Cuprates and Stripes

using Hubbard Model

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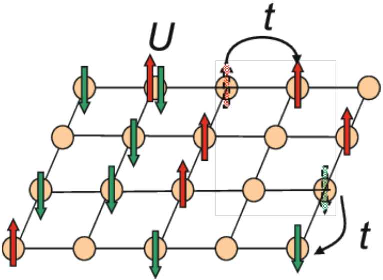


Objective

- Looking for the effects of electron-phonon coupling on the physics of stripes seen in Hubbard model for square lattice in 2D designed for Cuprates.
- Modelling the coupling using bond-SSH mechanism.
- In future,
  - plan to execute more "physical" mechanism, namely, optical-SSH;
  - looking for the possible similarities and differences with the results obtained from Holstein mechanism.

Model

- Hubbard model on 2D square lattice with nearest and next nearest neighbour hopping.
- Adding bond SSH coupling.*equation*

equation

- Relationship between α and λ.
- Working in hole doped regime. For starters, going till $p = 0.2$ and point of interest around $p = 0.125$ due to ...

Assesment of sign for different temperature

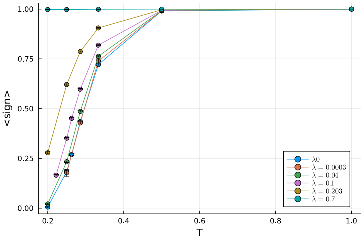


Figure: 1a. $\langle sign \rangle$ vs T

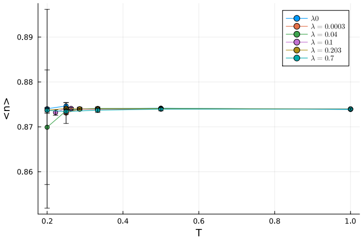


Figure: 1b. $\langle n \rangle$ vs T

NOTES: To check the limit on lower value of T, note: with varying T, important to keep <n> constant. $\langle n \rangle = 0.875, U = 6, t' = -0.25, t = 1$, varying T to check $\langle \text{sign} \rangle$ for a set of λ values set by α

Is Mott gap decreasing?

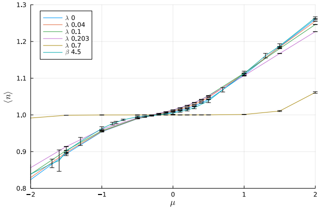
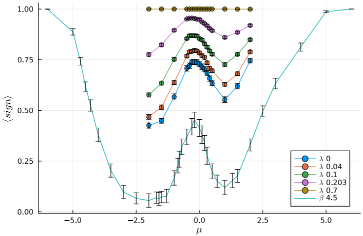
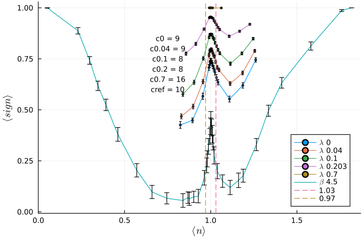


Figure: $\langle n \rangle$ vs μ

Initial assessment of Mott gap by looking at $\langle n \rangle$ vs μ curve. The trend of slope increasing with increasing λ indicates that the mott gap is decreasing.
Parameters used: $\beta = 3.5$ others are same as before.





- The sign gets worse very quickly as move away from half filling.
- Same distribution of chemical potential used for varying coupling strength to evaluate filling fraction.
- The denser the peak at half filling, more number of μ points near half filling, meaning larger the gap.
- c$\{\lambda\}$ (e.g., c0) counts such number within indicated upper and lower bounds and it again indicates decrease in Mott gap.
- This is not so evident from μ vs sign scan.

Structure factor

Direct look at the spin $S(\mathbf{Q}, \omega = 0)$ and charge density $N(\mathbf{Q}, \omega = 0)$ structure factor calculated for varying λ.
SDW for $q = (\pi/a, \pi/a)$ are found suppresed. As an example,

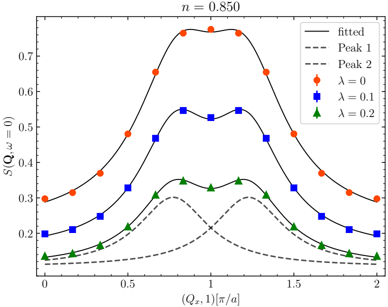
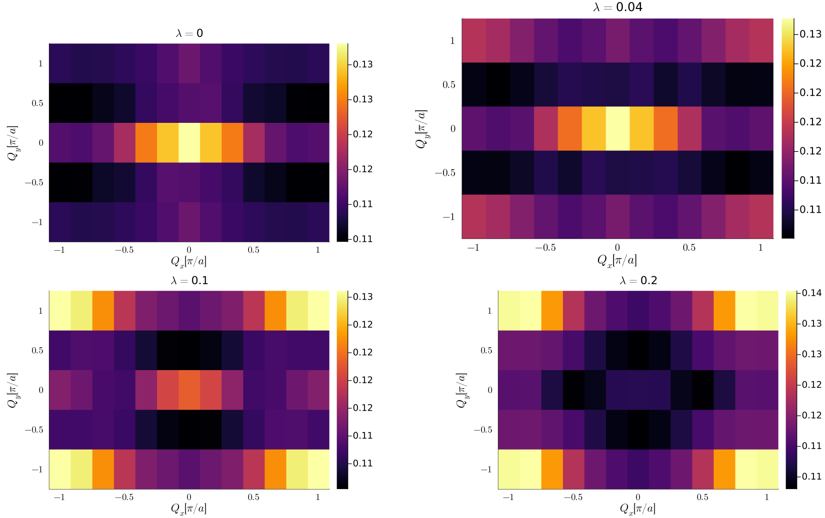


Figure: Spin structure factor along $(q_x, q_y = \pi/a)$

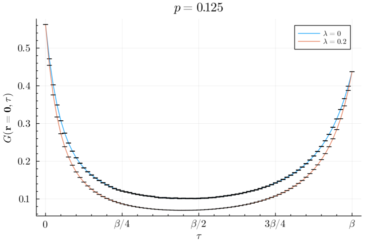
For the charge density wave, however the location of maxima shifts from $(0, 0)$ to $(\pi/a, \pi/a)$.

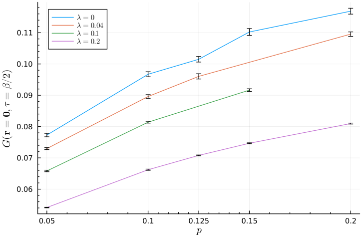


$p = 0.1, \beta = 4$

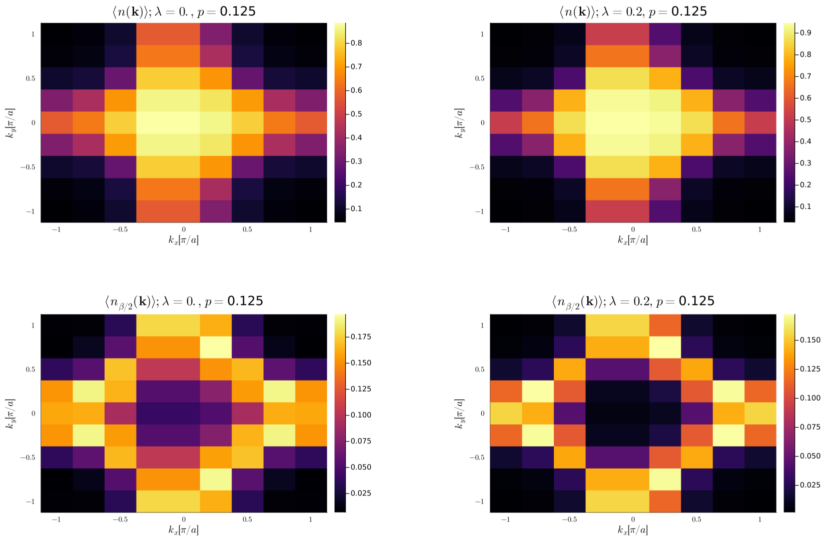
Studying Mott Gap

- $G(\mathrm{r}=0, \tau=\beta/2)$ gives the spectral weigh near fermi energy (μ at $T \neq 0$).
- $G(\mathrm{r}=0, \tau)$ records the cumulative spectral weighs over an energy range depending on τ.
- $G(\mathrm{k}, \tau)$ projects this on k-space, and with the model being single band, each k hosts non-degenerate single particle eigenstate.
- $G(\mathrm{k}, \tau=0^-) = 1 - \langle n_\mathrm{k} \rangle$, recording $\langle n_\mathrm{k} \rangle$





Both tell us that the states near fermi energy are moving away.
The former graph also indicates increase in Mott gap, contrary to what we (think) we see earlier in $\langle n \rangle$ vs μ graph.
To see clearer on what is happening, looking at $\langle n_{\mathrm{k}} \rangle$



where, $\langle n_{\mathbf{k}} \rangle = G(\mathrm{k}, \tau = \beta/2)$ captures the spectral weigh near fermi energy, making it clearer to see the fermi surface(FS).

Fermi surface(FS) appears to sharpen.

Hypothesis:

With Mott gap reducing and the FS sharpening, U might e effectively reducing.
(This has been already seen in Hubb-Holstein model)

Ideas to check this?

1. Looking for compressibility, $\kappa(= \partial\langle n\rangle/\partial\mu)$.
2. Direct comparison of ...(results) between low U, $\lambda = 0$ and high U with $\lambda \neq 0$.
3. Comparison with the weak-coupling physics, RPA limit results.

Compressibility

With increasing α, I find that μ required to fix specific $\langle n \rangle$(let us say, 0.8) shifts away from 0, and κ reduces as well, implying the rate at which $\langle n \rangle$is changing w.r.t μ is slowing down(slower the rate, lower the number of states).
Both of these lead to the conclusion that the Mott gap is increasing with e-ph coupling.

- Looking closely at the data of $\langle n \rangle, \kappa$ with varying μ, closer to half-filling, let us say ~1.004 or ~0.997 as the filling, κincreases with both fixed μ or $\langle n \rangle$ for increasing α; hinting decrease in Mott gap.
- On the other hand, the rough μ range for $\langle n \rangle$ to change from ~1.008 to ~ 0.997, the interval shifts toward lower values of μ but stay roughly same ~ 0.25 - 0.3.
- It should be noted that for this part of the analysis, better data is needed to conclude the statement with more confidence as the range interval has pattern of [0.3, 0.25, 0.25, 0.3] for [0,0.12,0.19,0.27] as α values. More number of alpha points and more number of μ points are needed at $\langle n \rangle \sim 1$(there were mostly 3-4 points).
- IDEA : Fine tune $\langle n \rangle - \mu$ map by running calc. for denser set of μ points. Result?

Result

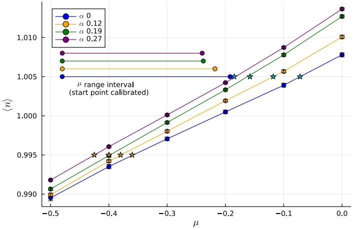


Figure: $\langle n \rangle$ vs μ

This shows much clearly and conclusively that the gap is reducing. μ range interval for $0.995 < \langle n \rangle < 1.005$.
As we move away from $\langle n \rangle = 0.99$,$\langle n \rangle$ drops drastically, hinting this is very close to Mott gap.
For further concrete comments, however, we need to look at DOS. >>> Analytic Contiuation!