The fermionic Hubbard model in an optical lattice

Pinaki Majumdar

Harish-Chandra Research Institute (HRI)

Allahabad, India

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Plan of the lecture

- Background: many body problems
- Repulsive Hubbard model
  - -A. Conjectured phase diagram
  - -B. The Neel state and Mott physics
  - -C. Effect of geometric frustration
  - -D. Mott shells in trapped fermions
  - -E. d-wave superfluidity?!
- Attractive Hubbard model
  - -A. Overall phase diagram
  - -B. BCS-BEC crossover in superfluids
  - -C. Superfluid-‘insulator’ transitions
  - -D. Inhomogeneous superfluid in a trap
- Conclusion

I. Many body systems

1. Weakly interacting many body systems

- Simplest case: ‘free’ fermi and bose systems!

  -‘many particle’ states are product states

  -many body character enters only through exchange statistics

  -fermions: $C_V \sim N(\epsilon_F)T$, $\chi \sim N(\epsilon_F)$, no phase transitions..

  -bosons: macroscopic occupation of ϵ_0 at $T \sim \frac{\hbar^2}{2m}n^{2/3}$.. BEC.

- The impact of weak interaction: (i) ‘normal’ state.

  -the ‘normal’ state corresponds to absence of any long range order ..

  -can use perturbation theory for ground state energy, damping ..

  -highly developed theory, but needs a small parameter!

- The impact of weak interaction: (ii) phase transitions, order..

  -even weak interactions can lead to ordering

  -weak attraction $\rightarrow$ pairing and superfluidity

  -weak repulsion can sometimes lead to antiferromagnetism

  -requires self-consistent treatment: ‘mean field’ (MF) theory ..

- Many systems **cannot** be understood within perturbation/MF theory..

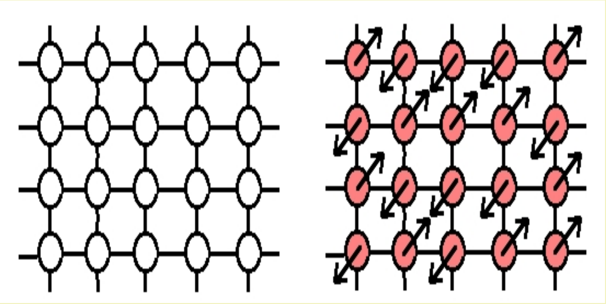
2. Correlated systems

Present effort: understand phenomena beyond straightforward perturbation theory.

The physics cannot be visualised in terms of 'independent' degrees of freedom.

Examples?

- Superfluid to Mott insulator transition in bose systems.
- Mott state and magnetic order for repulsive fermions.
- Possible superfluidity in doped fermionic Mott systems.
- The 'BEC' state in attractive fermionic systems.



Mott state: jamming! Motion of doped 'holes'.. superposition..

3. Models

Consider two artificially simple models of correlation.

These are approximately realised in the solid state.

They can be *engineered* in optical lattices!

- The repulsive (+ve U) Hubbard model

$$H = \sum_{ij} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} (V_i - \mu) c^{\dagger}_{i\sigma} c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- The attractive (-ve U) Hubbard model

$$H = \sum_{ij} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} (V_i - \mu) c^{\dagger}_{i\sigma} c_{i\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow}$$

t_{ij} denote hopping on the lattice, V_i is a potential .. ref fig..

If $U = 0$ we can diagonalise H in terms of Bloch states..

For $t_{ij} = 0$, the system is diagonal in a purely local basis..

If both t_{ij} and U are non-zero.. no exact solution for $d > 1$.

4. How is the model 'solved'?

- Mean field theory:

  -factorise $Un_{i\uparrow}n_{i\downarrow} \rightarrow U\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}\rangle c_{i\downarrow}c_{i\uparrow}$ or $U\langle c^{\dagger}_{i\uparrow}c_{i\downarrow}\rangle c^{\dagger}_{i\downarrow}c_{i\uparrow}$
  -superconducting or magnetic correlations.. compute self-consistently.
  -easy to implement, possibly large fluctuations.. incorrect in low d.

- Problems involving coupled quantum variables admit only two 'exact' methods:

  -(i) Exact diagonalisation (ED), (ii) Quantum Monte Carlo (QMC)

- ED is severely size limited. For a model with m basis states per site, and N sites, the matrix size $\sim m^N \sim e^{N lnm}$. With great effort one can solve for $N \sim 16$ for $m = 4$ (Hubbard model), exploiting all possible symmetries.

- Fermion QMC is usually implemented by rewriting the interaction in terms of an auxiliary HS variable, $\phi(\mathbf{r}, \tau)$, say.
  -'non-interacting' fermion problem is solved for sampled configs of $\phi(\mathbf{r}, \tau)$.
  -convergence is poor at low temperature due to the fermion sign problem.
  -state of art $\sim 8 \times 8$ on Hubbard, low T is inaccessible.

- ED and QMC are also used as 'solvers' within dynamical mean field theory (DMFT).

5. Hubbard physics: an outline

Why Hubbard? Simplest model of quantum correlation.

Single fermionic band with local interaction.

The attractive model describes s-wave superconductivity.

The repulsive model describes magnets and Mott insulators.

We will explore the following issues in the context of this model: (i) strong coupling, (ii) randomness, (iii) confinement, and (iv) frustration

- Optical realisation: (i) lattice and trap, (ii) bosons/fermions, (iii) tunable interaction!

- Experimental status ..

  -SF to Mott insulator transition in bosons

  -Strongly interacting fermi gases

  -s-wave superfluidity of fermions

- Challenges: (i) AF order in fermionic Mott systems, (ii) d-wave superfluidity ..

II. Repulsive Hubbard model

A. Conjectured phase diagram

The repulsive (+ve U) Hubbard model:

$$H = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} (V_i - \mu) n_i + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- Serves as the minimal model for Mott transition and antiferromagnetism.
- Also extensively studied as a candidate for d-wave superconductivity.
- The model is characterised by:

  NN hopping t, and longer range hoppings, t', t'', etc

  interaction U, we will use U/t as measure of coupling

  the density, n, controlled by μ

  possible disorder or confining potential V_i.

• Phases?

at $n = 1$ and NN hopping, AF insulator (Slater to Mott crossover)
at $n = 1$ on a *frustrated* lattice: complex magnetic order/MI trans
for $n \neq 1$ metal/superconductor/magnet..? no convincing theory
in a confining potential: Mott shells, 'metal-insulator' coexistence

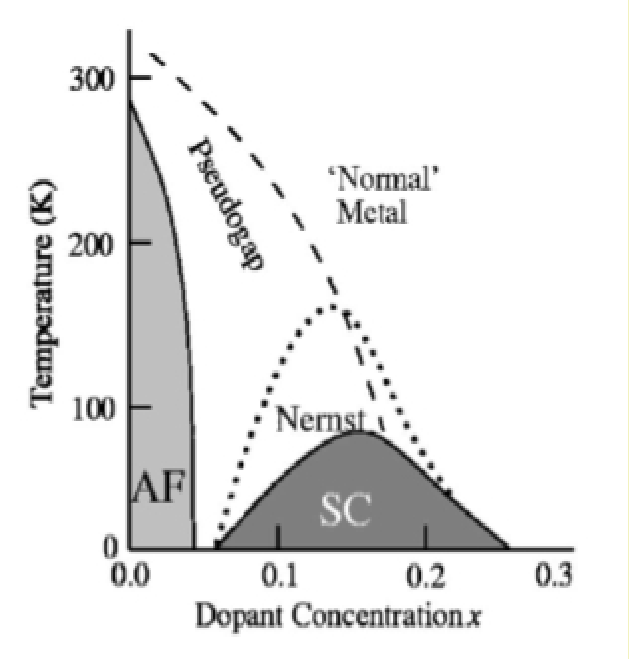


Figure 1: Doping-temperature phase diag at large U/t.. cuprates..

How do we proceed? many approx methods, we use the following ...

Recast as quadratic fermion problem!

Rewrite $n_{i\uparrow}n_{i\downarrow}$ in terms of n_i^2 and/or σ_{iz}^2.

$$n_{i\uparrow}n_{i\downarrow} = -\frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})^2 + \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow})$$

$$n_{i\uparrow}n_{i\downarrow} = +\frac{1}{2}(n_{i\uparrow} + n_{i\downarrow})^2 - \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow})$$

$$n_{i\uparrow}n_{i\downarrow} = \frac{1}{4}(n_{i\uparrow} + n_{i\downarrow})^2 - \frac{1}{4}(n_{i\uparrow} - n_{i\downarrow})^2$$

So? Still quartic?

We can use the identity below to 'linearise' an operator.. Hubbard-Stratonovich (HS)

$$\exp\left[\frac{1}{2}A^2\right] = \sqrt{2\pi}\int_{-\infty}^{\infty} dy \exp\left[-\frac{y^2}{2} - yA\right]$$

In Z, introduce a new variable at each (space-time) point, to be traced over.

For example, use ϕ_i coupling to n_i and m_i coupling to σ_{iz}..

We use the following (approximate) representation:

$$H = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} (V_i - \mu) n_i + U \sum_{i} n_{i\uparrow} n_{i\downarrow} = H_0 + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

'Magnetic' decomposition of the model..

$$H \approx H_0 + \sum_{i} [i\phi_i n_i - 2\vec{m}_i . \vec{\sigma}_i] + \sum_{i} \frac{\phi_i^2}{U} + \sum_{i} \frac{\vec{m}_i^2}{U}$$

The $i\phi_i$ is a problem! replace by saddle point value.. left with vector aux field $\vec{m}_i$.

B. The Neel state and Mott physics

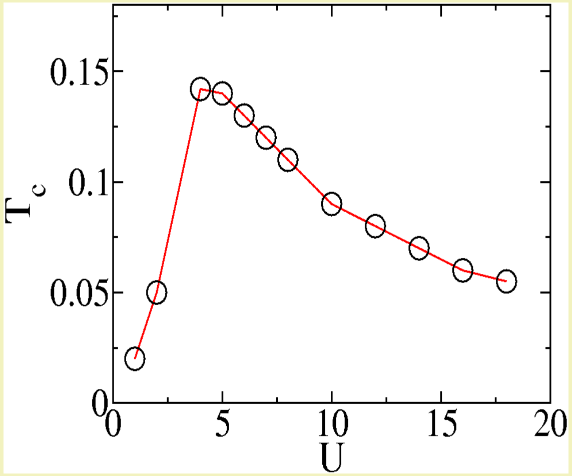
Consider the model on a square lattice with nearest neighbour hopping t.

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

At half-filling the ground state is insulating with $\{\pi, \pi\}$ AF order.. motivate..

Final effective Hamiltonian at half filling: fermions + classical HS field $\vec{m}_i$.

$$H = H_{kin} - \frac{U}{2} \sum_i \vec{m}_i \cdot \vec{\sigma}_i + \frac{U}{4} \sum_i \vec{m}_i^2$$



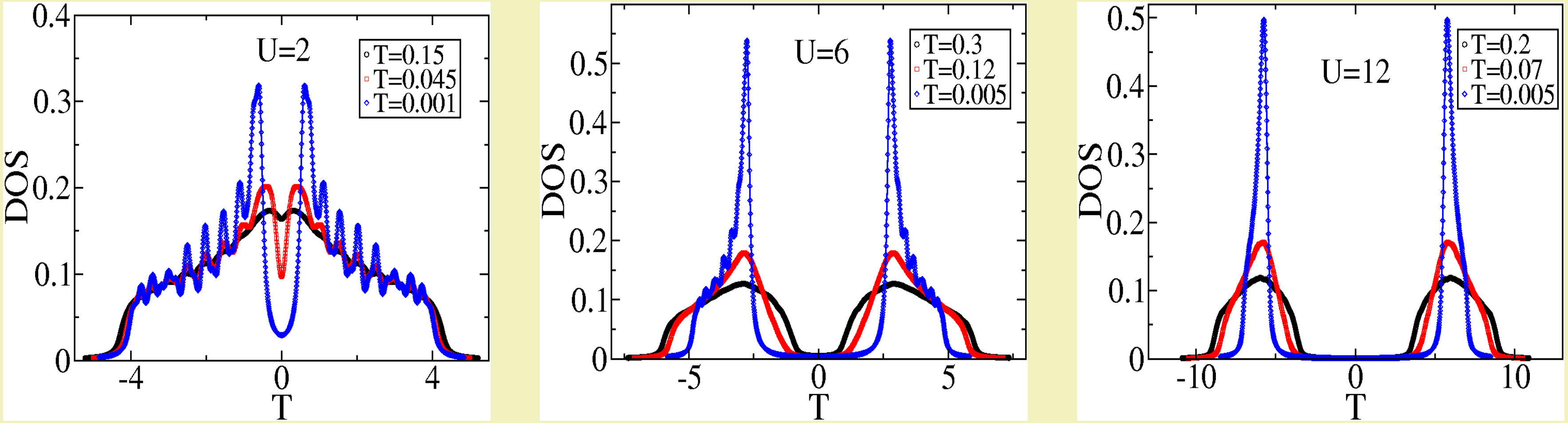
Physics of the AF crossover: MFT and fluctuation effects..

-Bipartite lattice: nesting driven small U SDW state, Slater insulator.

-Large U, localised electrons, Mott state, superexch driven Heis AF.

-With increasing T the weak U system loses AF order and ins character.

-Large U, low T_c Neel state, paramagnetic insulator above T_c.



Evolution of the DOS with U and temperature.

Fermions coupled to ‘local moments’ $\vec{m}_i$.

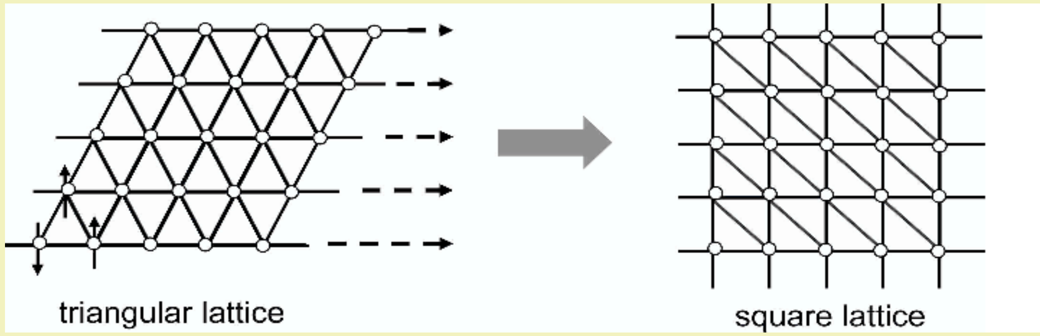
The ‘size’ of the moments depend on U, and also on T.

Local moment ‘formation’ at a U dep temperature scale..

Comment on the weak to strong coupling crossover..

C. Effect of geometric frustration

$$H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - t' \sum_{i*j, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



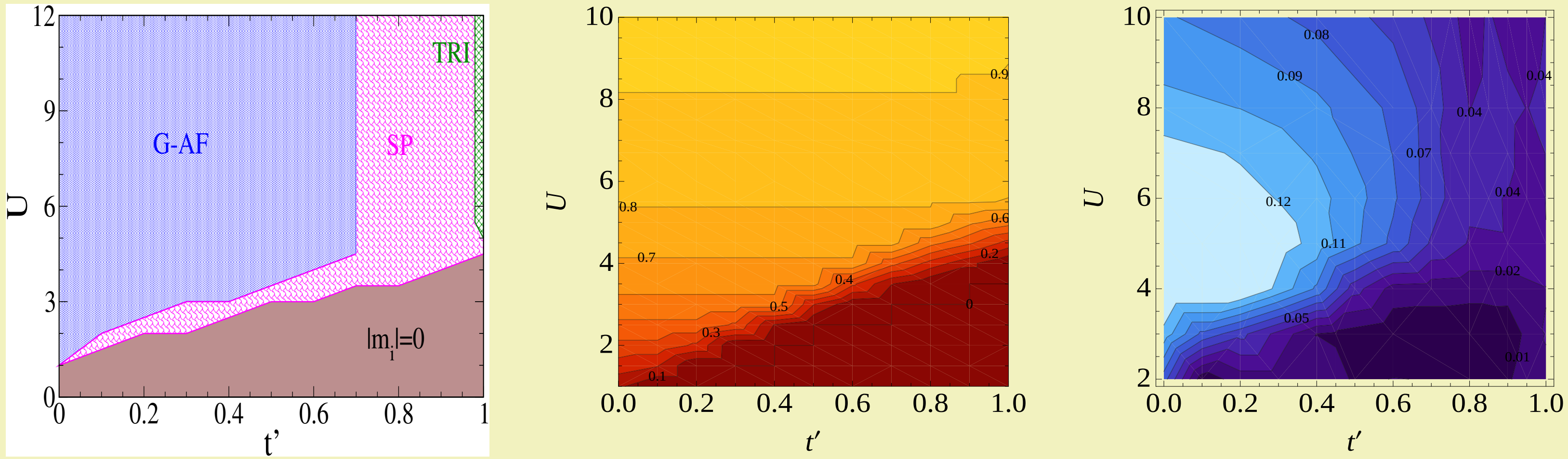
Left fig shows an triangular lattice, right: equiv square lattice.

We consider the square with ‘NN’ hopping t and diag hopping t'.

This is the *anisotropic* triangular lattice, $t' = t \rightarrow$ isotropic Δ lattice.

We have seen that for $t' = 0$, $n = 1$ is an AF insulator.

t' ‘frustrates’ AF order, consequence?



Left: phase diagram. Order destroyed by t' at small U.

Middle: size of the local moment, red: small, yellow: large.

Right: variation of the T_c, light -large, dark -small.

Reproduces known results, captures new finite T features.

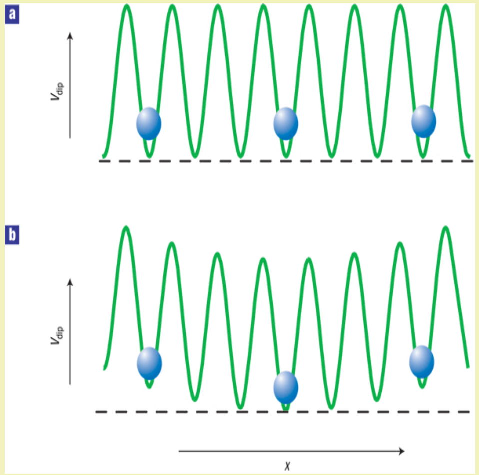
Metal-insulator transitions in the ground state, contrast $t' = 0$ ...

Unusual transport (Hall response) due to non-coplanar spin configs..

D. Mott shells in trapped fermions

Test case for inhomogeneity: Hubbard model + harmonic potential.

We explore the effect of a trap: $V_i = V_0(x_i^2 + y_i^2)$ on the Hubbard lattice.



Why interesting?

-The magnetic order in the Hubbard model is robust only at $n = 1$.

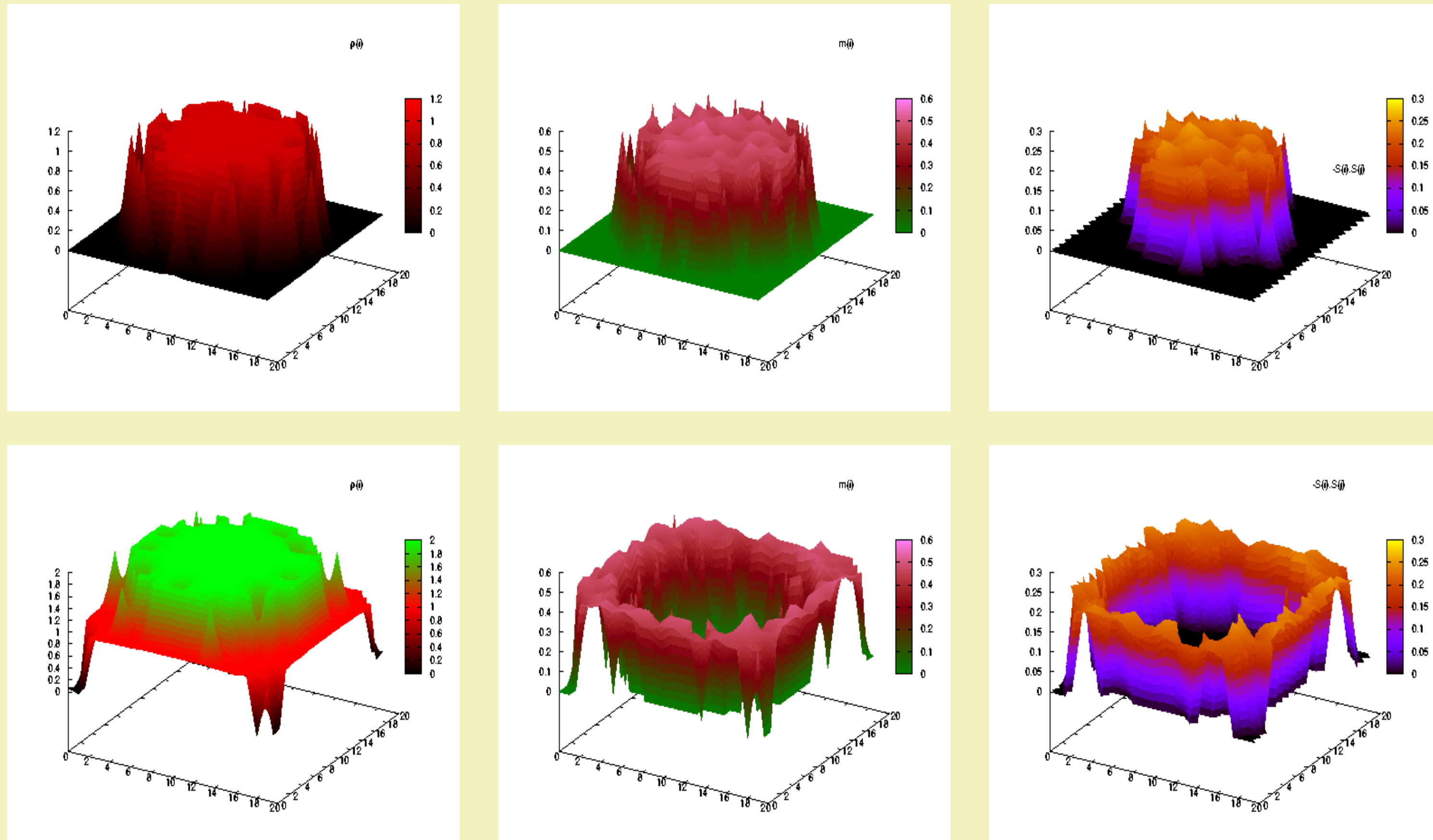
-$n = 1$ implies $n_i = 1$ in a homogeneous (flat) system.

-In a trap, n_i would be larger at the center and small at the boundary!

-How will the magnetic order/Mott character show up in such systems?!

Method: treat ϕ_i in terms of a thermal average..

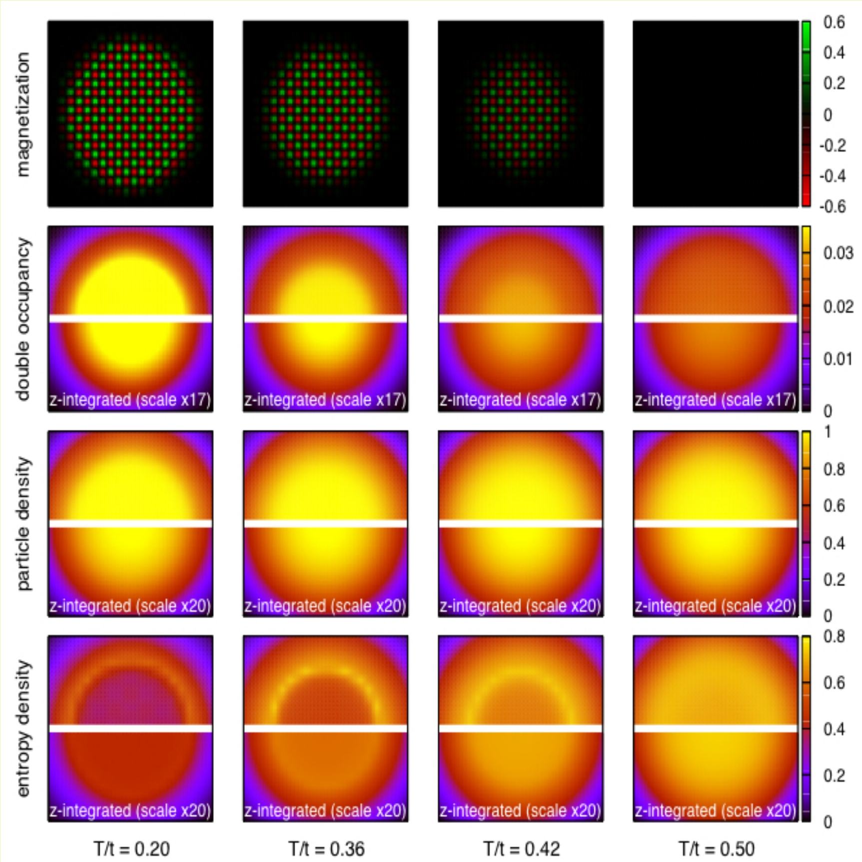
Variation of the density $n_{\mathbf{r}}$ (left), moment $|\vec{m}_{\mathbf{r}}|$ (center) and NN $\vec{m}_{\mathbf{r}}.\vec{m}_{\mathbf{r}'}$ (right).



Top row: density plateau's at $n = 1$ and $n = 0$, corresponding $|\vec{m}_{\mathbf{r}}|$ and $\vec{m}_{\mathbf{r}}.\vec{m}_{\mathbf{r}'}$.

Bottom: plateau's at $n = 2$, $n = 1$ and $n = 0$, and corresponding $|\vec{m}_{\mathbf{r}}|$ and $\vec{m}_{\mathbf{r}}.\vec{m}_{\mathbf{r}'}$.

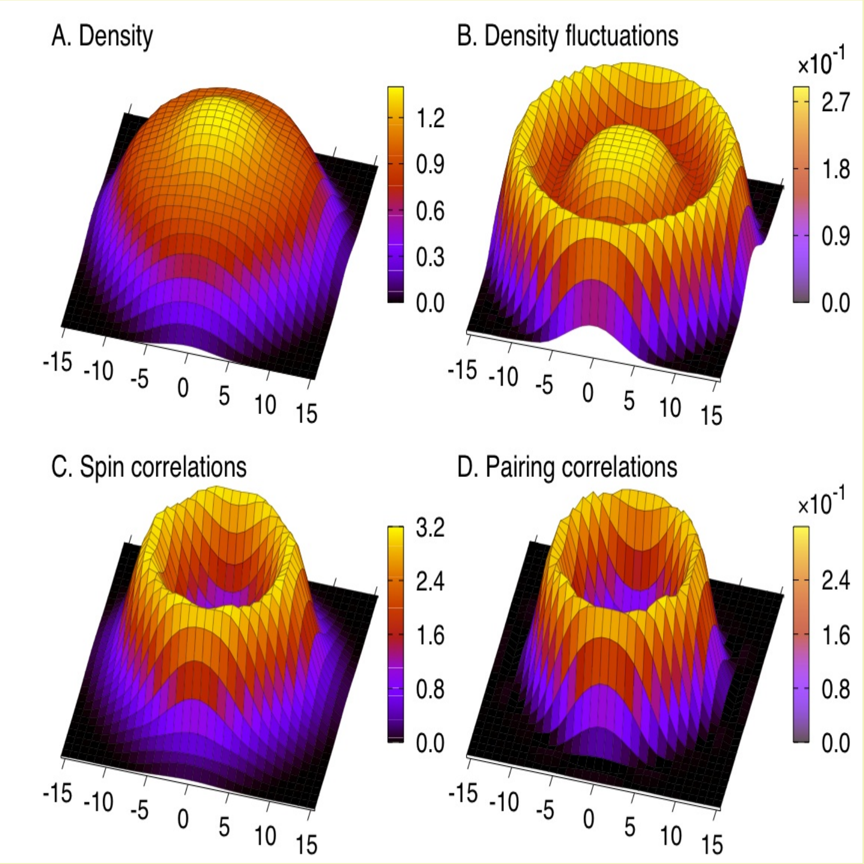
Results based on R-DMFT



Gorelik *et al.*, PRL (2010).

E. d-wave superfluidity of fermions

AF and superconducting correlations ...



Chiesa *et al.*, PRL (2011)

III. Attractive Hubbard model

A. Overall phase diagram

The -ve U Hubbard model is the simplest example of attractive interaction.

Somewhat artificial in condensed matter, more ‘real’ in cold atoms.

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

Involves electrons/atoms hopping between lattice sites and an on-site attraction.

- At all densities except $n = 1$ the ground state is superfluid.
- At $n = 1$ charge density wave (CDW) and superfluid correlations coexist.
- Weak coupling, $U/zt \ll 1$: momentum space pairing, ‘BCS superfluid’
- Strong coupling, $U/zt \gg 1$: BEC of molecular pairs (more soon)

Optical lattices nowadays allow tuning of the interaction strength.

They also bring in new features: inhomogeneity, spin imbalance ..

B. BCS-BEC crossover in superfluids

The method, quickly:

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

HS decouple in the Cooper channel (why!), neglect dynamics..

$$H \equiv H_{kin} + \sum_i (\Delta_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \Delta^\star_i c_{i\downarrow} c_{i\uparrow}) + \sum_i \frac{|\Delta_i|^2}{U}$$

$\Delta_i = \phi_i e^{i\theta_i}$ is a complex scalar field.

H is now quadratic in fermions for any configuration $\{\Delta_i\}$.

Can be solved via a Bogolyubov transformation (next slide)

BCS works exactly the same way, assumes $\Delta_i = \Delta$, constant.

Transform $c_{i\uparrow} = \sum_i (u_n^i \gamma_{n\uparrow} - v_n^{i\star} \gamma_{n\downarrow}^\dagger)$, $c_{i\downarrow} = \sum_i (u_n^i \gamma_{n\downarrow} + v_n^{i\star} \gamma_{n\uparrow}^\dagger)$

Canonical tranformation implies $\sum_n (|u_n^i|^2 + |v_n^i|^2) = 1 \; \forall i$ and

$$H = -\sum_i E_n + \sum_{i\sigma} E_n \gamma_{n\sigma}^\dagger \gamma_{n\sigma}$$

$E_n(\Delta_i)$ are nonnegative eigenvalues of the BdG equations

Effective 'Hamiltonian' in terms of the HS fields Δ_i

$$H_{eff}\{\Delta_i\} = \sum_i \frac{|\Delta_i|^2}{U} - \sum_n E_n - \frac{1}{\beta} \sum_n ln(1 - \exp(-\beta E_n))$$

The expansion of this, for uniform Δ, leads to Landau theory.

- How do we know the equilibrium configurations of $\{\phi_i, \theta_i\}$? Cluster MC..
- Mean field/BCS: phase locked uniform Δ_i state, 'superfluid' as long as $\Delta \neq 0$.
- Static HS $\equiv$ MFT for $T \rightarrow 0$, but very different at strong coupling and $T \neq 0$.

Let us characterise the superfluid state in terms of

(1) $\Delta(0)$, the gap at $T = 0$.
(2) $\xi(0)$, the $T = 0$ coherence length.
(3) the transition temperature: T_c.

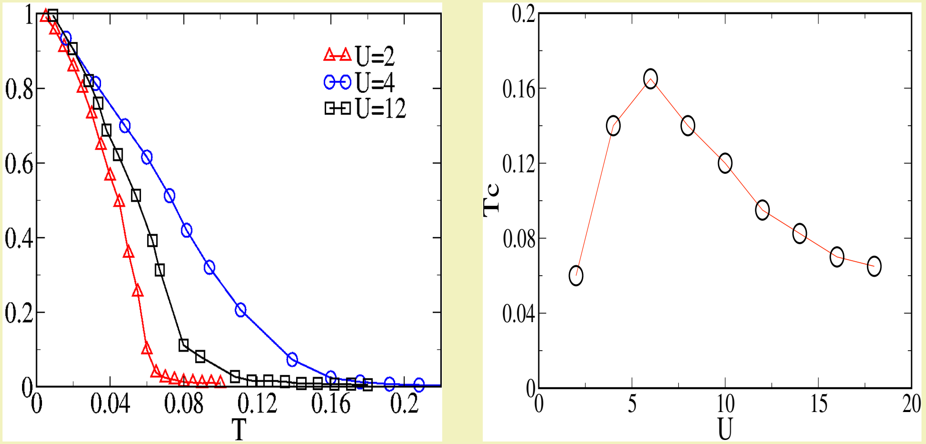
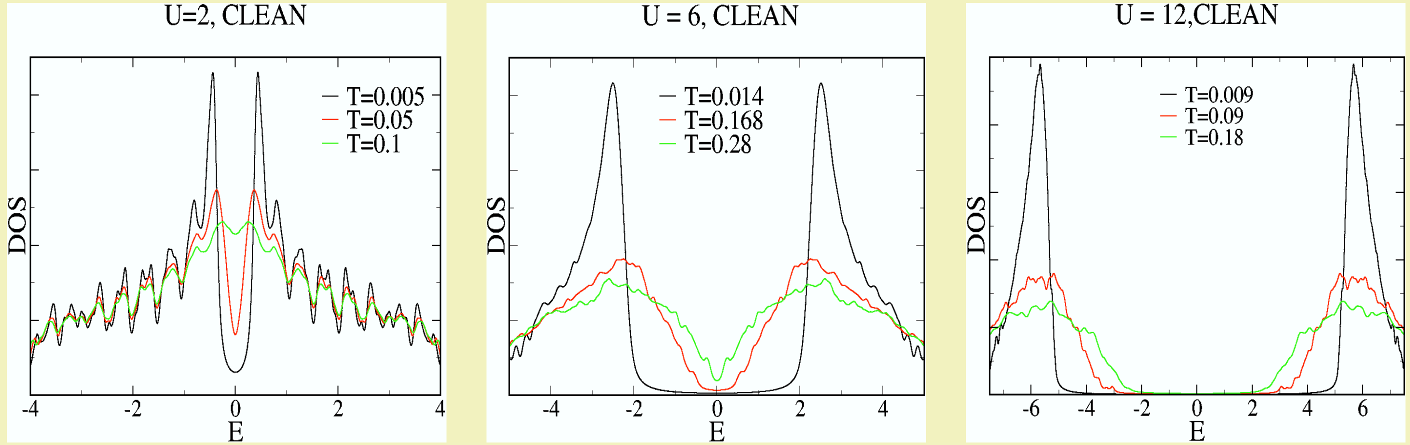


Figure 2: Left- T dep of SF order parameter. Right- non-monotonic $T_c(U)$.

$U/zt \ll 1$: BCS pairing, $\Delta(0) \sim e^{-1/N(\epsilon_F)U}$, $\xi(0)/a_0 \gg 1$, $k_B T_c/\Delta(0) \sim 3.5$

$U/zt \sim 1$: $\Delta(0)$ increases, smaller $\xi(0)$, $k_B T_c/\Delta(0) > 3.5$

$U/zt \gg 1$: 'BEC of pairs', $\Delta(0) \sim U$, $\xi(0) \sim a_0$, $k_B T_c/\Delta(0) \sim t^2/U^2$



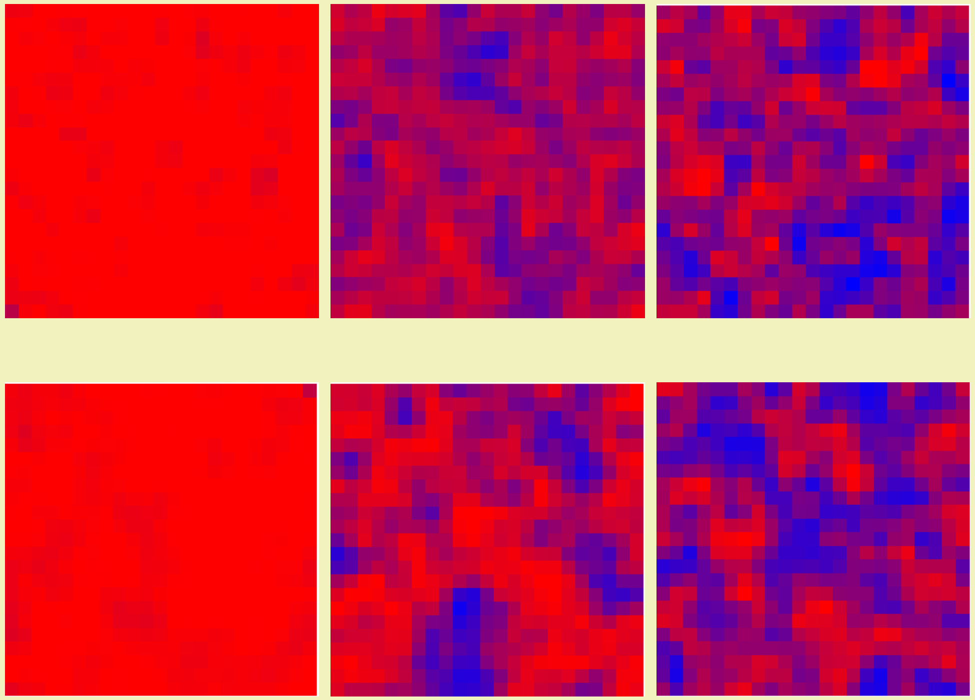
Highlight $U = 2$ (weak), $U = 6$ (intermediate), $U = 12$ (strong)

$U = 2$:
already $2\Delta(0)/k_BT_c \sim 10$, much greater than BCS!
gap closes with increasing T, band like DOS for $T > T_c$.

$U = 6$:
larger gap, $2\Delta(0)/k_BT_c \sim 20$, larger T_c
distinct pseudogap near T_c, persists to $T \sim 2T_c$
the ϕ's have a broad distribution at high T.

$U = 12$:
gap $\sim U$, suppressed $T_c \sim t^2/U$
clean gap persists to $T \gg T_c$.
the thermal transition is from an insulator to a SF

A further signature of correlations above T_c:



The correlation $\phi_0 \phi_i cos(\theta_0 - \theta_i)$ at $U = 2$ and $U = 12$ at three different T

Even $U = 2$ has significant ϕ_i amplitudes above T_c .. non BCS..

- Diff regimes at $U = 2$, $U = 6$ and $U = 12$. All have SC ground states.
- Even at $U = 2$ pairing amplitude survives at $2T_C$ and form domains. Already outside the BCS regime. No visible pseudogap.
- The $U = 6$ case shows qualitatively similar physics, but distinct pseudogap, and strong pair correlations at the highest T.
- $U = 12$ shows suppressed amplitude fluctuations, clean gap in the DOS. Phase fluctuations dominate.

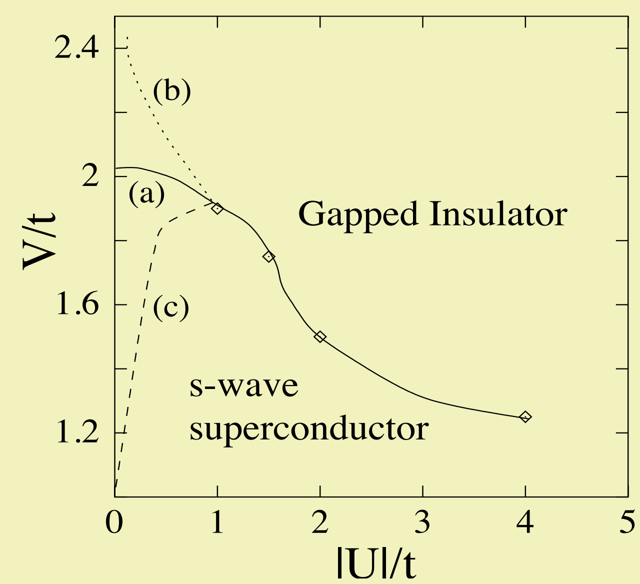
C. Superfluid-‘insulator’ transitions

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

The -ve U model with disorder describes SF-insulator transitions (SIT).

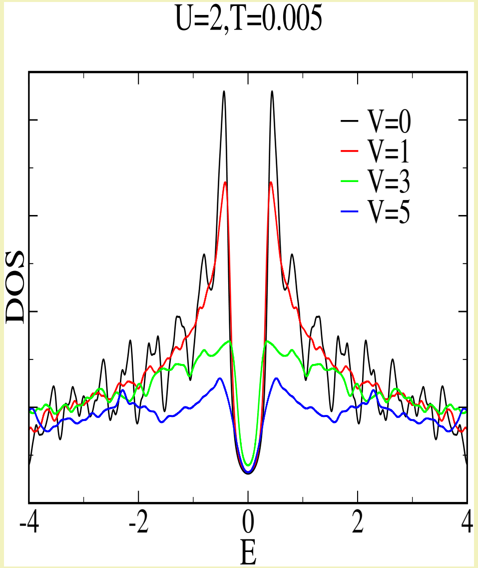
ϵ_i distributed between $\pm V$. Small V: disordered SF, large V: gapped insulator.

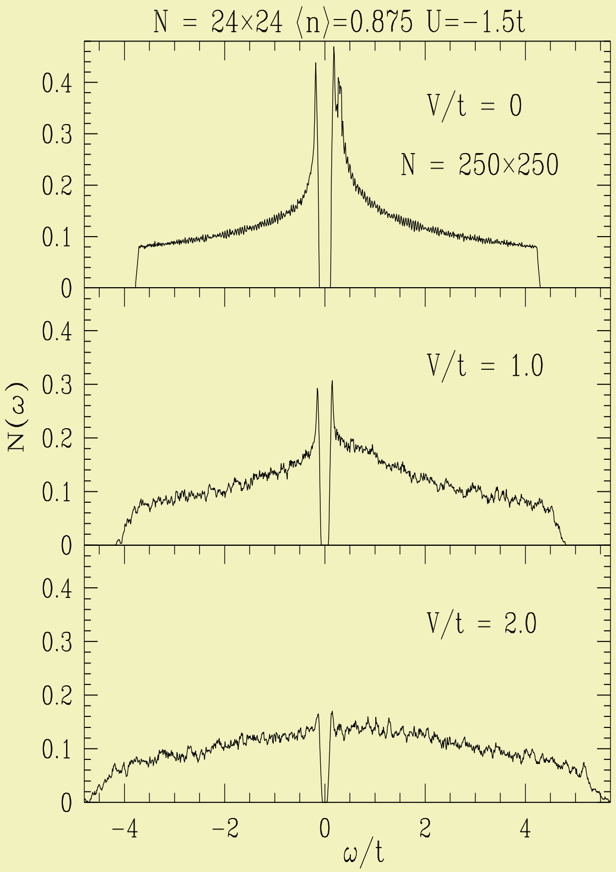
There is already a phase diagram based on a BdG + flucns theory



Ghosal, *et al.*, PRB (2001).

Illustrative result: Disorder at weak coupling, low T.

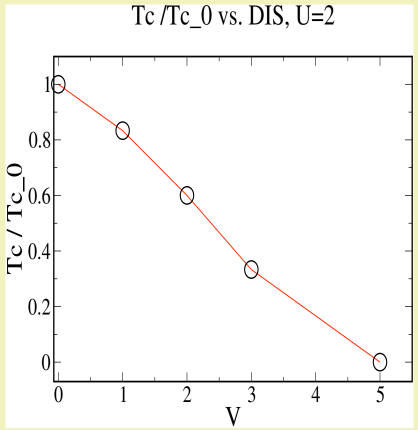


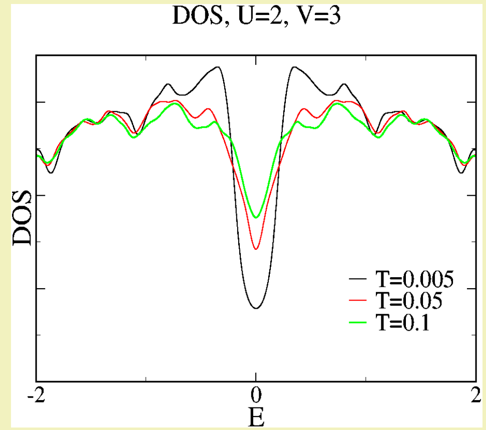


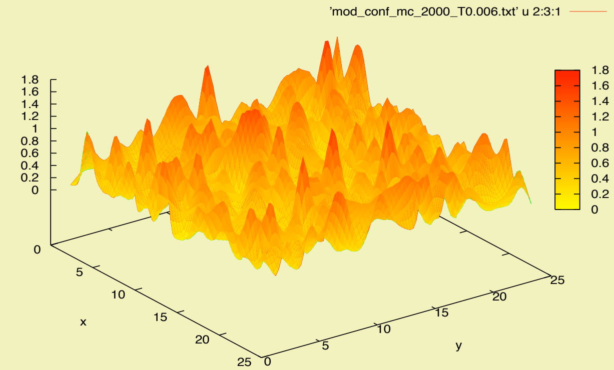
Loss of coherence peak in the DOS..

Can be captured within BdG as well (Ghosal..)

But the thermal physics?







Three benchmark results:

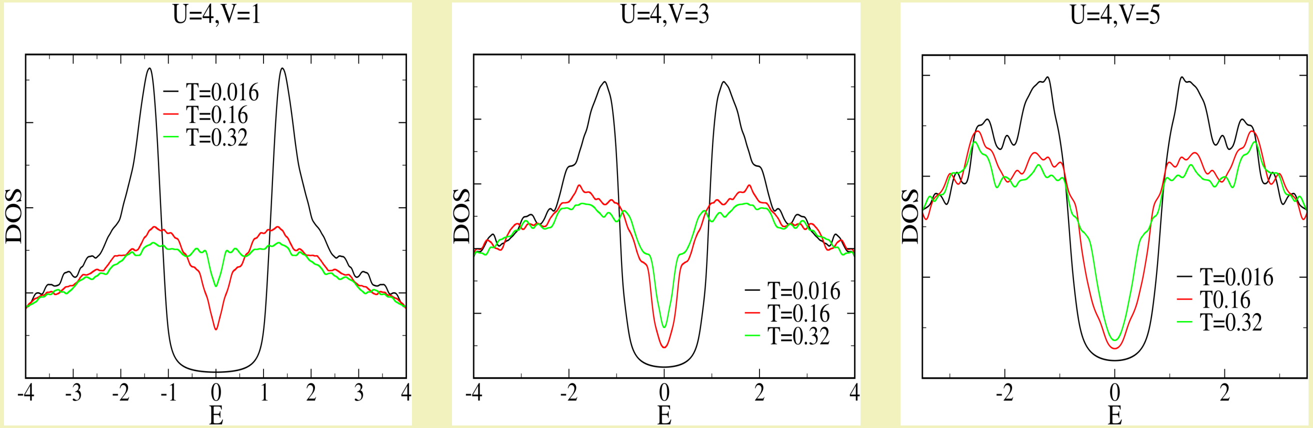
(i) Suppression of T_c with disorder (left), albeit slower than full QMC.

(ii) The presence of a 'pseudogap' in the DOS even above T_c (middle).

(iii) The formation of superconducting islands, in the disordered system

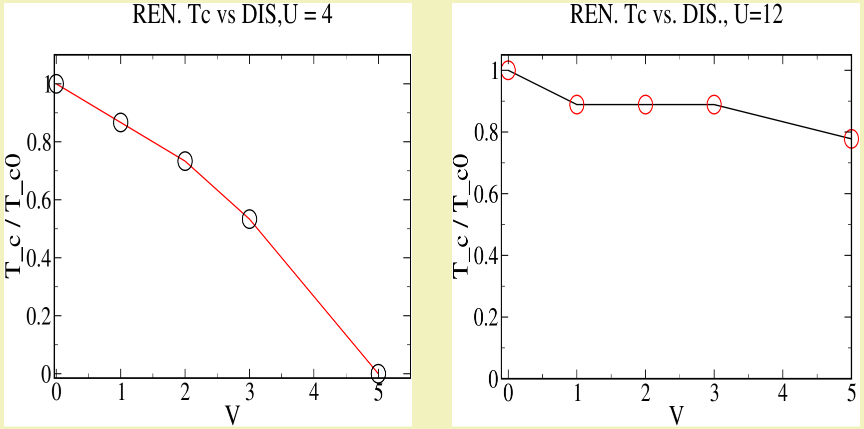
What is our advantage with respect to (disordered) BdG theory?

The HS based approach is equiv to BdG at low T, captures amplitude and phase flucns at finite T.



Disorder dependence of the DOS at intermediate coupling.

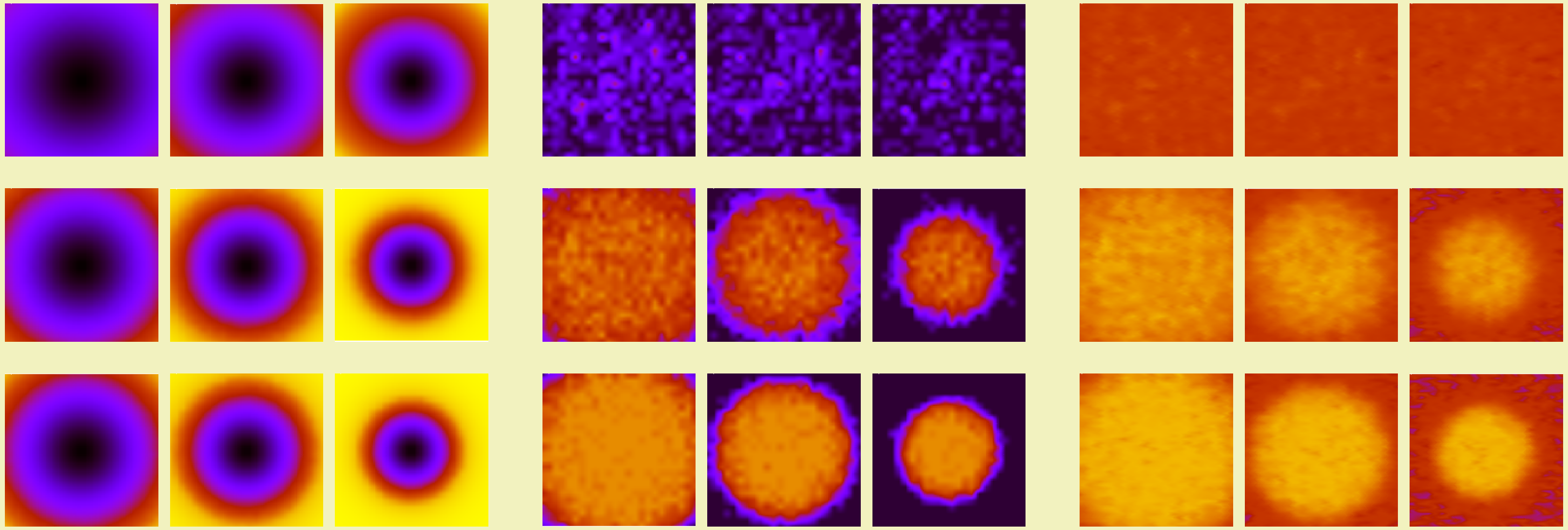
Prominent pseudogap even at low temperature.



Disorder suppression of T_c at intermed and strong coupling.

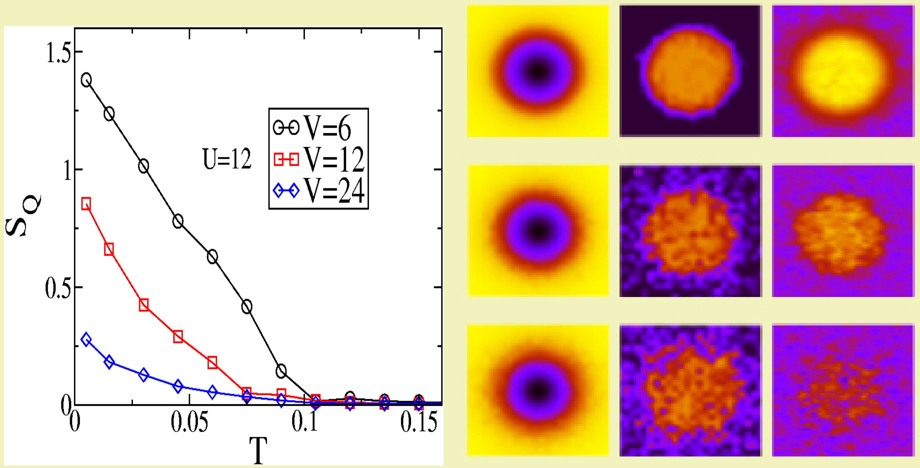
D. Inhomogeneous superfluid in a trap

$$H = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + V_0 \sum_{i\sigma} (x_i^2 + y_i^2) n_{i\sigma} - \mu \hat{N} - U \sum_i n_{i\uparrow} n_{i\downarrow}$$

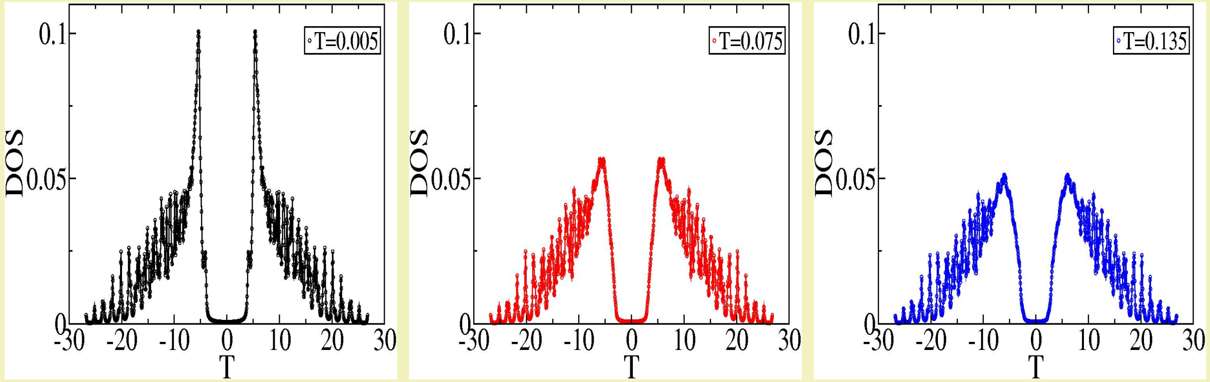


We explore $U = 2,\ 6, 12$, $\mu = -U/2$, and $V_b = U/2,\ U,\ 2U$.

T dependence at strong interaction $U = 12$, $V_b = 2U$.



Quasiparticle density of states: T dep at strong coupling, $U = 12$, $V_b = 2U$.



- the coherence feature at low T and its T dependence
- the persistent gap in the spectrum above T_c
- the confinement induced oscillations, T indep

Conclusion

-Optical lattices allow controllable realisation of many body models.

-They can be used as ‘analog simulator’ for correlated systems.

-May be used to study dynamics and non-equilibrium effects as well.

-The *inhomogeneity* is an essential feature: novelty, difficulty..

-We have a method that handles strong coupling, disorder and confinement.

-Easy extension to d-wave pairing, FFLO states, vortex lattices ...

-More measurement tools, and theoretical concepts need to be developed..

Huge literature! two references..

Jaksch and Zoller, Ann. Phys., 315, 52 (2005)

Bloch, Dalibard and Zwerger, Rev. Mod. Phys. 80, 885 (2008)