - isn't. But can be made by Hubbard-Stratonovich transformation:

$$e^{-U\Delta\tau(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})} = \frac{1}{2} e^{-\frac{U\Delta\tau}{4}} \sum_s e^{\lambda s (n_\uparrow - n_\downarrow)},$$

$\cosh\lambda = e^{\frac{U\Delta\tau}{2}}$, $s = \pm 1$.

Infinite U in Hubbard and related models

$U = \infty$: Hard-core particles.

$t - J$ model:

$$\hat{H} = -t \sum_{<ij>\sigma} (\hat{a}^\dagger_{i\sigma} \hat{a}_{j\sigma} + H.c.) + J \sum_{ij} \vec{S}_i \cdot \vec{S}_j$$

- in the subspace with no doubly occupied sites.

Approach 1: $U \to \infty$

Doesn't work well in DQMC: with U increasing, calculations become unstable.

Richard Fye: Approach 2: $U = \infty$

$$H = H_1 + H_2,$$

$$H_1 = -t \sum_{<ij>\sigma} (\tilde{c}^{\dagger}_{i,\sigma} \tilde{c}_{j,\sigma} + H.c.)$$

$$H_2 = J \sum_{<ij>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j)$$

$$\tilde{c}_{i,\sigma} = c_{i,\sigma}(1 - n_{i,-\sigma})$$

Fye keystones:

Projection operator

$\tilde{c}$ operator

Projection operator

$P_0 \equiv$ Operator which destroys state with any double occupied site, otherwise acts as the identity operator.
Approximation:

$$P_0 \approx P = \prod_j e^{-U_P n_{j\uparrow} n_{j\downarrow}}$$

- If double occupancy for some j, $n_{j\uparrow} = n_{j\downarrow} = 1$, then for large U_P: $\quad P \approx 0$.

$$Z \approx Tr\left\{ e^{-\beta(H_1 - \mu N)} P \right\}$$

We find $U_P \sim 10$ is large enough for simulations.

$\tilde{c}$ operator

$$\tilde{c}_{i,\sigma} \equiv c_{i,\sigma}(1 - n_{i,-\sigma})$$

The use of $\tilde{c}_{i,\sigma} = c_{i,\sigma}(1 - n_{i,-\sigma})$ prevents one starting with a state with no double occupations and ending with a state with a double occupation.

$$c_i^\dagger c_j \rightarrow \tilde{c}_i^\dagger \tilde{c}_j$$

Shortcoming: quadratic term becomes power 6.
Can be simplified: With no double occupation result the same as

$$c_i^\dagger c_j \rightarrow \tilde{c}_i^\dagger c_j$$

- quartic

$\tilde{c}$ operator

For one time slice

$$e^{-\Delta\tau H_1} \approx \prod_{<ij>} \prod_{\sigma=\pm 1} e^{t\Delta\tau \tilde{c}^\dagger_{i\sigma} c_{j\sigma}} e^{t\Delta\tau \tilde{c}^\dagger_{j\sigma} c_{i\sigma}}$$

$$= \prod_{<ij>} \prod_{\sigma=\pm 1} e^{t\Delta\tau c^\dagger_{i\sigma} c_{j\sigma}(1-n_{i,-\sigma})} e^{t\Delta\tau c^\dagger_{i\sigma} c_{j\sigma}(1-n_{j,-\sigma})}$$

- May be decoupled using Hubbard-Stratonovich transformation, applying the general formula

$$e^{\alpha c_1^\dagger c_2 n_3} = e^{-\alpha_2 n_3} \left(\frac{1}{2}\right) Tr_\sigma e^{\sigma(\alpha_4 n_3 + \alpha_3 c_1^\dagger c_2)}$$

where
α_4 - arbitrary (and recommended $\approx \sqrt{t\Delta\tau}$),
$e^{\alpha_2} = \cosh(\alpha_4)$,
$\alpha_3 = \frac{\alpha}{\tanh(\alpha_4)}$.

First step: making DQMC code for Hubbard Model

Need: working Hubbard Model DQMC, then work on modifications.

$\Rightarrow$ Write my own Hubbard DQMC code.

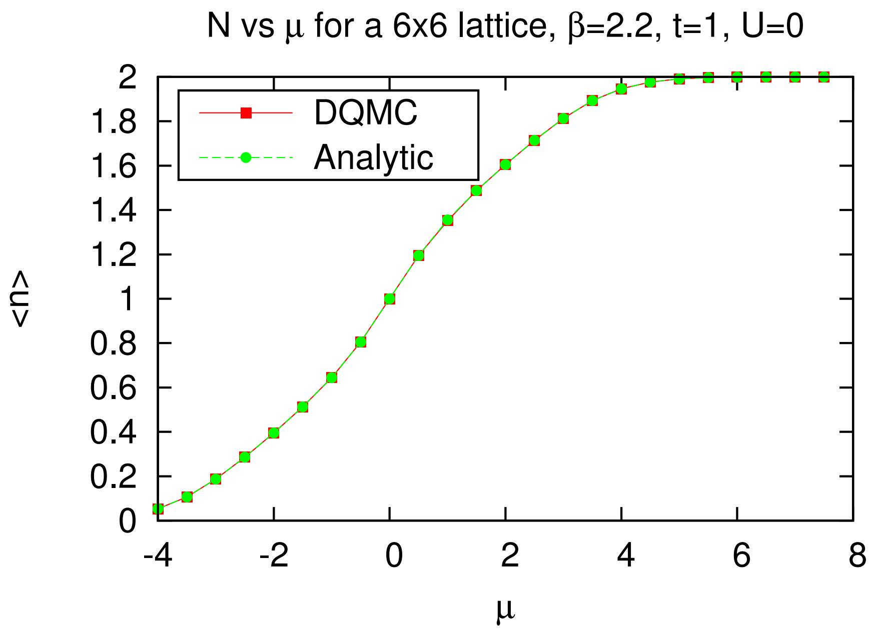
Checks of code

$U = 0$

Analytically: total occupancy

$$< n > = \sum_k \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}$$

$$\epsilon_k = -2t(\cos k_x + \cos k_y)$$

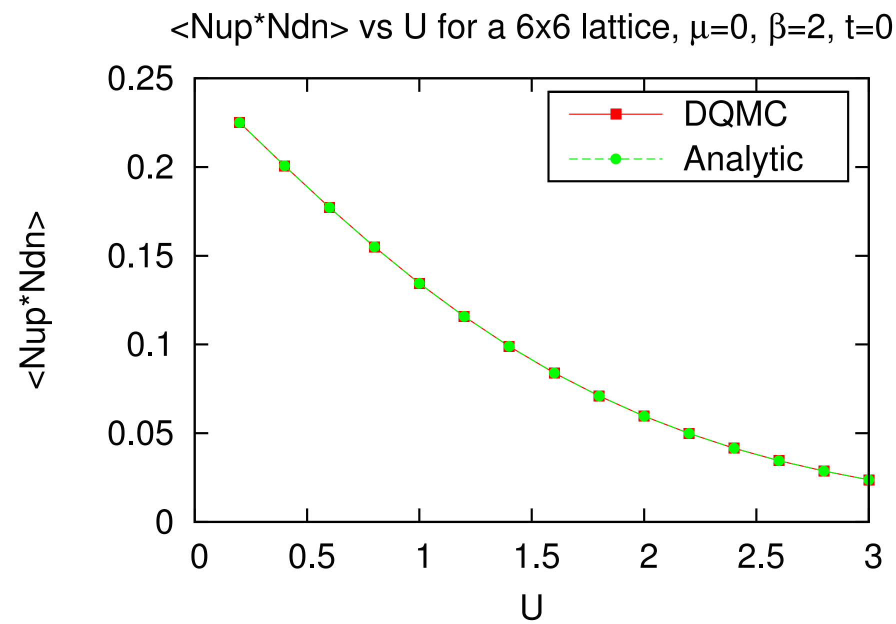


$t = 0$

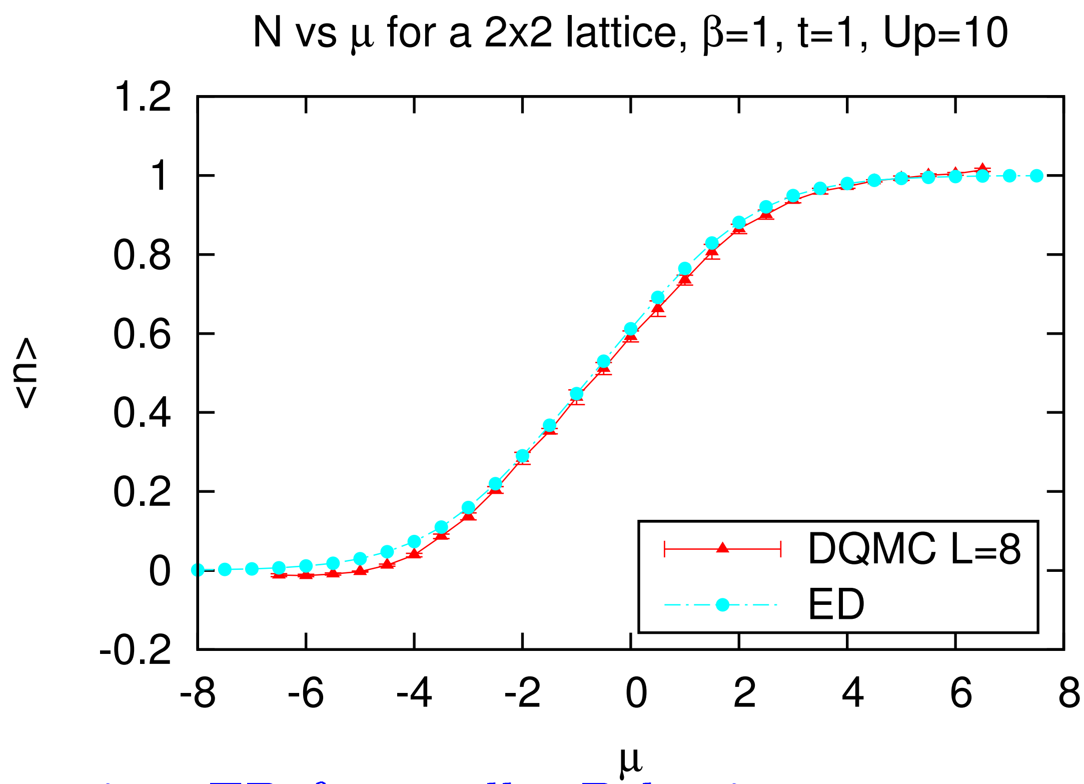
Analytically:

$$Z = Z_1^N$$

$$Z_1 = \sum \frac{1}{e^{\beta(\epsilon_i - n_i \mu)}}$$

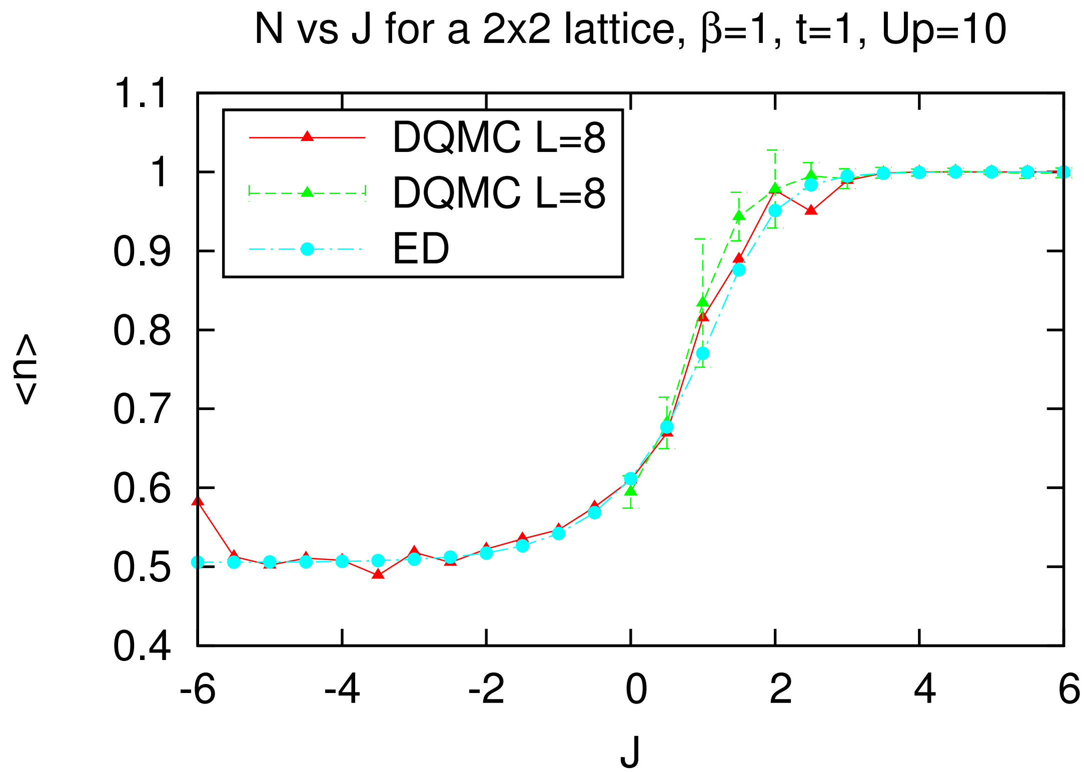


Checks of "Infinite U" Hubbard model against exact diagonalization



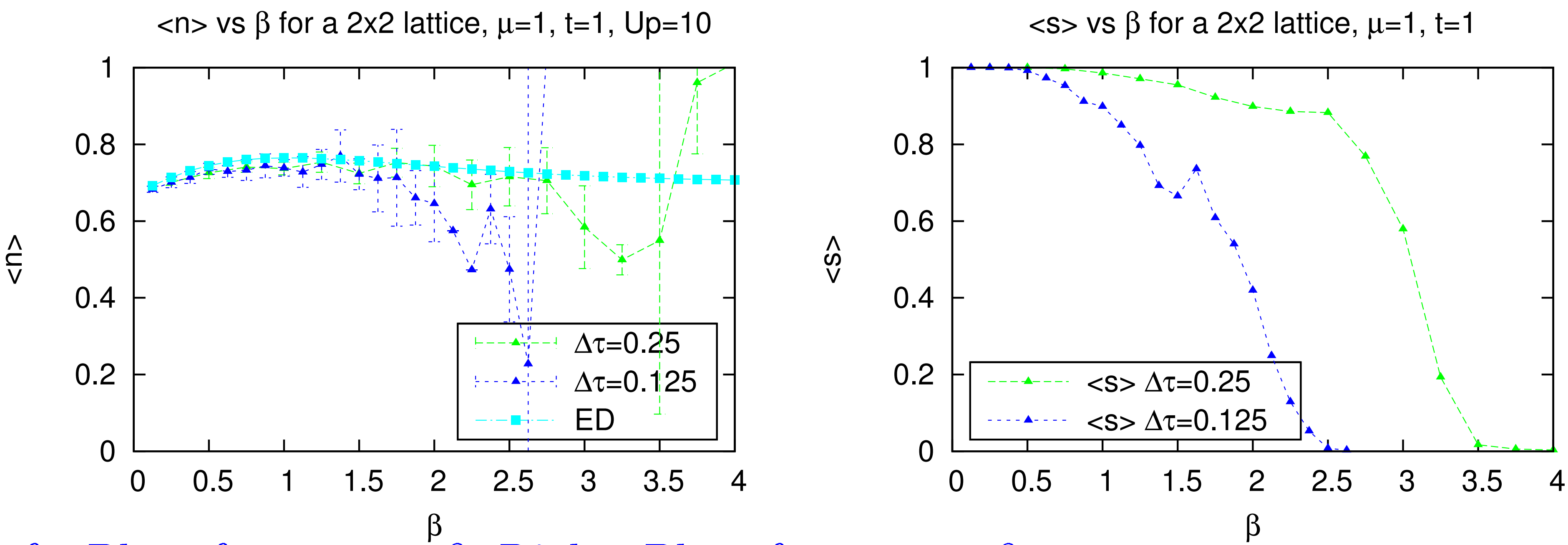
Checks of DQMC against ED for small 2-D lattice.

Spin part of the Hamiltonian



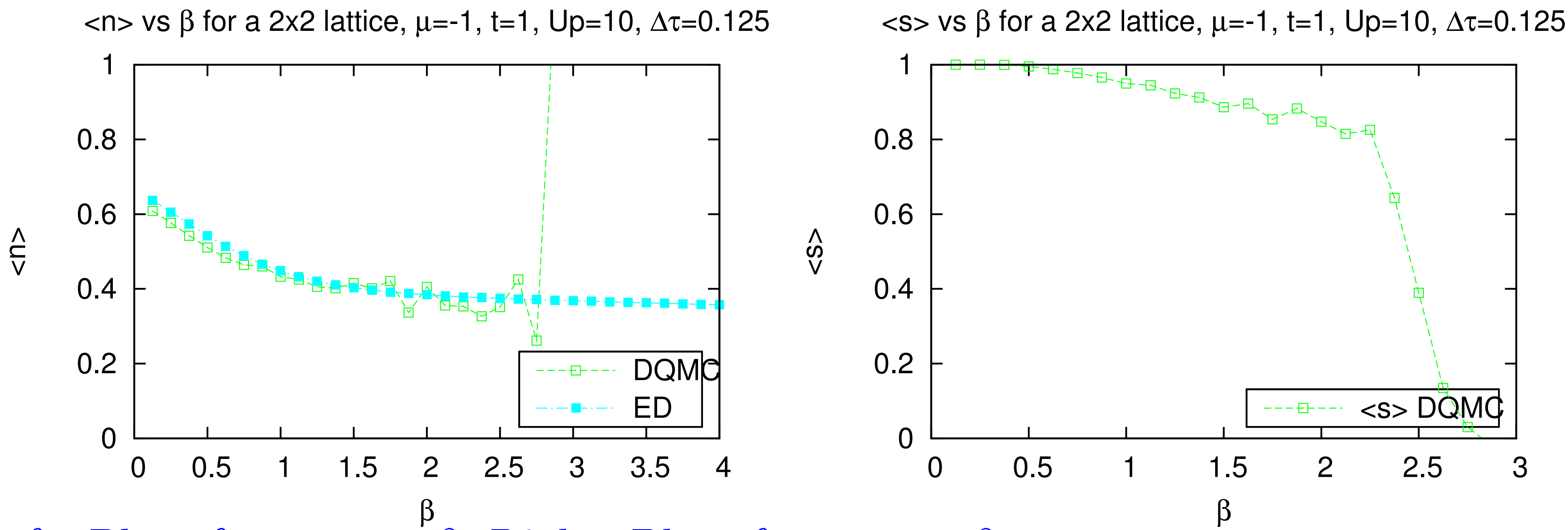
Plot of $< n >$ vs J without $S_{ix}S_{jx}$ and $S_{iy}S_{jy}$ part.

Sign Problem

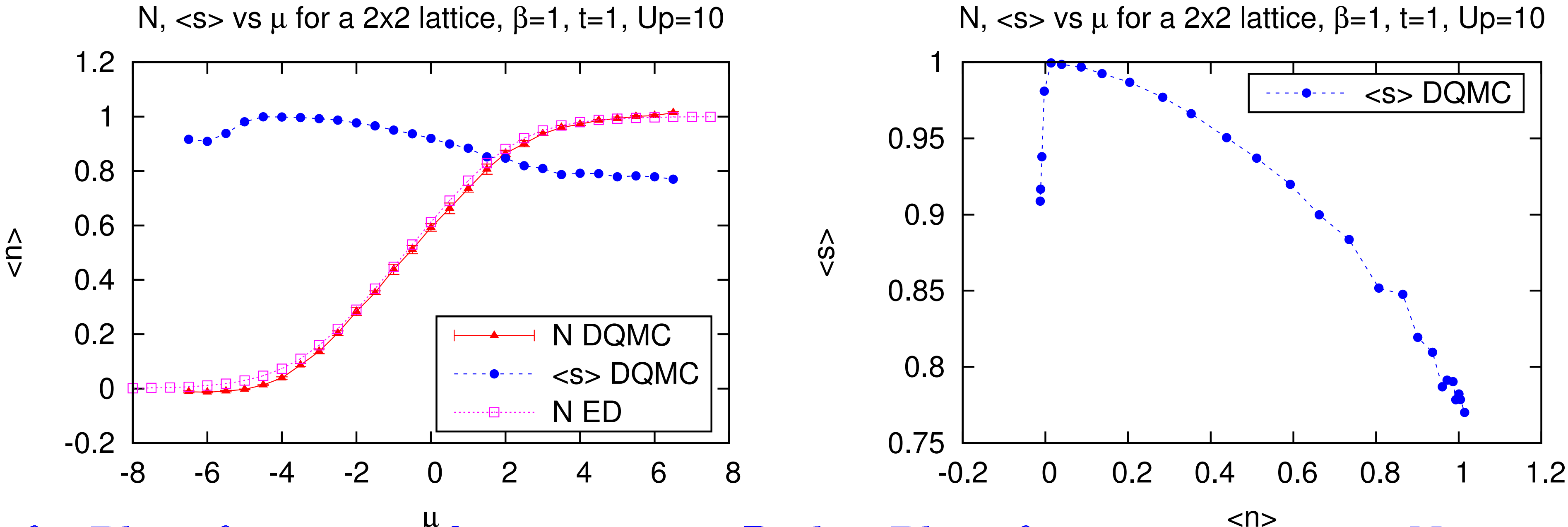


Left: Plot of $< n >$ vs β. Right: Plot of $< s >$ vs β.
As can be seen, $< s >$ falls too soon with increasing of β.

It was pointed out that I chose n so that the sign is the worst.
Trying with $\mu = -1$.



Left: Plot of $< n >$ vs β. Right: Plot of $< s >$ vs β.
Checking dependence of $< s >$ on $< n >$.



Left: Plot of $< n >$ and $< s >$ vs μ. Right: Plot of $< s >$ vs $< n >$. Not quite what is supposed to be: minimum of $< s >$ at $< n > \sim 0.8$.

For acceptable simulations, we need $< s > \geq \ 1/3$, for at least $\beta \ \leq \ 4$.

Summary

- Presented Infinite U approach to $t - J$ model
- Work on its realization
- Encountered serious sign problem

Next?

Sign problem: Major obstacle.

• H-S decoupling we used was non-Hermitian. May it be the reason for a bad sign problem? One possibility Fye suggests is to try a Hermitian break-up.

• Try to tune parameters? $\Delta\tau$, c_4, U_P, number of projection operators. The sign depends on them, but doesn't look like there may be a major difference. I however didn't do systematic investigation.