Luttinger theorem breaking in the repulsive Fermi Hubbard model

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Introduction

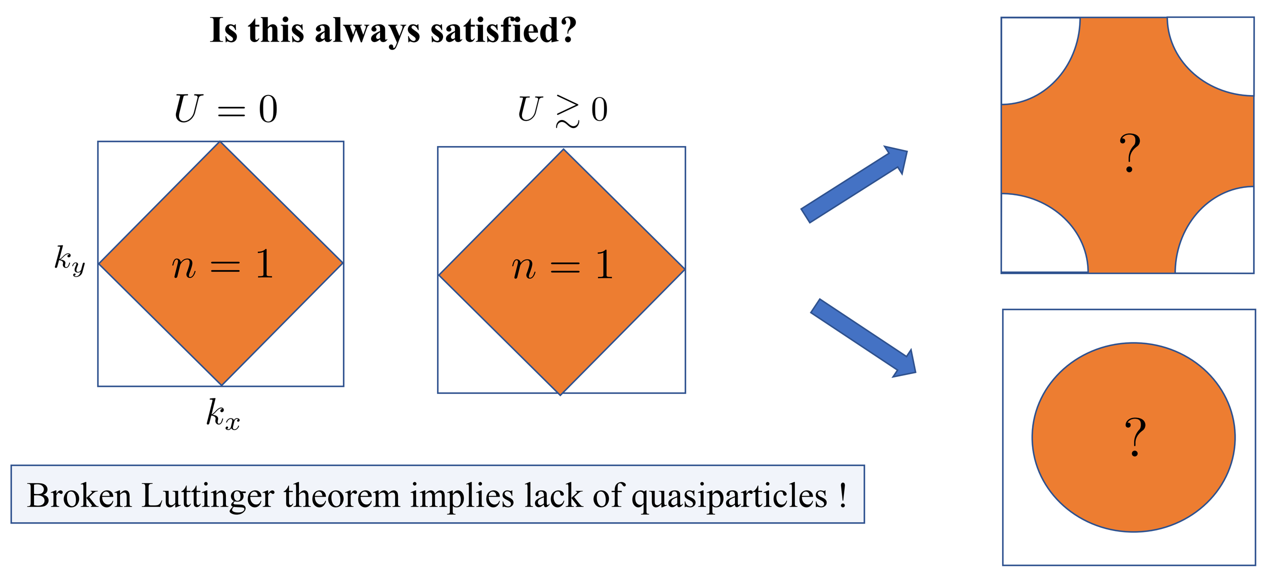
Luttinger's theorem:

$$\frac{1}{V}\langle\sum_k c_k^\dagger c_k\rangle = \frac{1}{V}\sum_k \oint \frac{d\omega}{2\pi}\frac{e^{i\omega 0^+}}{i\omega-\epsilon(k)-\Sigma(k,\omega)} = \sum_k \Theta(\mathrm{Re}G(k,\omega=0))$$

n Fermi surface volume

Proof by Luttinger(1960) (Perturbative)[1], Oshikawa(2000) (Non perturbative)[2]

Is this always satisfied?



Broken Luttinger theorem implies lack of quasiparticles !

$U>>0, n>1$

Model and methodology

Fermi Hubbard model (parent model of high T_c superconductors):

$$H = -\sum_{\langle i,j\rangle,\sigma}(t_{ij}\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma}+\mathrm{h.c}) - \mu\sum_{i,\sigma}\hat{n}_{i,\sigma} + U\sum_{i,\sigma}(\hat{n}_{i,\uparrow}-\frac{1}{2})(\hat{n}_{i,\downarrow}-\frac{1}{2})$$

nearest neighbor hopping — sets doping — particle hole symmetry

Investigate by discrete Ising Hubbard Stratonovich DQMC: (Determinantal Quantum Monte Carlo)

- Partition function $Z=\sum_n\langle n|\prod_l e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}}|n\rangle$
- Evaluate Z with HS transformation (with $\cosh(\nu)=e^{\frac{U\Delta\tau}{2}}$)

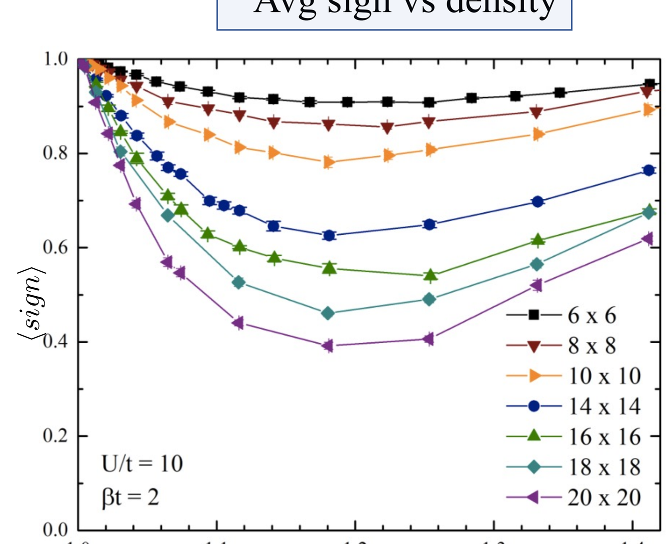
$$e^{-U\Delta\tau(\hat{n}_{i,\uparrow}-\frac{1}{2})(\hat{n}_{i,\downarrow}-\frac{1}{2})} = C\sum_{h_i=\pm1} e^{\nu h_i(n_{i,\uparrow}-n_{i,\downarrow})}$$

- Transforms Z into: $Z=Tr_{\{h\}}\prod_{\sigma=\uparrow,\downarrow}\mathrm{Det}(I+\prod_l e^{-\Delta\tau K}e^{-\Delta\tau V^\sigma_l(\{h\})})$
- Fermion determinants not always > 0. Source of sign problem.

We work at intermediate temperature:

- Temperature is high enough to avoid spontaneously symmetry broken ground states.
- Sign problem is not a hindrance.

Avg sign vs density



Results from G(k, $\tau=\beta/2$)

Relation between Green's function and spectral function:

$$G(k,\tau)=\int d\omega\frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}A(k,\omega)$$

$$G(k,\tau=\beta/2)=\int d\omega\frac{1}{2\cosh(\beta\omega/2)}A(k,\omega)$$

For variation in A(k,ω) at scale, $\beta\Omega>>1$ [4]

$$A(k,\omega=0)=\frac{\pi}{\beta}G(k,\tau=\beta/2)$$

Accessible by ARPES — Accessible by DQMC

Interacting Fermi surface, defined by contour where $A(k,\omega=0)$ is maximized

$$(\mathrm{F.S})_I = \oint_k dk[|\hat{k}\cdot\nabla_k G(k,\tau=\beta/2)=0]$$

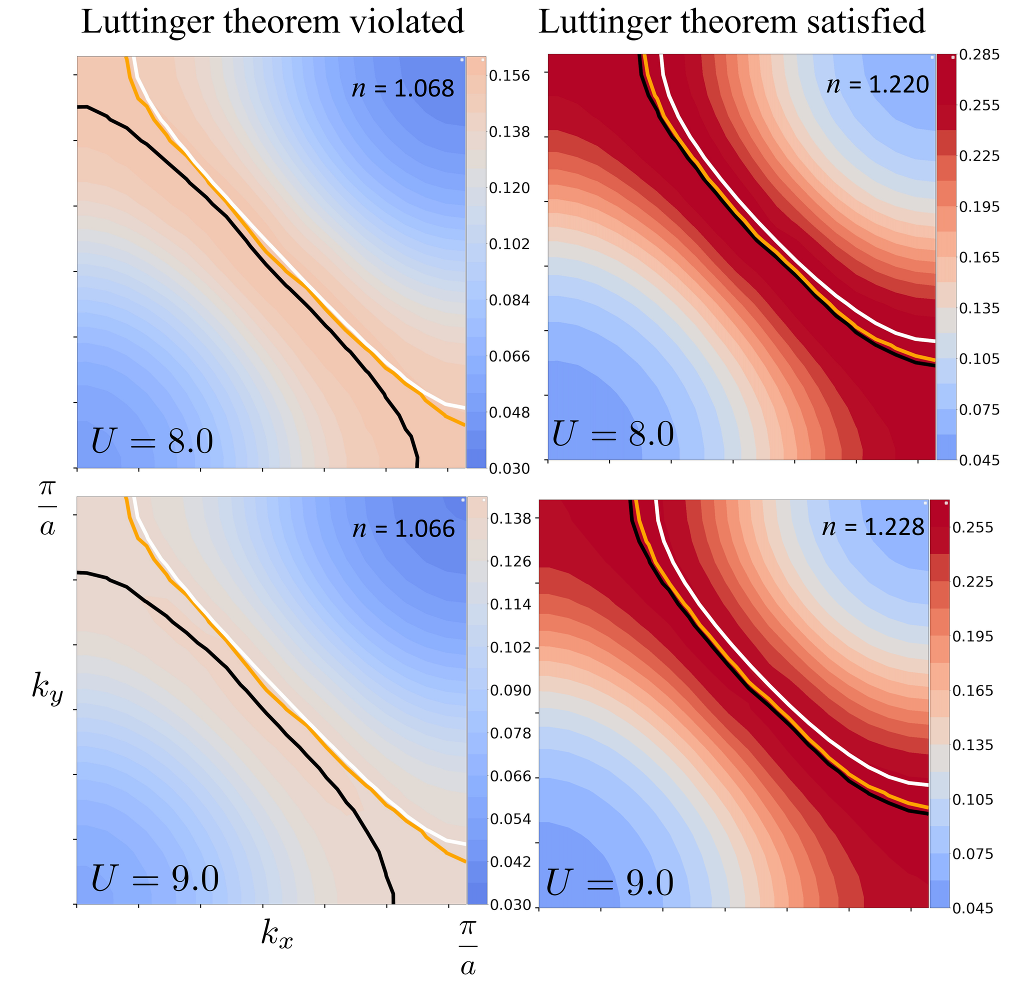
(black contour)

Non interacting Fermi surface, defined by $\epsilon(k)=\mu$

$$G(k,\tau=\beta/2)_{N.I} = \int d\omega\frac{1}{2\cosh(\beta\omega/2)}2\pi\delta(\omega)=\frac{1}{2}$$

(i) $(\mathrm{F.S})_{N.I}=\oint_k dk[|\hat{k}\cdot\nabla_k G(k,\tau=\beta/2)_{N.I}=0]$ (orange contour) (ii) $(\mathrm{F.S})_{NI}=\oint_k dk[n(k)=0.5]$, where $n(k)=\langle c^\dagger_k c_k\rangle$ (white contour)

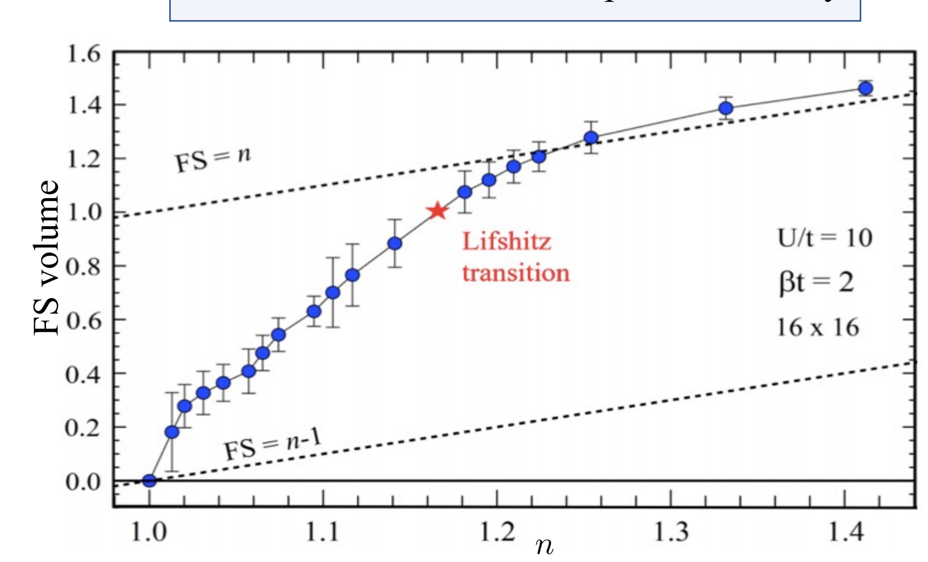
Contour plots of $G(k,\tau=\beta/2)$



[Plots are for 16x16 sites at $\beta=2$]

Fermi surface reconstruction by over-doping Fermi Hubbard Model:

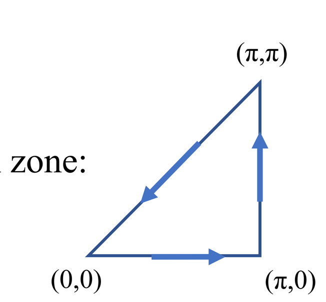
Fermi surface volume vs particle density



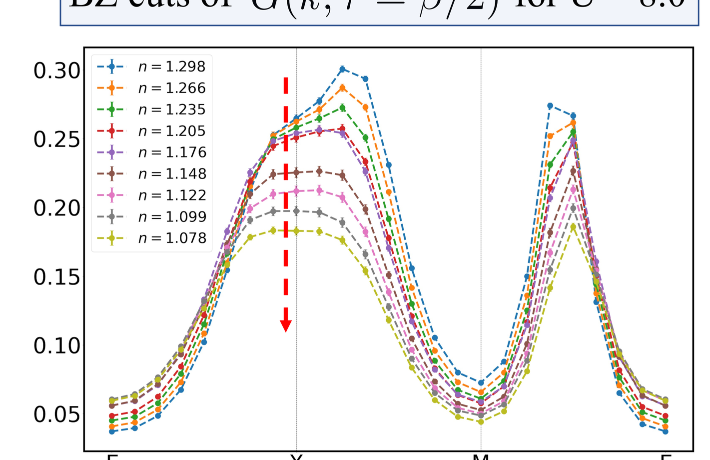
- Fermi surface volume shows a departure from Luttinger count at critical density $n_c=1.2$
- Electron like Fermi surface secedes to smaller volume (or hole like) below $n_c=1.2$
- Fermi surface is 0 at the Mott Insulator limit

Distribution of spectral weight in the Brillouin zone:

Path in Brillouin zone:

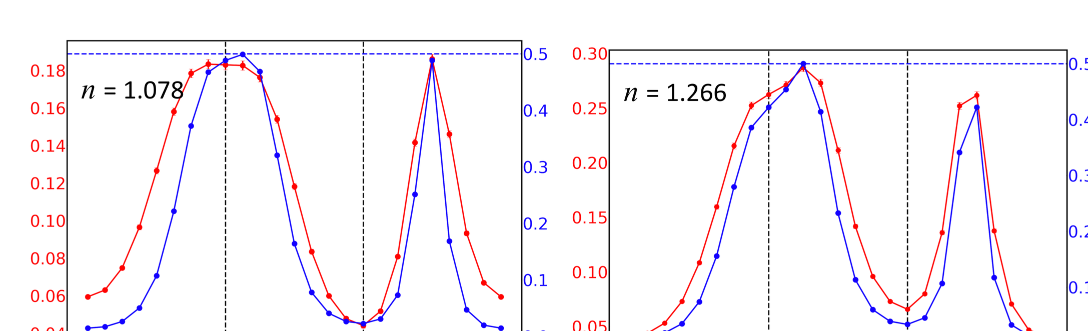


BZ cuts of $G(k,\tau=\beta/2)$ for U = 8.0



Quasiparticle weights decrease on entering LB phase

BZ cuts of $G(k,\tau=\beta/2)$ for U = 9.0, U = 0.0



Luttinger theorem violated — Luttinger theorem satisfied

Results from Analytic Continuation

Non interacting Fermi Surface:

$(\mathrm{F.S})_{N.I}=\oint_k dk[\epsilon(k)=\mu]$ (orange contour)

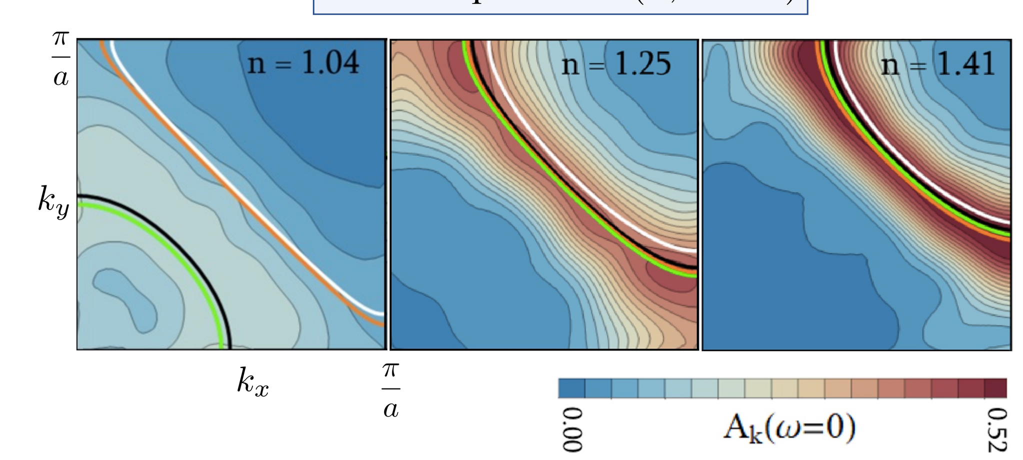
$(\mathrm{F.S})_{N.I}=\oint_k dk[n(k)=0.5]$ (white contour)

Interacting Fermi Surface:

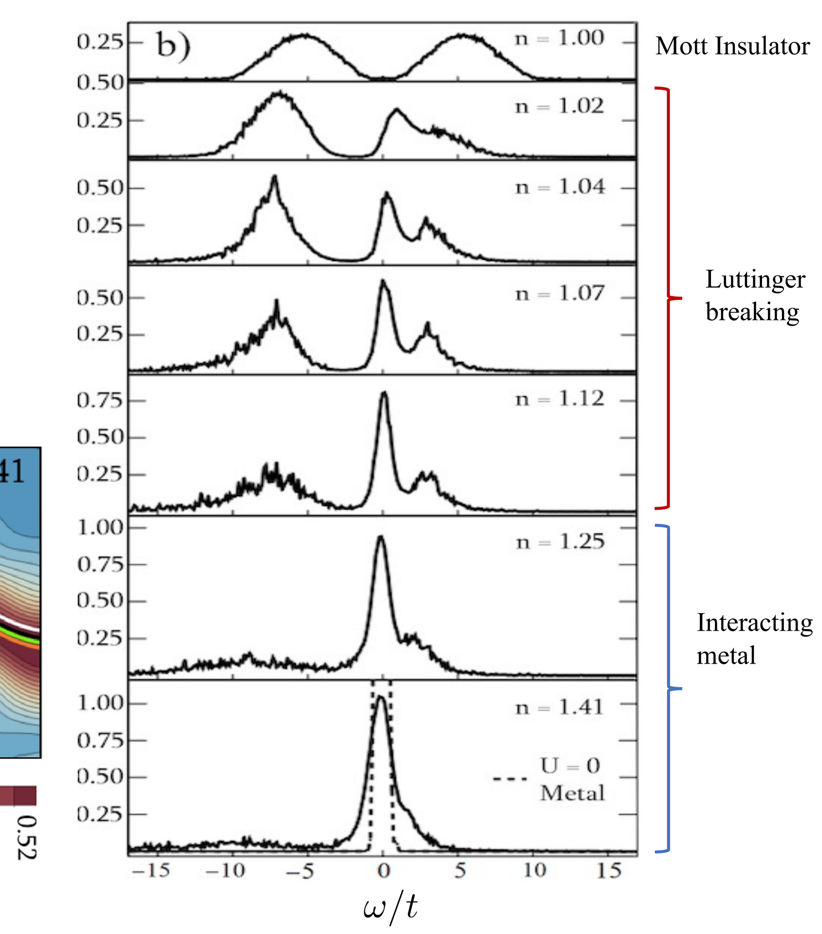
$(\mathrm{F.S})_I=\oint_k dk[|\hat{k}\cdot\nabla_k A(k,\omega=0)=0]$ (black contour)

$(\mathrm{F.S})_I=\oint_k dk[\mathrm{Re}(G(k,\omega=0))=0]$ (green contour)

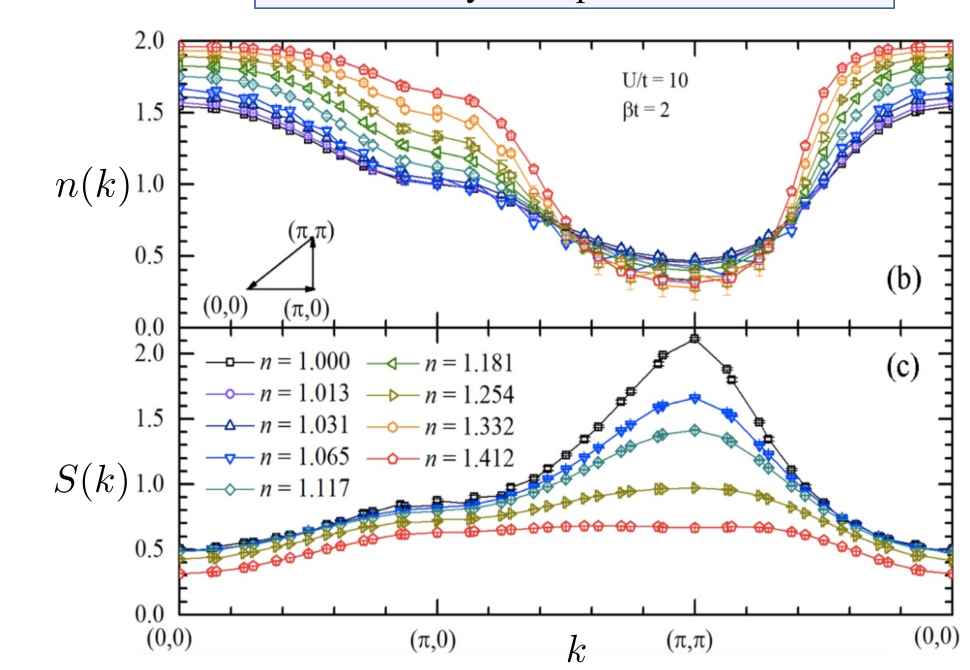
Contour plots of $A(k,\omega=0)$



Normalized plots for $\frac{1}{S}\int dk A(k,\omega)$



Static density and spin structure factors



No CDW in Luttinger breaking phase

No SDW in Luttinger breaking phase

[Plots are for 16x16 sites at $\beta=2$]

Conclusion

1) Repulsive Fermi Hubbard model shows restructuring of the Fermi surface as a function of doping, while approaching the Mott limit from the metallic side.

2) Restructuring of single particle spectral weight across Brillioun zone on transitioning between Luttinger breaking and metallic phase.

3) No broken U(1) symmetry. No charge density or spin density wave formation. Possible topological order?

Acknowledgment and References

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