Magnetic phases of the Hubbard model

some answers from quantum simulations, the “old-fashioned” way

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Outline

- Itinerant ferromagnetism in Fermi gas - connect. w. Hubbard model
- Recent advances in quantum Monte Carlo
  - Phaseless appr. controls sign/phase problem in auxiliary-field QMC
  - Improves QMC accuracy, better convergence to thermodynamic limit
- Ferromagnetism in dilute Hubbard model?
- Antiferromagnetism in Hubbard models (connection with high-Tc?)
  - Optical lattices: **experimental simulation**? Advances in QMC --> synergy
  - What happens to the antiferromagnetic order upon doping?
    - prediction: incommensurate spin-density waves

Research Group:

- Chia-Chen Chang
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- Wirawan Purwanto
- Eric Walter
- Dorothy Xu

Support:

- ARO; NSF; DOE (QMC-endstation; ThChem; cmsn); NSF PRAC

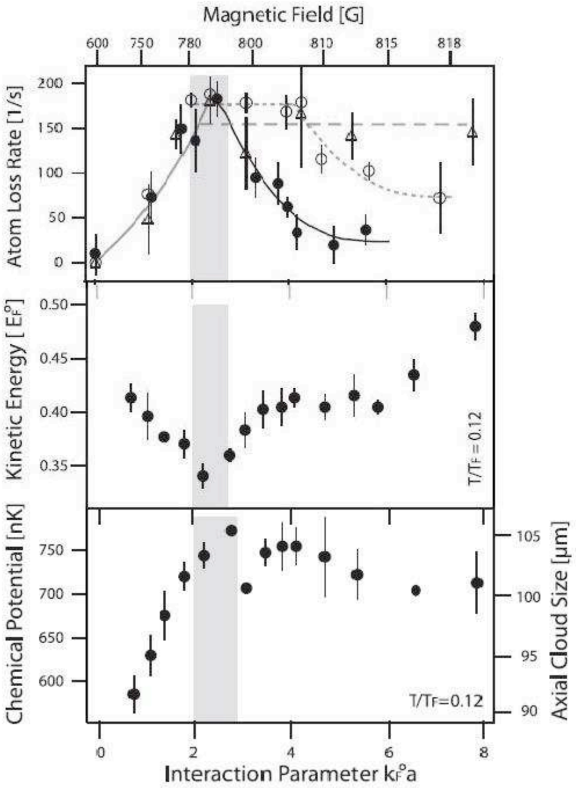
Some references: (http://physics.wm.edu/~shiwei)

- Zhang & Krakauer, PRL '03
- Al-Saidi et. al., PRB '06; JCP '06; JCP '06; JCP `07
- Suewattana et. al., PRB '07
- Kwee et. al., PRL `08
- Purwanto et. al., JCP '08; JCP '09
- Chang, Zhang & Ceperley, PRA (R) '10
- Chang & Zhang, PRB '08; PRL '10

Motivation

- What is the physical basis for ferromagnetism in metals?
- New interests: Expt aimed at emulating the Stoner Hamiltonian: hints of ferromagnetic instability observed in trapped Fermi gas

Jo et. al., Science ('09)



- At $T/T_F = 0.12$ (lowest used)
- A maximum in atom loss rate:

$$k_F^0 a \approx 2.5$$

- A minimum in kinetic energy:

$$k_F^0 a \approx 2.2,$$

- A maximum in cloud size.

$$\Downarrow$$

Indirect evidence of ferromagnetic ordering

Motivation

- Summary of expt: (Jo et. al., 2009)
    - ✦ equal mixture of F=1/2 hyperfine states of Li^6
      => 2-component Fermi gas with short-range interaction
    - ✦ a>0, i.e., excited state branch (molecular bound state below)
    - ✦ Transition point ka ~ 1.9(2)
    - ✦ No observation of FM domains
- Interpretation has been debated (Ho, Zhai, ...)
- Recent MIT expt (Zwierlein et al)

Motivation

- The 3-D Hubbard model is a reasonable representation of the Stoner Hamiltonian

  itinerant electrons + local interaction

- Caveats!
  - Hubbard model: Ground state, repulsive interaction, equilibrium
    Experiment: Excited states, attractive interaction, dynamic (quench)
  - The scattering length on a lattice is bounded by lattice spacing
    (Castin 2004)

$$a_{lattice} = \frac{a_s}{1 + 3.173 a_s}$$

- Does the model have an instability towards ferromagnetism?
  (What is the minimal model for itinerant FM in metals?)

Introduction: Hubbard model

- Simplest model combining band structure and interaction:

$$H = K + V = -t \underbrace{\sum_{\langle ij\rangle\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma})} + \underbrace{U \sum_i n_{i\uparrow} n_{i\downarrow}}$$

Electrons on a lattice:

- near-neighbor hopping
- on-site repulsion

Size N=L^d

$$\text{Filling } n = \frac{N_\uparrow + N_\downarrow}{N}$$

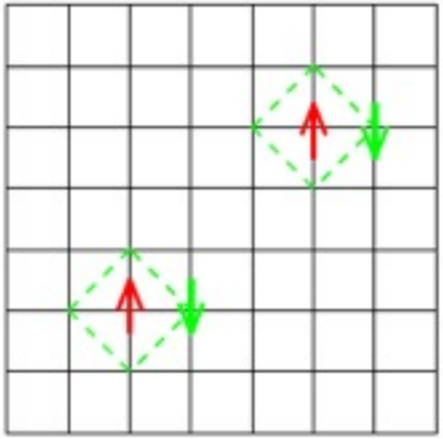
Half-filling: n=1

Consider:

- T=0K
- $N_\uparrow = N_\downarrow$

Parameters:

- U/t >0 (t=1)
- n=(0,1]; doping h=1-n



- Optical lattice emulator?
- Extremely difficult computational problem

Introduction: Hubbard model

- Simplest model combining band structure and interaction:

$$H = K + V = -t \underbrace{\sum_{\langle ij\rangle\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma})} + \underbrace{U \sum_i n_{i\uparrow} n_{i\downarrow}}$$

Electrons on a lattice:

- near-neighbor hopping
- on-site repulsion

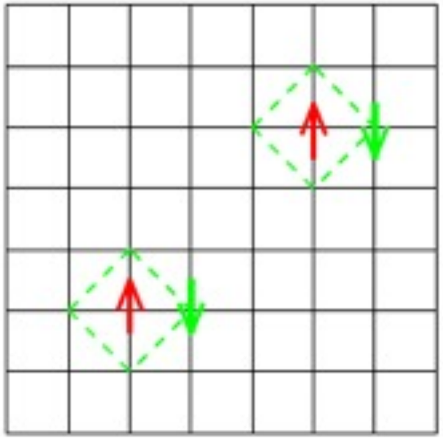
Size N=L^d

$$\text{Filling } n = \frac{N_\uparrow + N_\downarrow}{N}$$

Half-filling: n=1

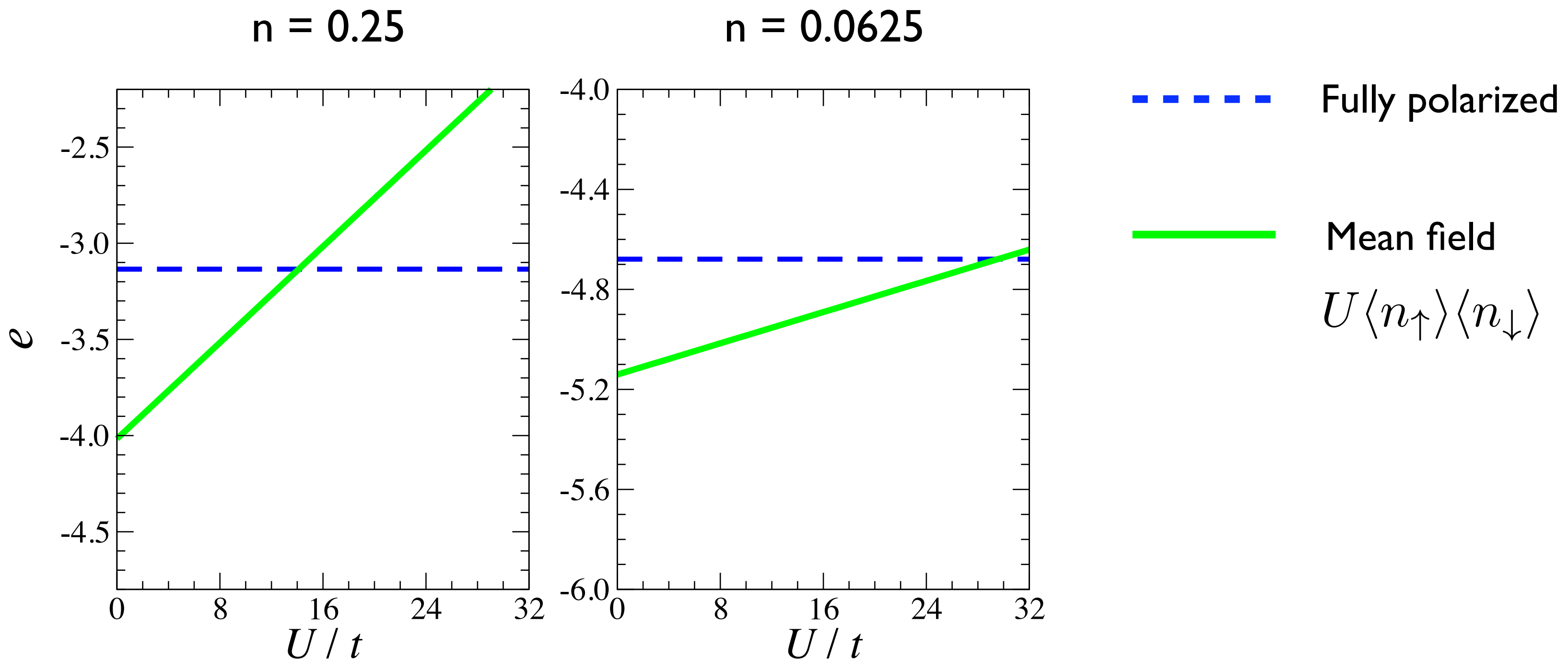
Does it have a ferromagnetic instability?

- Neither K nor V term favors FM alone
- Academic case: Nagaoka-Thouless:
  1 hole, U=infty, bipartite: yes



Mean-field theory

- Stoner's criterion $U \cdot N(\epsilon_F) > 1$

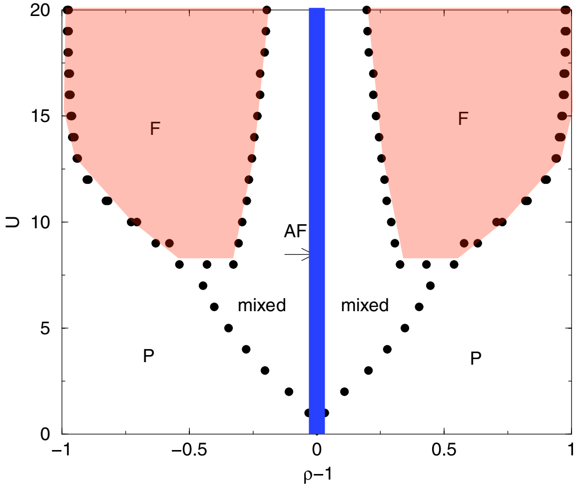


$$H = -t \sum_{\langle \mathbf{i}\,\mathbf{j}\rangle,\sigma} c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

Mean-field theory

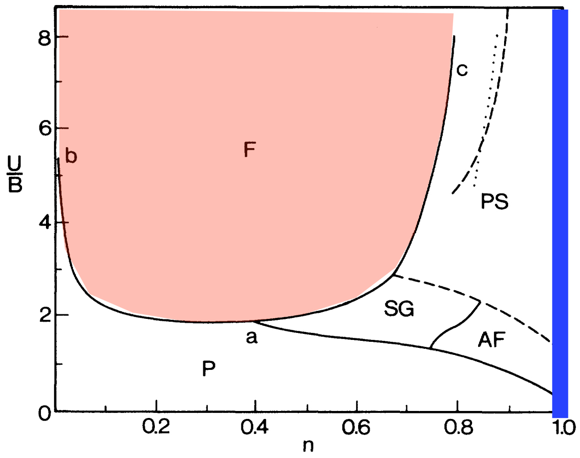
- Stoner's criterion $U \cdot N(\epsilon_F) > 1$

2D Hubbard



Langmann & Wallin (2007)

3D Hubbard



Andriotis et al. (1993)

- The ground state is antiferromagnetic at half-filling n = 1
- Phase diagram has large domain of ferromagnetism

How does correlation modify this?

Constrained path auxiliary field QMC

To obtain ground state, use projection in imaginary-time:

$$|\Psi^{(n+1)}\rangle = e^{-\tau \hat{H}} \, |\Psi^{(n)}\rangle \quad \xrightarrow{n\to\infty} \quad |\Psi_0\rangle$$

τ: cnst, small $\quad |\Psi^{(0)}\rangle$: arbitrary initial state

Hamiltonian:

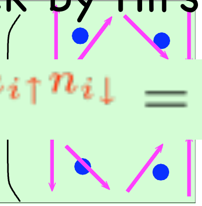
$$\hat{H} = \hat{H}_1 + \hat{H}_2 = -t \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow}\, n_{i\downarrow}$$

Hubbard–Stratonovich transformation

$$e^{-\tau \hat{H}} \quad \longrightarrow \quad e^{-\tau \hat{H}_1} \int e^{-x^2/2} \, e^{x\sqrt{\tau}\,\hat{v}} \, dx \qquad \hat{v}: \text{ one-body}$$

interacting system → $\sum$ (non-interacting system in auxiliary fields)

E.g., trick by Hirsch:



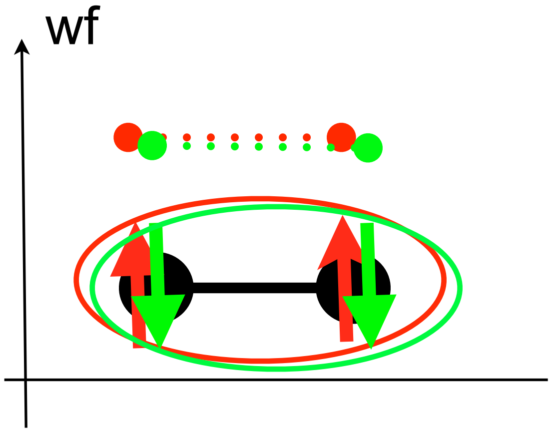
$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} = e^{-\tau U (n_{i\uparrow}+n_{i\downarrow})/2} \sum_{x=\pm 1} \frac{1}{2} e^{\gamma x\,(n_{i\uparrow}-n_{i\downarrow})}$$

next →

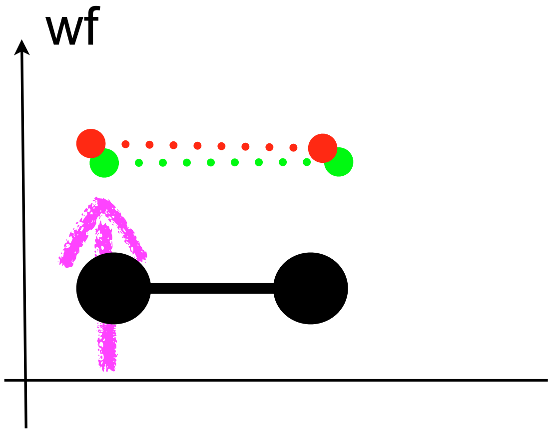
Toy system: Hubbard model

Illustration of how AFQMC works:

H2 molecule



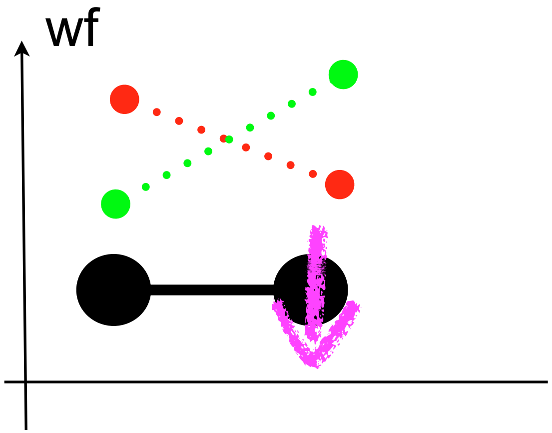
mean-field



auxiliary-field QMC

- Formalism similar to LGT
- But sign problem severe in most problems of interest
- Reformulated into open-ended random walks

+



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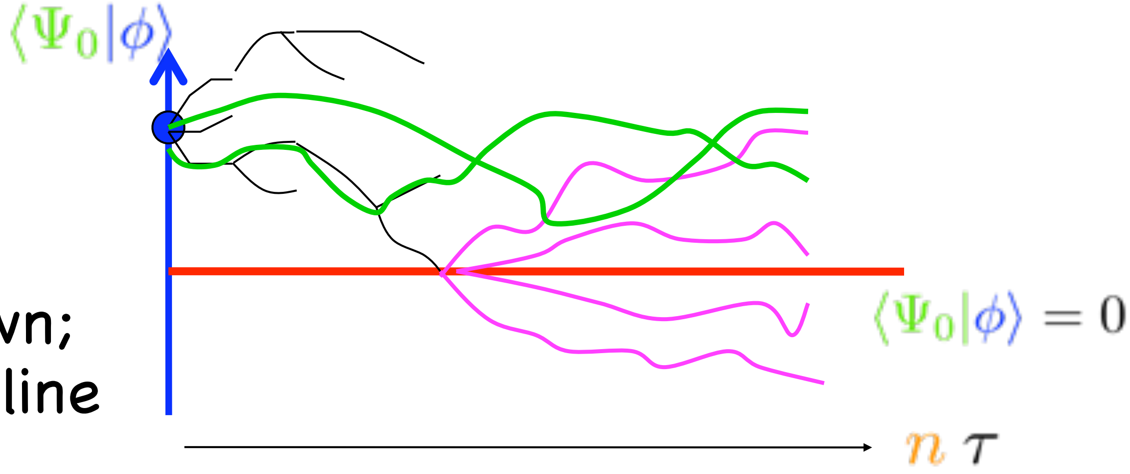
The sign problem

E.g., in Hubbard:



- $e^{-\tau\hat{H}}$ → paths in Slater determinant space

- Suppose $|\Psi_0\rangle$ is known; consider "hyper-node" line

- If path reaches hyper-node

$$\langle\Psi_0|\phi\rangle = 0$$
$$\Rightarrow \langle\Psi_0|\underline{e^{-n\tau\hat{H}}|\phi\rangle} = 0$$

then its descendent paths collectively contribute 0

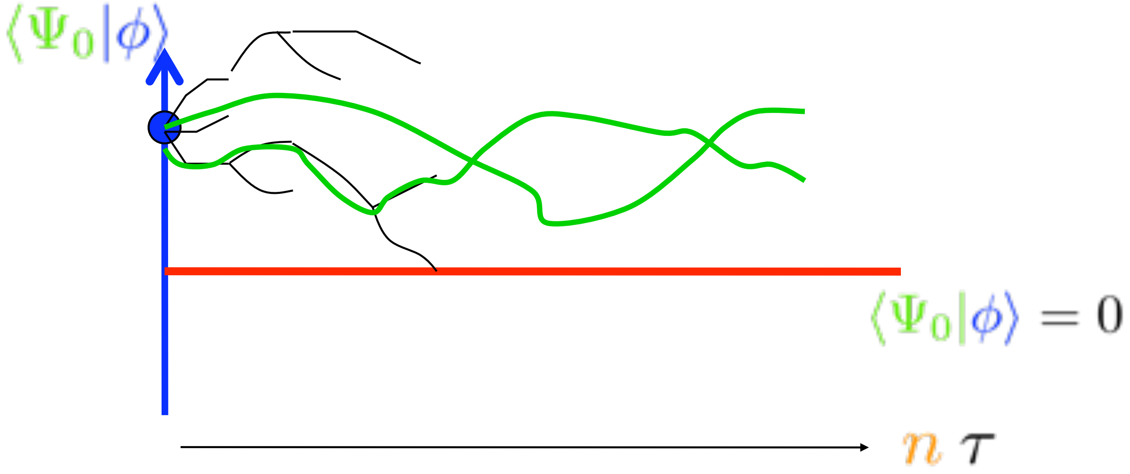
- MC signal is exponentially small compared to noise

In special cases (1/2 filling, or U<0), symmetry keeps paths to one side → no sign problem

next →

How to control the sign problem?

- Constrained path appr.



keep only paths that never reach the node

Zhang, Carlson, Gubernatis, '97

require $\langle \Psi_{\mathbf{T}} | \phi \rangle > 0$

Zhang, '00

Trial wave function used to make detection

- Phaseless approximation *Zhang & Krakauer, '03; Chang & Zhang, '08*

general interaction: complex HS --> phase problem

twisted boundary condition: removes shell effects --> complex w.f.

next →

Benchmark

- Sampling 1000 random TABCs

  3x3: Largest relative error:

    ~ 0.2% for U/t = 4

    ~ 1.0% for U/t = 8

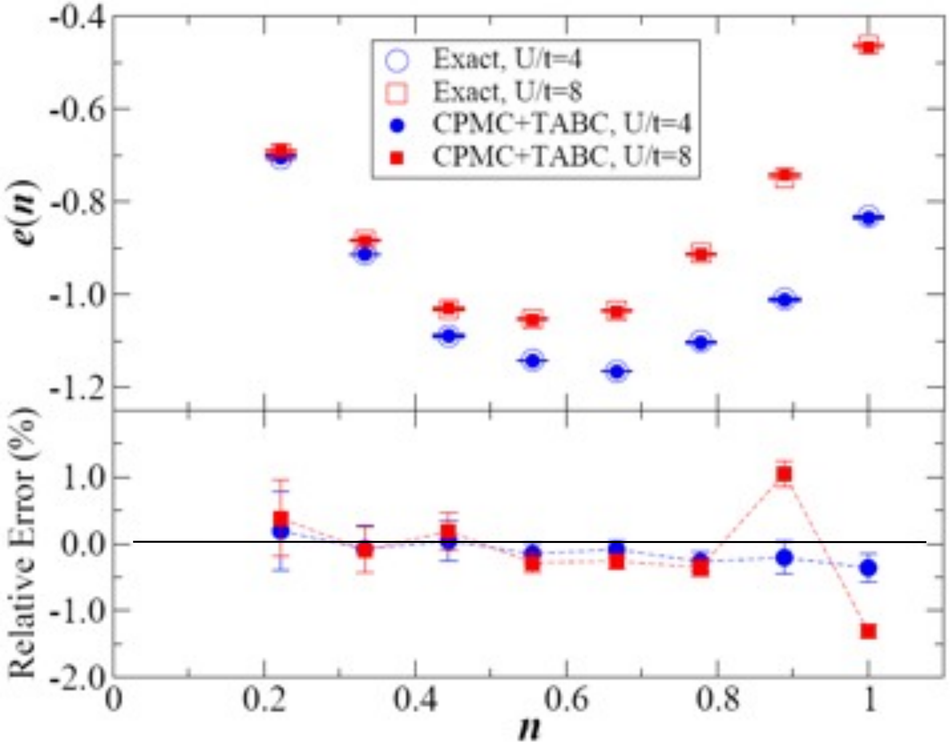
  dilute 4x4 at n=0.25

    ~ 0.2% for U/t = 16

    ~ 0.6% for U/t = 30

- Summary: CPMC + TABCs
  - ➢ controls sign problem
  - ➢ many benchmarks (including ab initio electronic structure)
  - ➢ Most accurate many-body method available at intermediate interactions for large systems (2- & 3-D)

Equation of state for 3x3 Hub

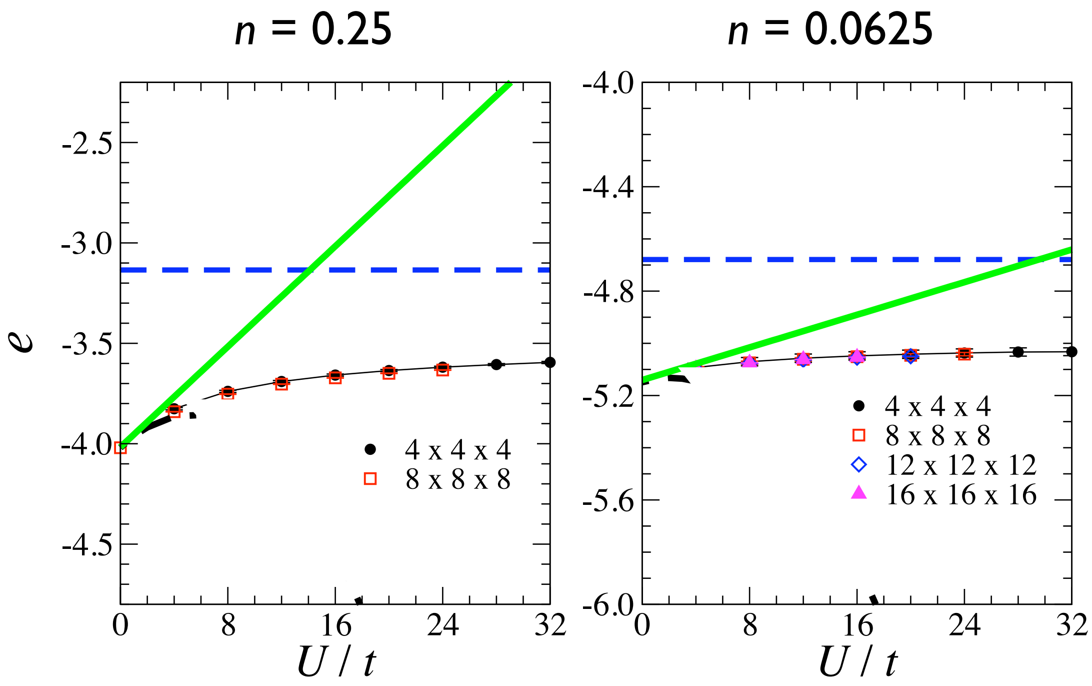


$$\text{Relative error\%} = \frac{e_{QMC}(n) - e_{Exact}(n)}{|e_{Exact}(n)|}$$

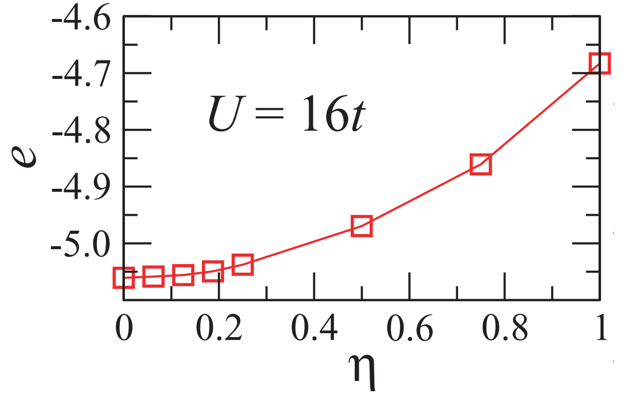
Chang & SZ, PRB ’08

Ferromagnetism in 3D dilute Hubbard model?

Energy results:



Essentially no finite size effects in the QMC data



- No FM transition was found: 0 < n < 0.5
- Partially polarized state is unlikely to be stable

$$\eta = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

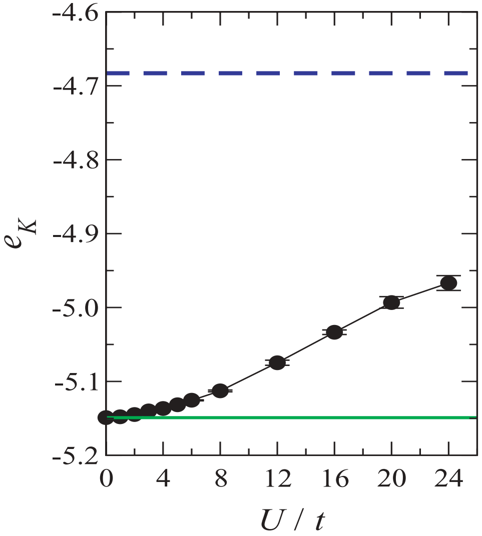
Individual energy components

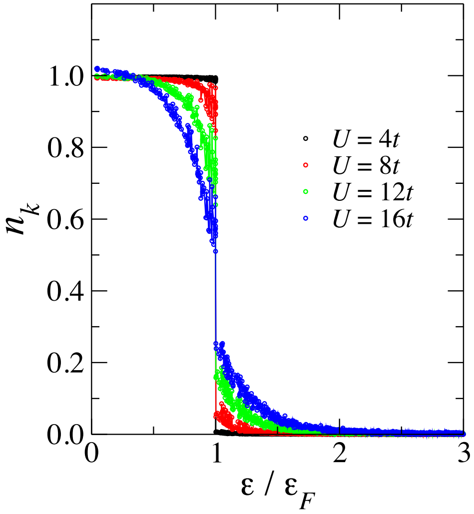
- Interaction creates excitations beyond the Fermi surface, increasing the kinetic energy

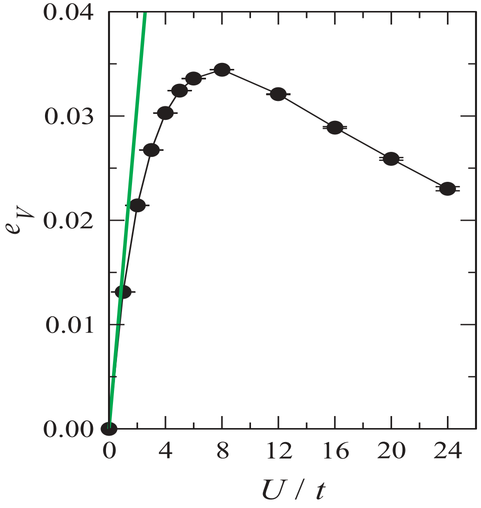
- At large U, the interaction energy is lowered by correlation:

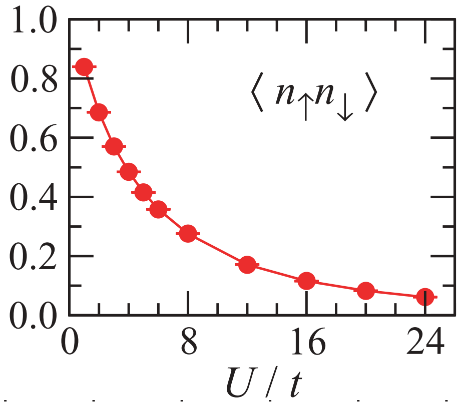
  reduced double occupancy

8x8x8, *n* = 0.0625



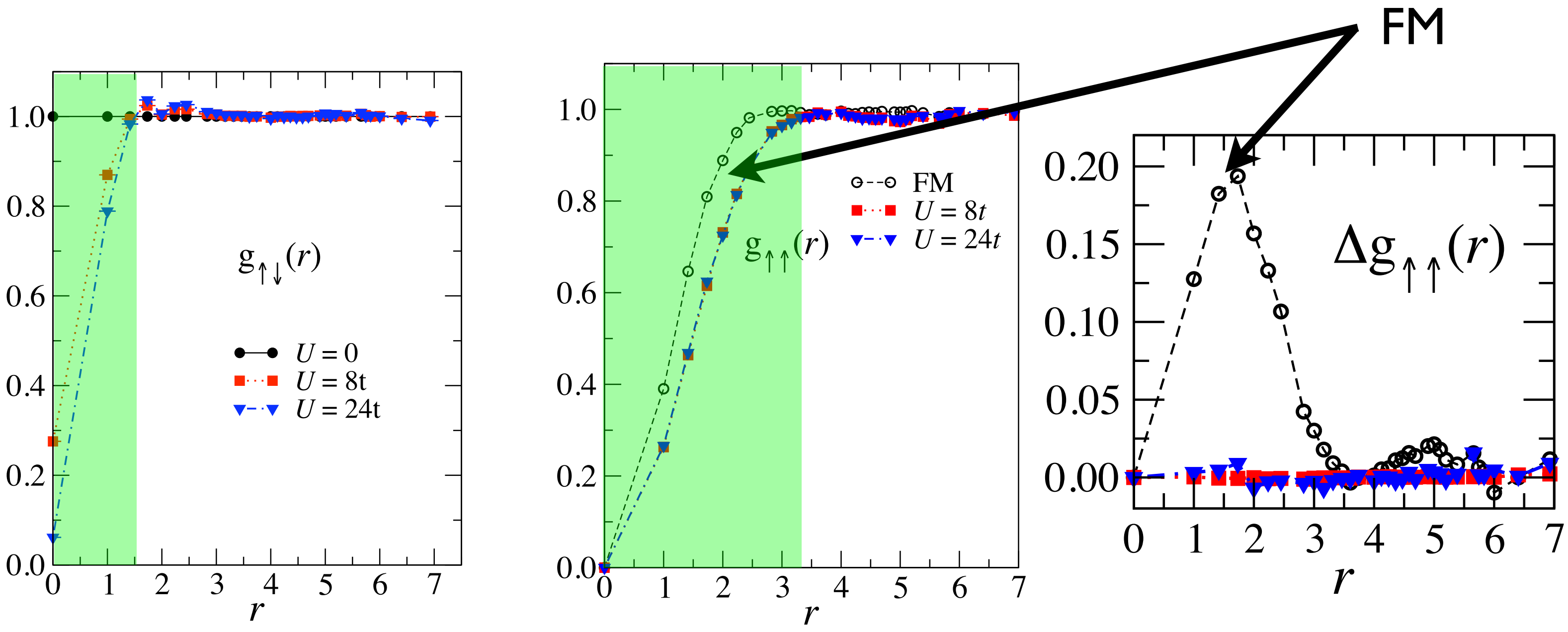






Correlation effects

Pair-correlation function:



correlation hole

exchange hole

- Enhanced ferromag. corr, but short-range, weaker than in FM phase
- Consistent with a paramagnetic Fermi liquid

Comment & connection to other calculations

- Expt:
  - ✦ Transition point ka ~ 1.9(2)
  - ✦ Quench of excited state (dynamics?)
- Other calculations/theory:
  - ✦ Mean-field in continuum gives ka~1.5; fluctuation correction: ka~1
  - ✦ Diffusion Monte Carlo: ka=0.8-0.9
    Conduit et al, '09; Pilati et al, '10; Chang et. al. '09
  - ✦ **However,** all used "hard-sphere" potential (scattering length appr.) to remove molecular states. This over-estimates trends for FM and can cause errors

    \- see **Zhou, Ceperley, SZ: arXiv/1103.3534**

Summary on itinerant FM in Fermi gas

- No ferromagnetism is found in the dilute 3-D Hubbard model up to U~30t, with density up to n=0.5.

- Energy is lowered by creating correlation holes (cf. Wigner, electron gas)

Chang, SZ, Ceperley, PRA, 82, 061603(R) (2010)

- Caveats:
  - ✦ ground state; repulsive contact int.; equilibrium (calc) vs. excited state; attractive int. (a>0); dynamic (expt)
  - ✦ scattering length in our model (repulsive 3D Hubbard) is bounded by latt. spacing

Magnetic properties at larger density?

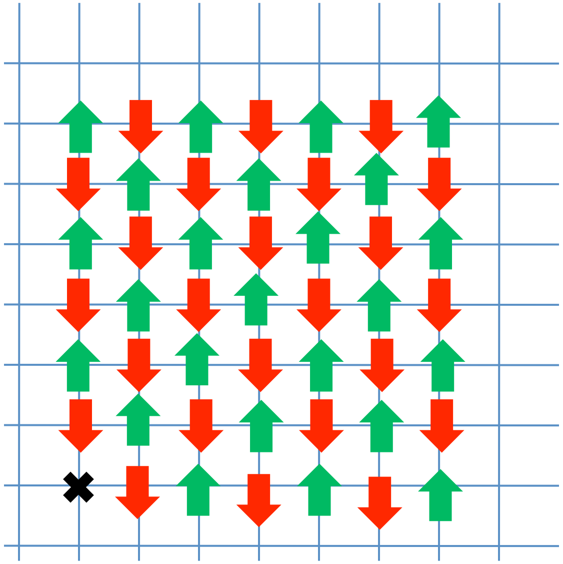
- Half-filling: antiferromagnetic (AF) order

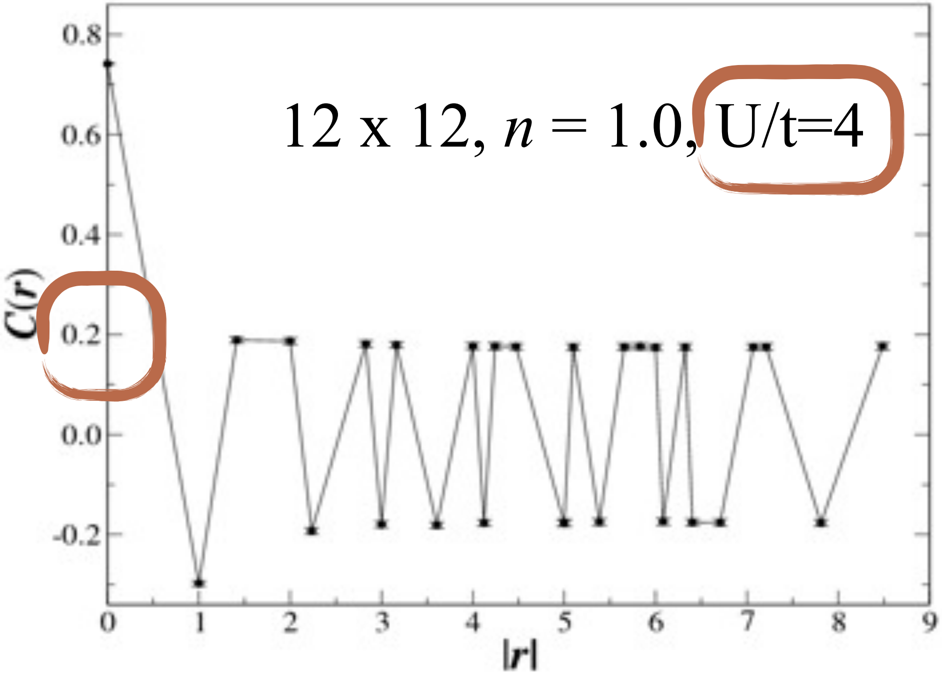
  (Furukawa & Imada 1991; Tang & Hirsch 1983; White et al, 1989; ….)

- Model for high-Tc? Must understand magnetism and its fluctuations first!

Calculate AF correlation:

$$C(\mathbf{r}) = \frac{1}{L \times L} \sum_{\mathbf{r}'} \langle \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\mathbf{r}'} \rangle$$



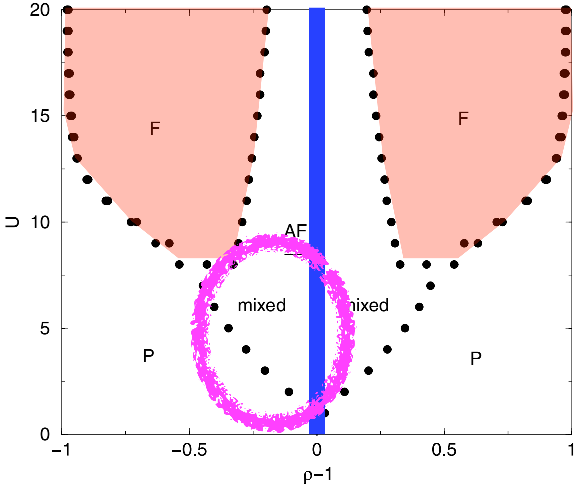


What happens to the AF order with doping?

next →

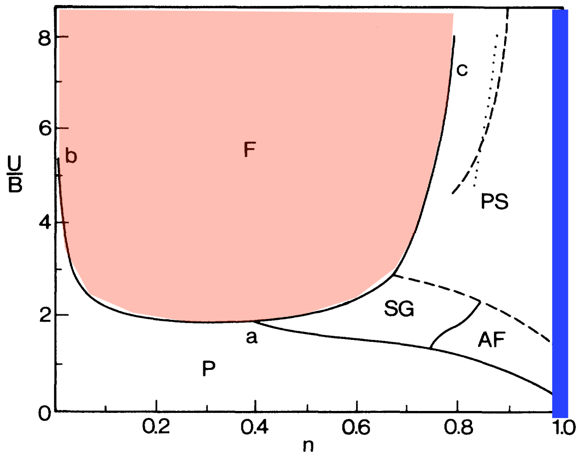
Mean-field theory

2D Hubbard



Langmann & Wallin (2007)

3D Hubbard



Andriotis et al. (1993)

- Note even the HF answer has not been unambiguous

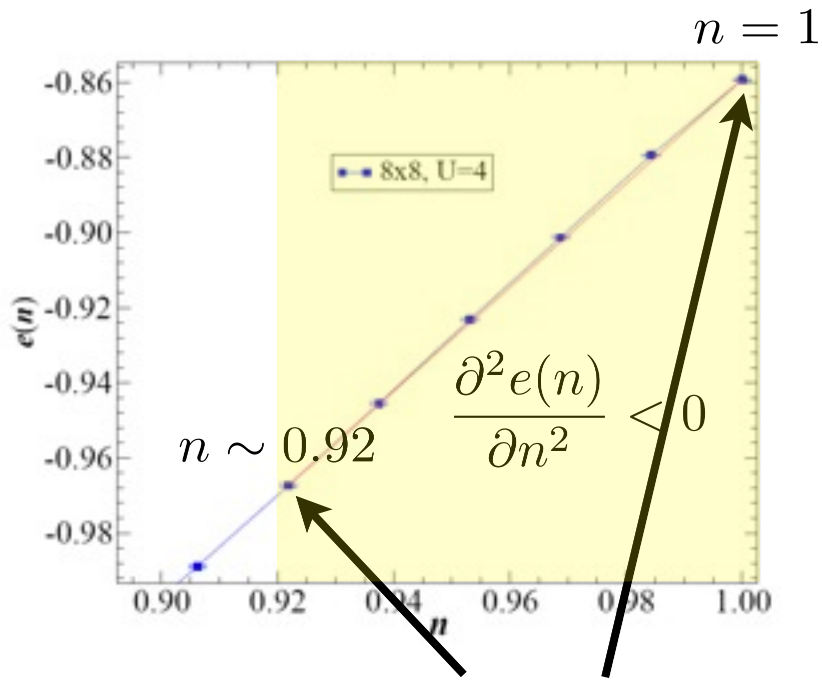
Xu, Chang, Walter, SZ, 2011

How does correlation modify this?

Equation of state in 2D

- Free-electron trial w.f.
- Use 20 ~ 300 random twist angles
- Data of different lattice sizes has good agreement at n < 0.9

- "Unstable" region is found on 8x8, 12x12, 16x16



$n = 1$

$n \sim 0.92$

$$\frac{\partial^2 e(n)}{\partial n^2} < 0$$

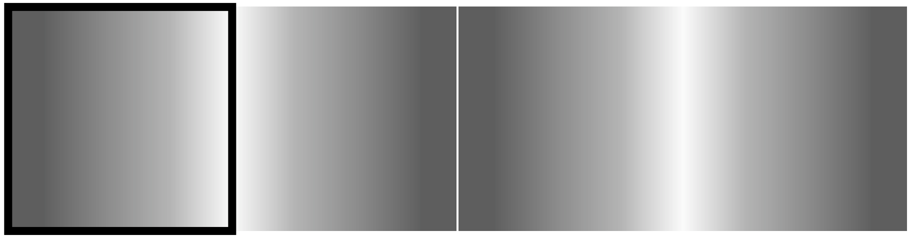
U=8t

U=6t

U=4t

U=2t

U=0



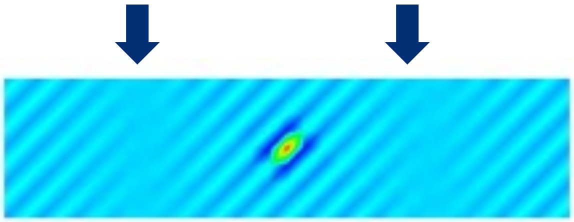
frustrated long wavelength mode ?

phase separation ?

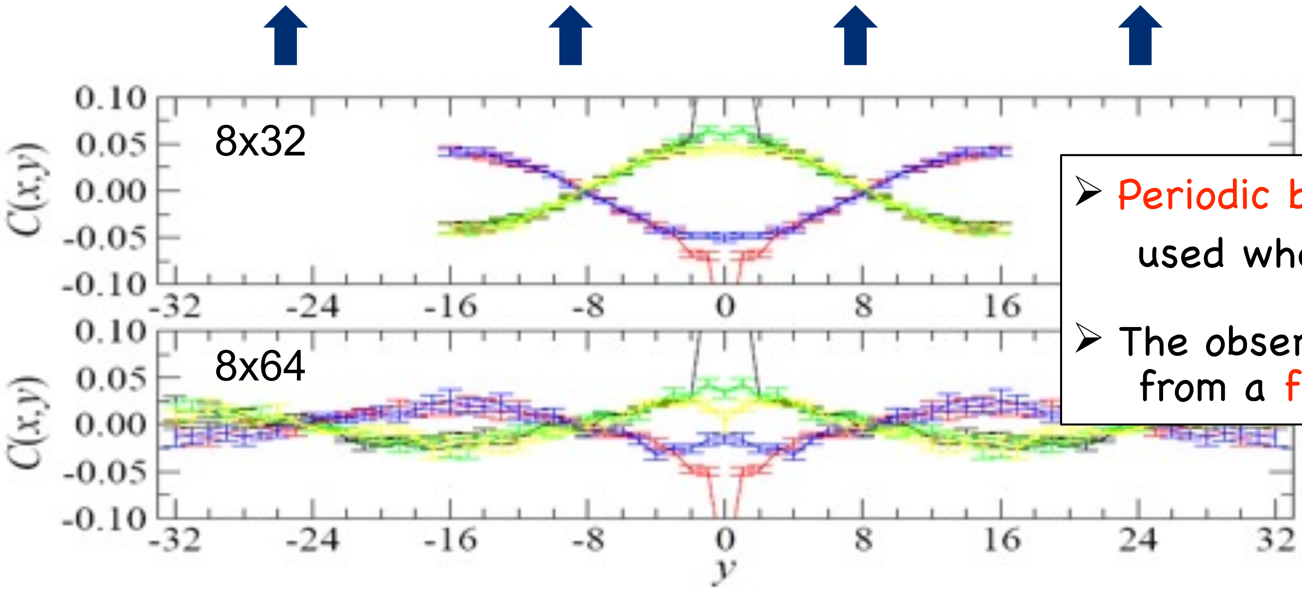
Spin-spin correlation

- Use rectangular lattices to probe correlation length L > 16
- Up to 8x128 supercell (dimension of CI space: 10^600 !)
- Detect spatial structures using correlation functions

8x32
n = 0.9375



$$C(\mathbf{r}) = \frac{1}{N_s}\sum_{\mathbf{r}'}\langle \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\mathbf{r}'}\rangle$$

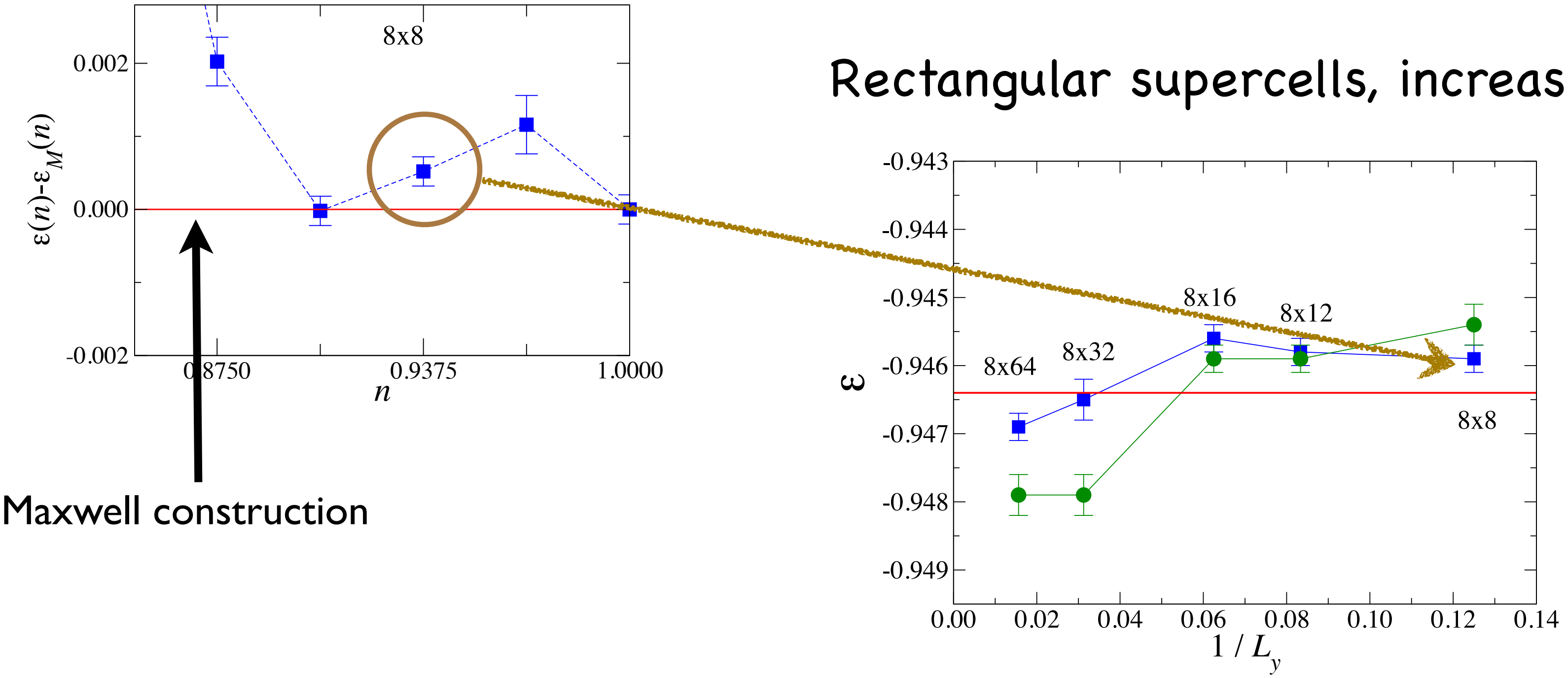


- ➢ Periodic boundary condition is used when calculating C(**r**)
- ➢ The observed structure emerges from a free electron trial state

"staggered":
(-1)^y C(x,y)

Equation of state, again

- TABC removes one-body shell effects, but not two-body finite-size effects:



Rectangular supercells, increasing Ly

Maxwell construction

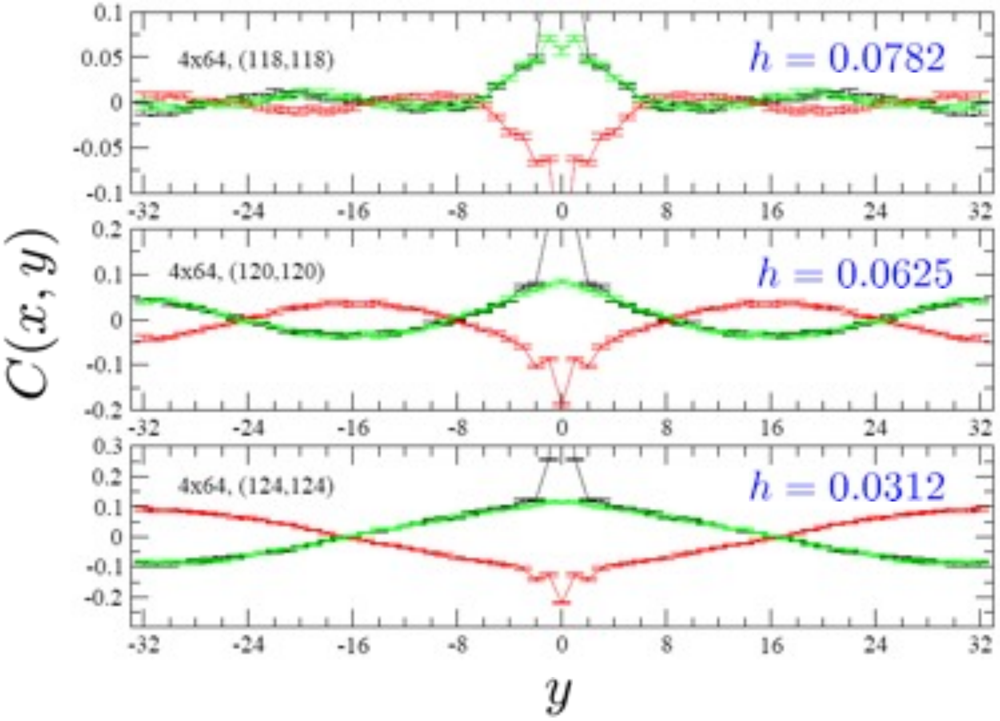
- Instability is from frustration of SDW due to finite size
- At n = 0.9375, need L>~32 to detect SDW state

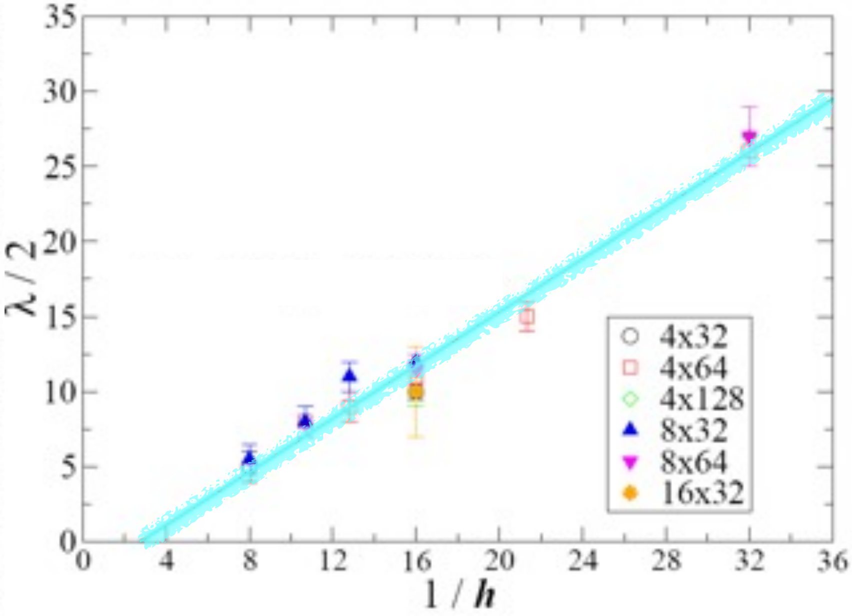
(Previous calculations: Ly~12, with large shell effects)

Wavelength versus doping

Doping h = (1-n) dependence

4x64, U/t = 4.0





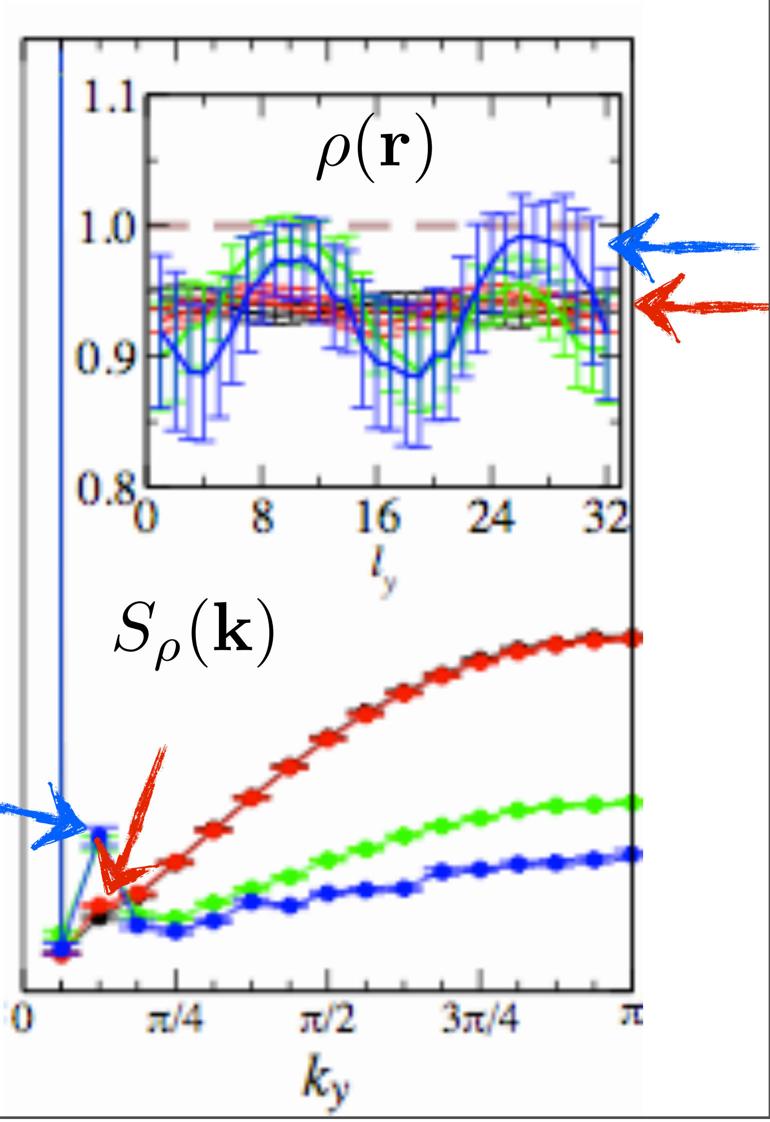
- Wavelength decreases with doping; as does the amplitude
- SDW terminates at finite doping (~0.15), enters paramagnetic state
- Wavelength appears $\propto 1/h$

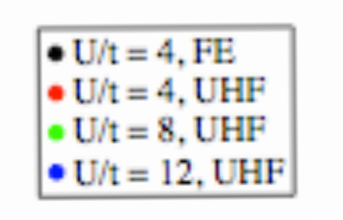
Chang & SZ, PRL 104, 116402 (2010)

Dependence on U

- At U/t=4, charge is uniform:
  - No peak in charge struc. factor
  - holes fluid-like (de-localized)

- At U/t=8-12, CDW develops:
  - Peak in structure factor
  - Clumps of density=1, separated by dips (SDW nodes)
  - Consistent with DMRG results at large U/t (White et al, ’03, ’05)
  - holes Wigner-like (localized)





Summary

- Magnetic phases in repulsive Hubbard model using CPMC + TABCs
  - Accurate QMC results
  - No ferromagnetism in 3D up to n~0.5; paramagnetic Fermi liquid?
  - Near half-filling, in 2D, at low to intermediate U/t:
    - AF spin density wave (SDW) with long wavelength modulation
    - Wavelength decreases with doping (infinity at half-filling)
    - SDW amplitude decreases with doping, vanishes at n~0.85(5)
    - Charge-charge correlation almost uniform
  - LO state in spin-imbalanced **attractive** optical lattice ?