Cuprates and Stripes
using Hubbard Model

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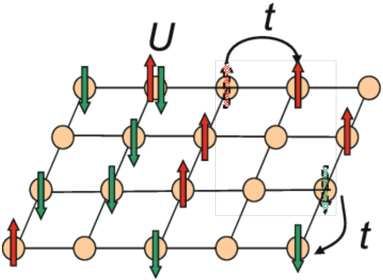
12th December, 2023



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

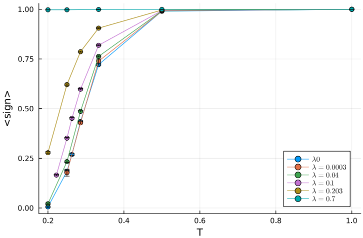


Figure: 1a. $\langle sign \rangle$ vs T

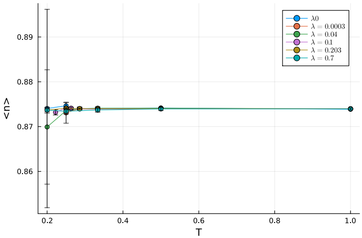


Figure: 1b. $\langle n \rangle$ vs T

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?

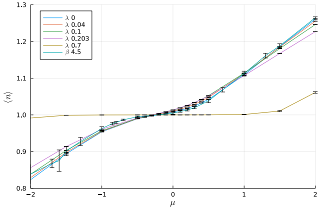
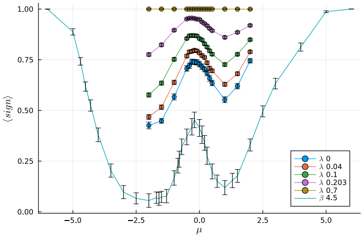
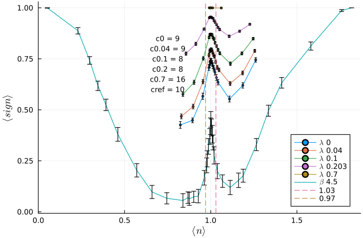


Figure: $\langle n \rangle$ vs μ

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.
<u>Parameters used:</u> $\beta = 3.5$ 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{λ} (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,

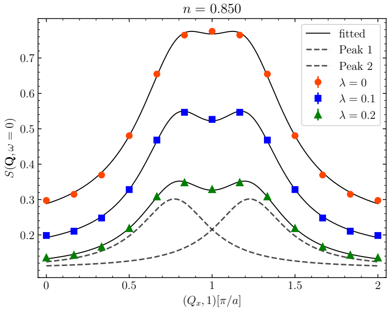
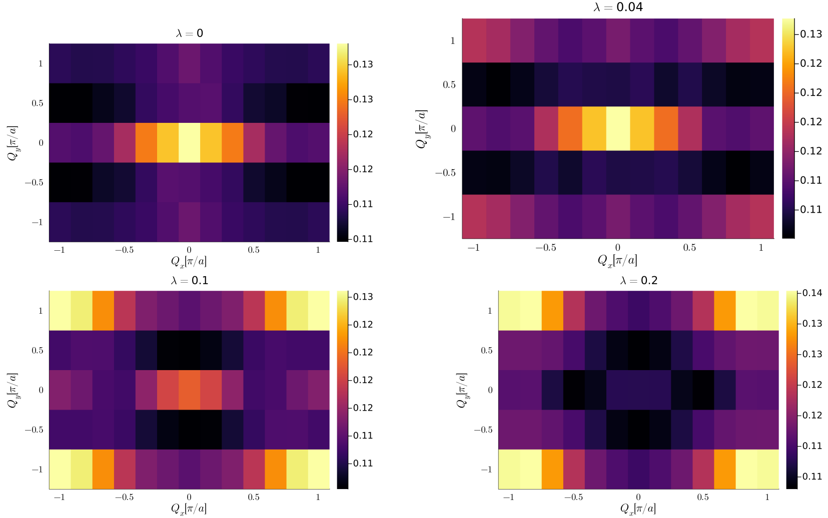


Figure: Spin structure factor along $(q_x, q_y = \pi/a)$

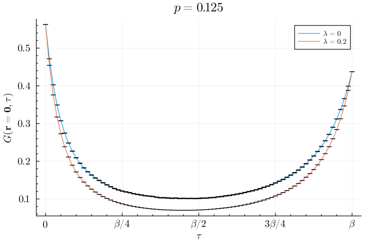
For the charge density wave, however the location of maxima shifts from $(0, 0)$ to $(\pi/a, \pi/a)$.

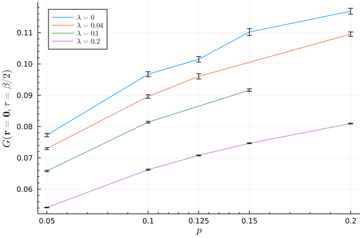


$p = 0.1, \beta = 4$

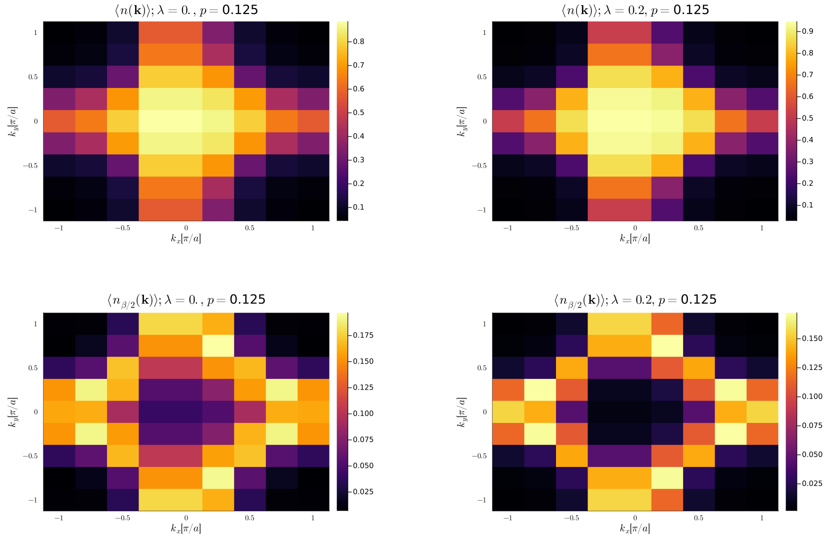
Studying Mott Gap

- $G(\mathrm{r}=0, \tau=\beta/2)$ 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

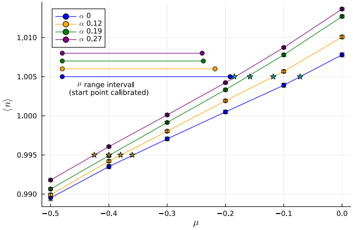
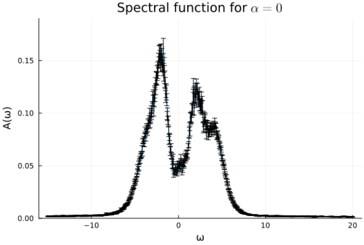
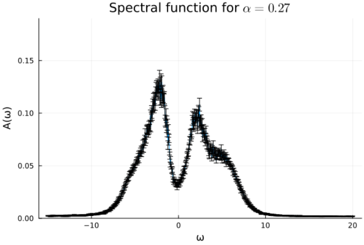


Figure: $\langle n \rangle$ vs μ

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!

DOS using DEAC





Note: It peaks are getting less sharper, moving more into the coherent states. Though the depth of the valley (at low temp, clear gap) is increasing, the curvature is increasing as well. By extrapolation to lower temperature, I infer that the gap is reducing.