



UCDAVIS



# Charge Density Wave Order and Superconductivity in the Disordered Holstein Model

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- 3. Phonons with Dispersion
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Funding:

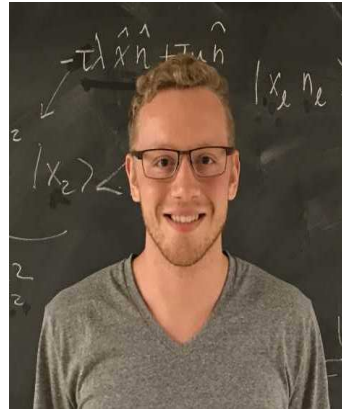
Department of Energy DE-SC0014671 and DE-NA0002908.



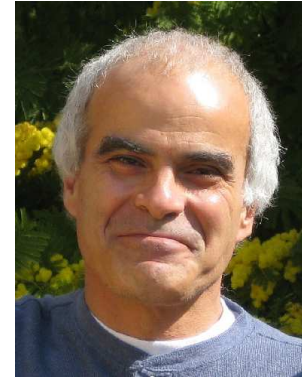
Natanael  
Costa



WeiTing  
Chiu



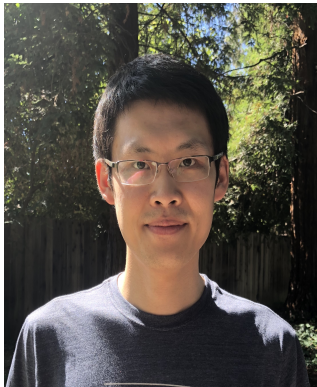
Thomas  
Blommel



George  
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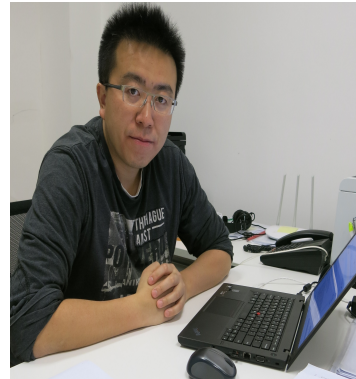
Ehsan  
Khatami



Bo  
Xiao



YuXi  
Zhang



ZiYang  
Meng

“Phonon dispersion and the competition between pairing and charge order”, N.C. Costa, T. Blommel, W.-T. Chiu, G.G. Batrouni, and RTS, Phys. Rev. Lett. 120, 187003 (2018).

“Charge Order in the Holstein Model on a Honeycomb Lattice,” Y.-X. Zhang, W.-T. Chiu, N.C. Costa, G.G. Batrouni, and RTS, Phys. Rev. Lett. 122, 077602 (2019).

“Localization, Charge Ordering, and Superfluidity in the Disordered Holstein Model,” B. Xiao, E. Khatami, N. Costa, G. Batrouni, and RTS, submitted to Phys. Rev. Lett.

## 0. Mark and My First Car

In my third year in grad school at UCSB I bought my first car, a 1974 Mazda 808.



It cost \$500 and was not in great shape.

(The paint job looked nothing like the photo above.)

I think Mark was way more excited than I was.





I had owned the car 5 nanoseconds  
when Mark came rushing into the office,

“Let’s change the oil!”

Actually, I don’t have **nearly enough**  
exclamation points there . . .

“Let’s change the oil!!!!!!!!!!”

So we started. (Well, Mark did.)

About ten minutes into the process Mark stuck his head out from under the car,  
an **absolutely ecstatic** look on his face.

“They put the wrong size oil filter on! It’s going to be **really hard** to get off!”

**It’s hard to overestimate how delighted this made Mark.**

Everyone here knows that side to Mark: The joy at encountering a tough problem.



## Mark and Holstein:

“Holstein model in infinite dimensions,” J.K. Freericks, [Mark Jarrell](#), and D.J. Scalapino, Physical Review B 48, 6302 (1993).

“Two-dimensional Hubbard-Holstein bipolaron,” A. Macridin, G.A. Sawatzky, and [Mark Jarrell](#), Physical Review B69, 245111 (2004).

“Iterated perturbation theory for the attractive Holstein and Hubbard models,” J.K. Freericks and [Mark Jarrell](#), Physical Review B50, 6939 (1994).

“Synergistic polaron formation in the Hubbard-Holstein model at small doping,” A. Macridin, B. Moritz, [Mark Jarrell](#), and T. Maier, Physical Review Letters 97, 056402 (2006).

“Spectral properties of Holstein and breathing polarons,” C. Slezak, A. Macridin, G.A. Sawatzky, [Mark Jarrell](#), and T.A. Maier Physical Review B73, 205122 (2006).

“Effect of long-range hopping on  $T_c$  in a two-dimensional Hubbard-Holstein model of the cuprates,” E. Khatami, A. Macridin, and [Mark Jarrell](#), Physical Review B78, 060502 (2008).

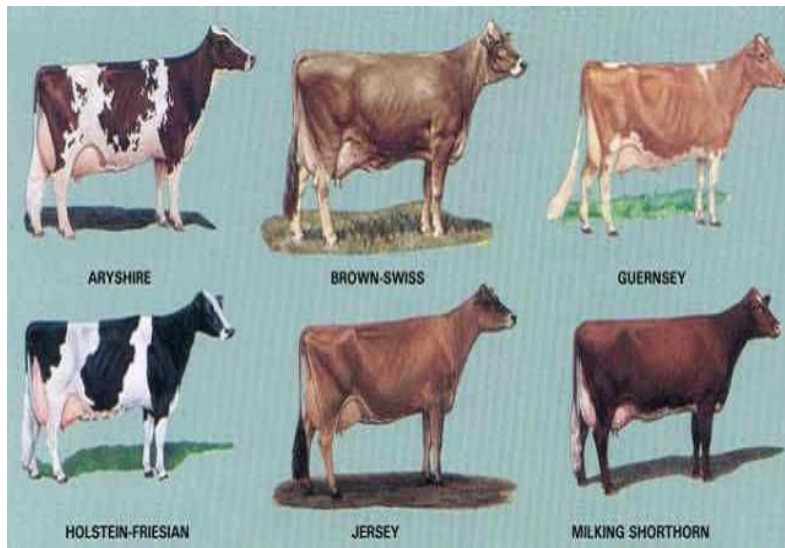
“Periodic Anderson model with Holstein phonons for the description of the cerium volume collapse,” E. Li, S. Yang, P. Zhang, K.M. Tam, [Mark Jarrell](#), and J. Moreno, Physical Review B99, 155147 (2019).

Theorists have a reputation for oversimplification:



In that sense the **Holstein** model is an unfortunate name . . . .

Holsteins originated in Holland more than 2,000 years ago, and were brought to America in the 1850's.



The Holstein model:

“Studies of polaron motion: Part II.  
The ‘small’ polaron”  
Annals of Physics 8, 343 (1959).

This talk: somewhat more realistic  
‘cows’!

## 1. Hubbard to Holstein

Noninteracting electron kinetic energy:

$$\hat{H}_{\text{el-ke}} = -t \sum_{\langle ij \rangle \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} \right)$$

**Hubbard:** Spin  $\uparrow, \downarrow$  electrons on same site  $i$  interact with each other:

$$\hat{H}_{\text{el-el}} = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

**Holstein:** Spin  $\uparrow, \downarrow$  electrons interact with boson displacement on site  $i$

$$\hat{H}_{\text{el-ph}} = \lambda \sum_i \hat{X}_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) \quad H_{\text{boson}} = \frac{1}{2} \omega_0^2 \sum_i \hat{X}_i^2 + \frac{1}{2} \sum_i \hat{P}_i^2$$

Bosons local  $\Rightarrow$  energy independent of momentum (**dispersionless**)  $\omega(q) = \omega_0$ .

Similarly, electron-boson coupling is local  $\Rightarrow$  independent of momentum.

**Dimensionless coupling:**  $\lambda_D = \lambda^2 / (\omega_0^2 W)$  where  $W$  = electronic bandwidth.



Slightly technical: Understanding **Hubbard-Holstein** Connection  
**Quantum Monte Carlo** at finite temperature- **Partition function**:

$$Z = \text{Tr} [ e^{-\beta \hat{H}} ] = \text{Tr} [ e^{-\Delta\tau \hat{H}} e^{-\Delta\tau \hat{H}} \dots e^{-\Delta\tau \hat{H}} ]$$

Path integral: Insert complete sets of boson coordinate states.

$$\frac{1}{2} \omega_0^2 \hat{X}_i^2 \Rightarrow \frac{1}{2} \omega_0^2 X_i^2 \quad \hat{P}_i^2 \Rightarrow \left[ \frac{X_i(\tau + \Delta\tau) - X_i(\tau)}{\Delta\tau} \right]^2$$

**Adiabatic approximation** (ignore boson kinetic energy).

Complete square on every site  $i$  and time slice  $\tau$ :

$$\frac{1}{2} \omega_0^2 X^2 + \lambda X (\hat{n}_\uparrow + \hat{n}_\downarrow) = \frac{1}{2} \omega_0^2 \left( X + \frac{\lambda}{\omega_0^2} (\hat{n}_\uparrow + \hat{n}_\downarrow) \right)^2 - \frac{\lambda^2}{2 \omega_0^2} (\hat{n}_\uparrow + \hat{n}_\downarrow)^2$$

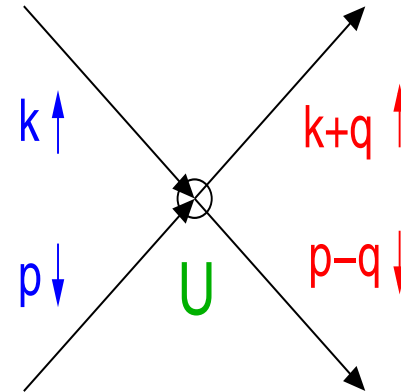
Integrate out bosons: effective on-site interaction *between electrons*.

$$-\frac{\lambda^2}{2 \omega_0^2} (\hat{n}_\uparrow + \hat{n}_\downarrow)^2 = -\frac{\lambda^2}{2 \omega_0^2} (\hat{n}_\uparrow + \hat{n}_\downarrow) - \frac{\lambda^2}{\omega_0^2} \hat{n}_\uparrow \hat{n}_\downarrow$$

**Holstein**: Close connection to **attractive Hubbard** model.  $U_{\text{eff}} = -\lambda^2 / \omega_0^2$ .

Hubbard Model in momentum space:

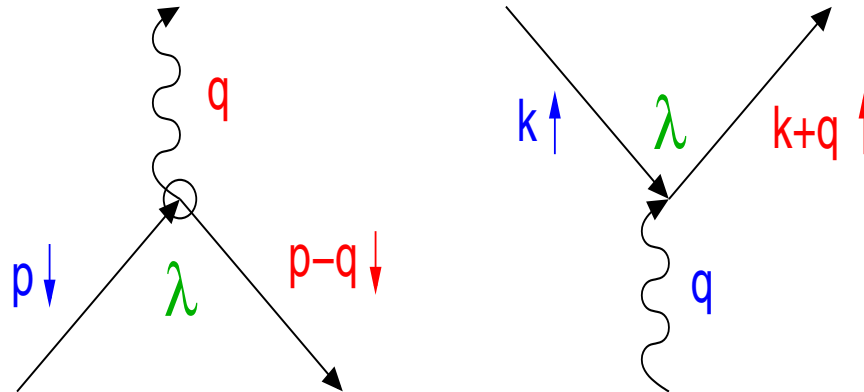
$$\hat{H}_{\text{el-el}} = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \frac{U}{N} \sum_{kpq} \hat{c}_{p-q\uparrow}^\dagger \hat{c}_{k+q\downarrow}^\dagger \hat{c}_{p\uparrow} \hat{c}_{k\downarrow}$$



Holstein Model in momentum space:

$$\frac{\lambda}{N} \sum_{pq} \hat{X}_q \hat{c}_{p-q\sigma}^\dagger \hat{c}_{p\sigma} =$$

$$\frac{\lambda}{N} \sum_{pq} (\hat{a}_q^\dagger + \hat{a}_{-q}) \hat{c}_{p-q\sigma}^\dagger \hat{c}_{p\sigma}$$

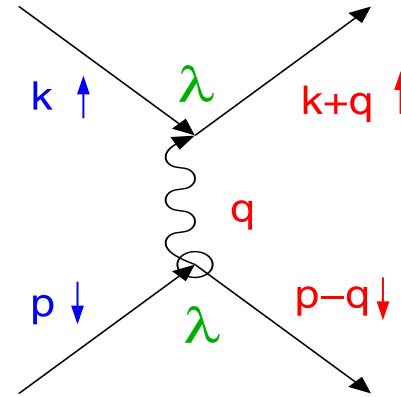


Let's tie the boson lines together...

To second order in  $\lambda$ , interaction is

$$U_{\text{eff}} = \lambda^2 D_0(q, w) = \lambda^2 \frac{1}{\omega^2 - \omega_q^2}$$

$D_0(q, \omega)$  is free boson propagator.



Suppressing  $\omega$  dependence, and, for Holstein, setting  $\omega_q = \omega_0$ :

$$U_{\text{eff}} = \lambda^2 D_0(q, w) = -\frac{\lambda^2}{\omega_0^2}$$

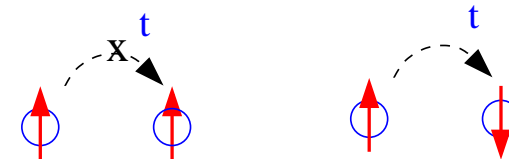
Effective el-el coupling  
(reproducing previous argument).

Repulsive interaction ( $+U$  Hubbard):

Local moments form.

up/down spin alternation favored by  $J$ :

Antiferromagnetism.

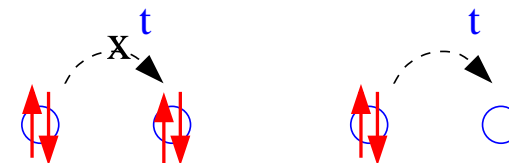


Attractive interaction ( $-U$  Hubbard; Holstein):

Local pairs form.

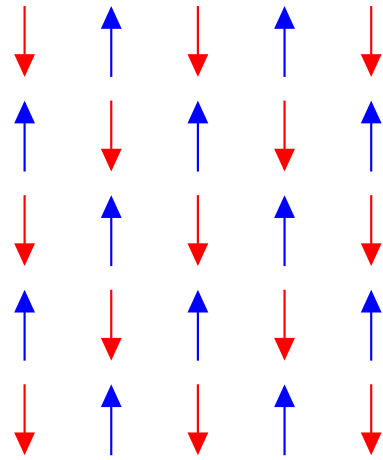
Double occupied/empty alternation favored:

Charge Density Wave.

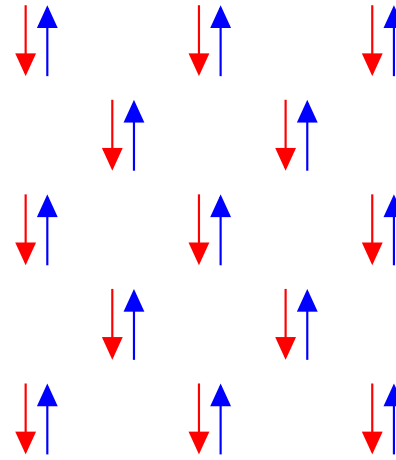




Local order can become **long range** if thermal/quantum fluctuations reduced.



Repulsive (AF)



Attractive (CDW)

### Holstein Model:

- Charge order at half-filling (bipartite lattice).
- Superconducting order when doped.

CDW transition at **finite  $T$**  in 2D (Ising universality class).

Contrast to Hubbard: AF order only at  **$T = 0$**  in 2D (Heisenberg universality).

**Quantitative values for  $T_c$  obtained for square lattice only recently!**

Weber and Hohenadler, Phys. Rev. B 98, 085405 (2018).

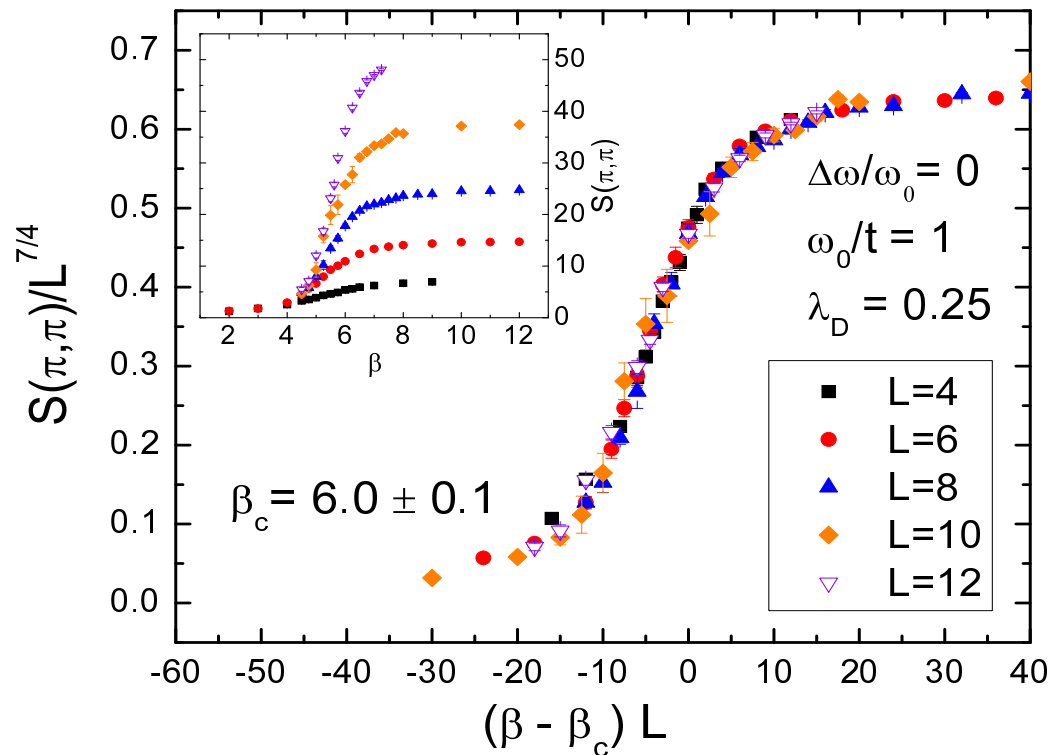
# Square Lattice Holstein model

## Structure factor

$$S_{\text{cdw}}(\pi, \pi) = \frac{1}{N} \sum_{i,j} \langle n_i n_j \rangle (-1)^{i+j} \quad \leftrightarrow \quad S_{\text{af}}(\pi, \pi) = \frac{1}{N} \sum_{i,j} \langle S_i^z S_j^z \rangle (-1)^{i+j}$$

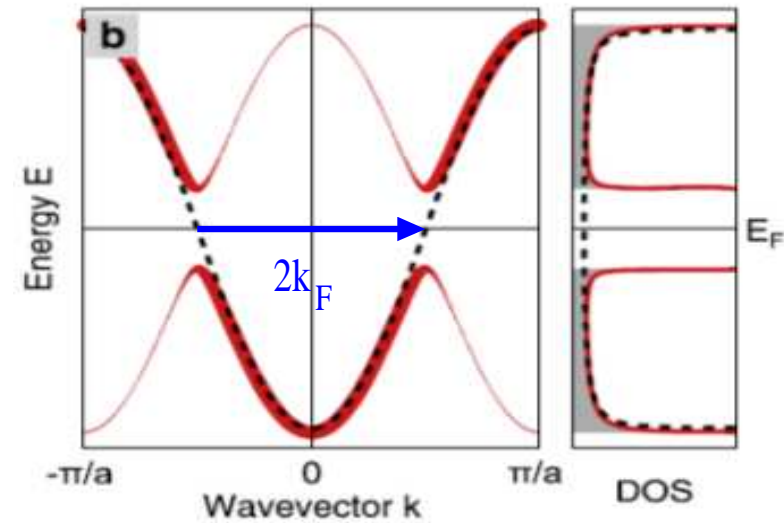
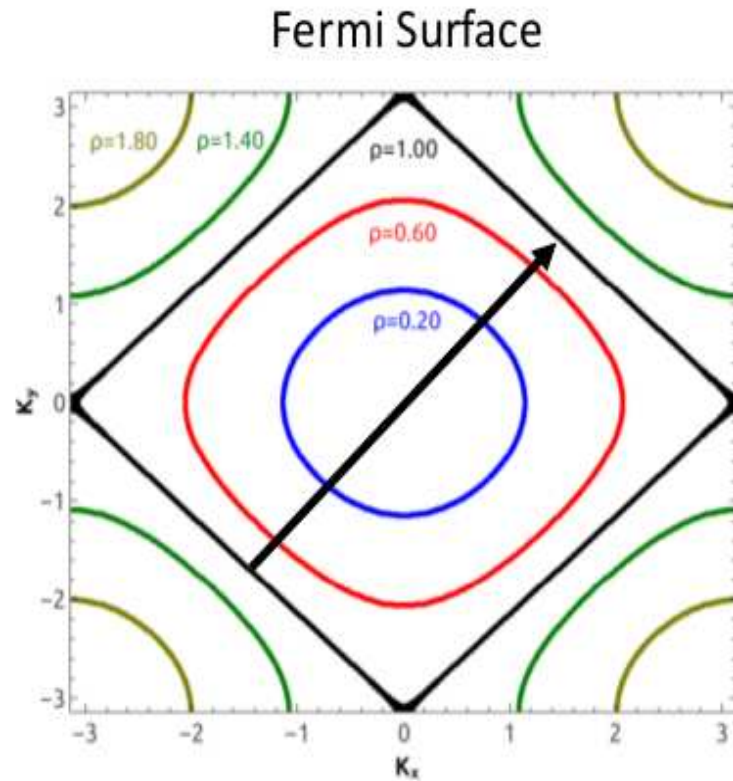
High  $T$ :  $\langle n_i n_j \rangle \sim e^{-|i-j|/\xi} \Rightarrow S(\pi, \pi)$  independent of  $N$ .

Low  $T$ :  $\langle n_i n_j \rangle \sim \text{constant} \Rightarrow S(\pi, \pi) \propto N$ .



Finite size scaling collapse  
determines  $T_c = 1/\beta_c$ .

Order at  $\mathbf{q} = (\pi, \pi)$ : **Fermi-Surface Nesting** (FSN) for half-filled 2D square lattice.



In 1D, always have FSN at  $q = 2k_F$ .

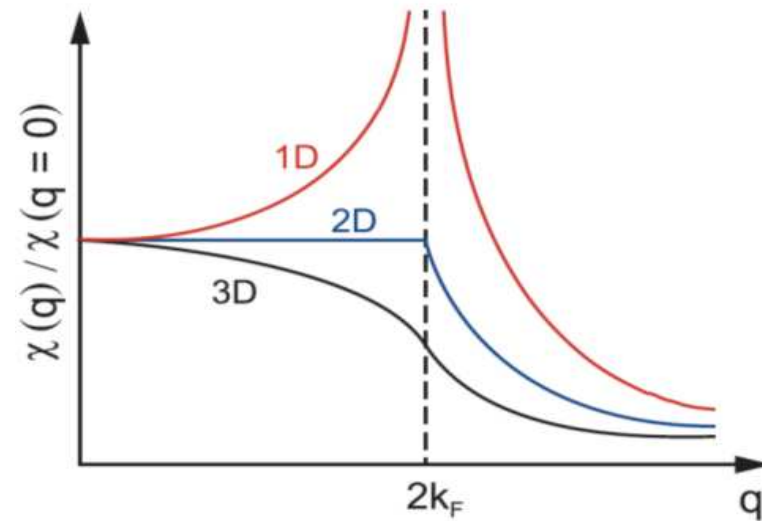
Lattice distortion lowers electronic energy more than bond stretching energy cost.



## 2. Peierls Picture of CDW Transition

**Peierls Instability:** FSN in one dimensional system creates very high susceptibility to lattice distortion at  $2k_F$ .

$$\chi(q) = \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k}+\mathbf{q}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}}$$



Widely used and useful picture! However:

- CDW in NbSe<sub>2</sub>: no sign of FSN.

Attributed instead to momentum dependent electron-boson coupling.

- Charge order (e.g. stripes etc) in cuprates.

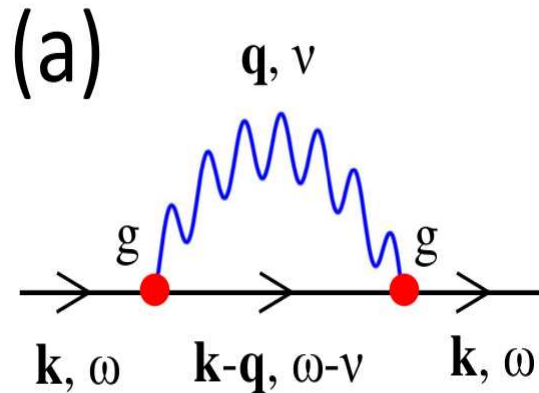
Attributed instead to electron-electron interactions.

### 3. Phonons with Dispersion

We explored momentum dependence of **boson dispersion**.

Easy to implement in Determinant QMC.

A ‘close cousin’ of momentum dependent coupling.



$$\Sigma^g(k, \omega) \sim \int dq d\nu |g(q)|^2 \frac{1}{\omega - \nu - \epsilon(k-q)} \frac{2\omega_0}{\nu^2 - \omega_0^2}$$

$$\Sigma^\omega(k, \omega) \sim \int dq d\nu |g_0|^2 \frac{1}{\omega - \nu - \epsilon(k-q)} \frac{2\omega(q)}{\nu^2 - \omega(q)^2}$$

$\Sigma^g$ : momentum dependent **electron-boson coupling**.

$\Sigma^\omega$ : momentum dependent **boson dispersion**.

$\nu \rightarrow 0$  (boson carries no energy):  $\Sigma^g = \Sigma^\omega$  if  $|g(q)|^2/\omega_0 = |g|^2/\omega(q)$ .

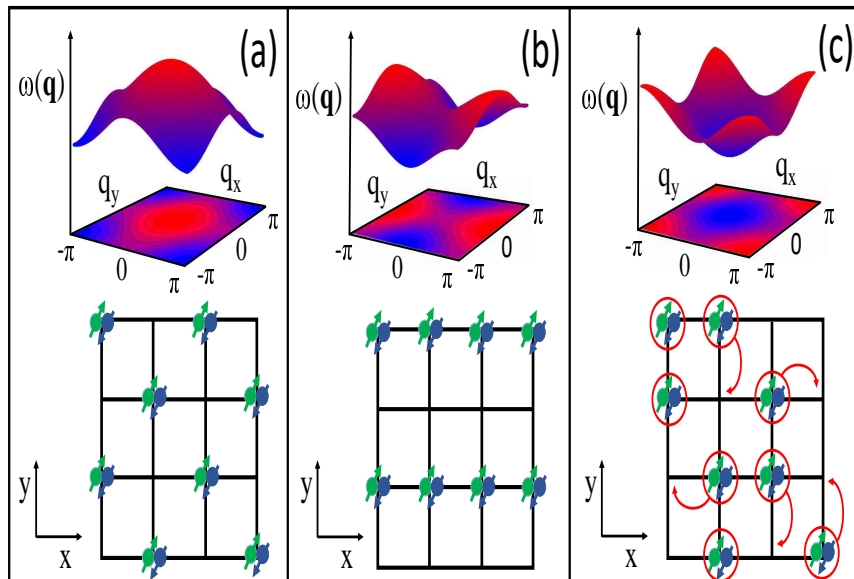
(For nonzero  $\nu$  the two self-energies are not equal.)

## Conventional Holstein Model:

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + \lambda \sum_i \hat{X}_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) + \frac{1}{2} \omega_0^2 \sum_i \hat{X}_i^2 + \frac{1}{2} \sum_i \hat{P}_i^2$$

An **intersite** boson coupling introduces  $\mathbf{q}$  dependence in boson energy.

$$\hat{H}_2 = \frac{1}{2} \omega_2^2 \sum_{\langle i,j \rangle} (\hat{X}_i \pm \hat{X}_j)^2$$



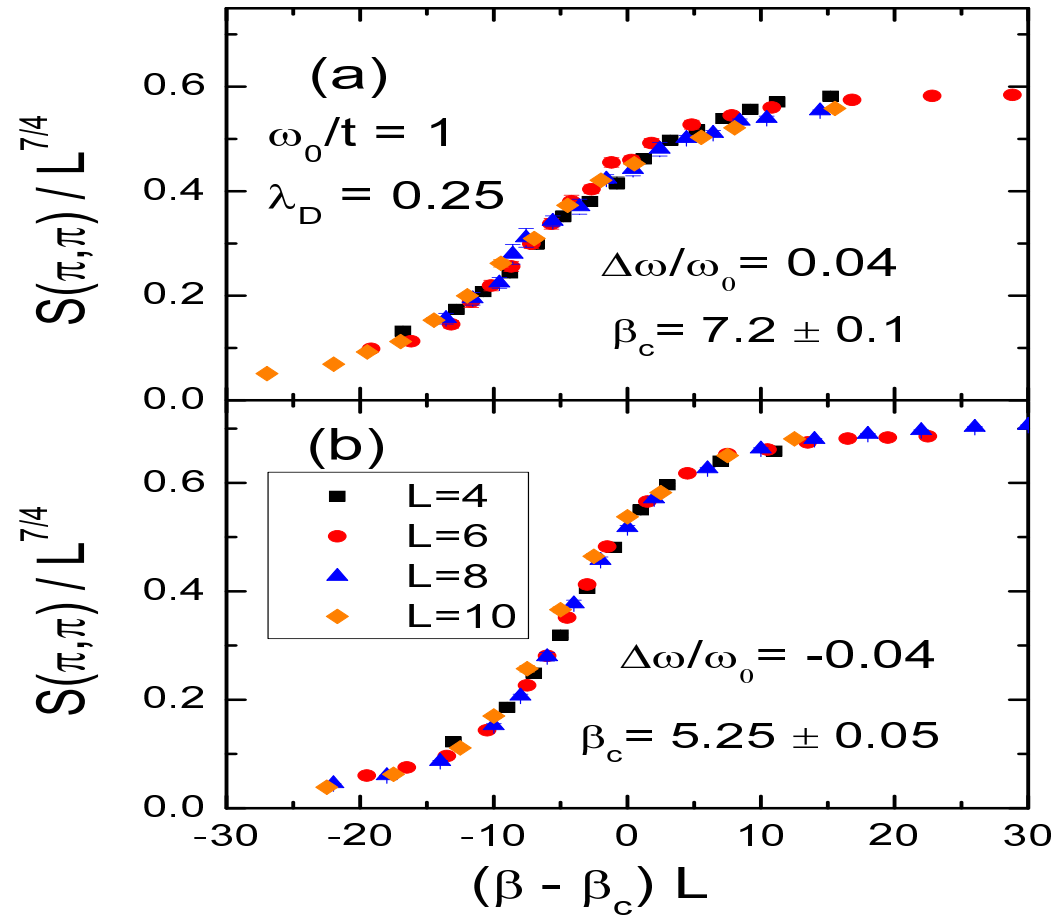
- a.  $\hat{X}_i + \hat{X}_j$ : lowers  $\omega(\mathbf{q} = (\pi, \pi))$   
(Checkerboard CDW).
- b. Mixed signs in  $x, y$  directions:  
lowers  $\omega(\mathbf{q} = (0, \pi))$   
(Stripe CDW).
- c.  $\hat{X}_i - \hat{X}_j$ : raises  $\omega(\mathbf{q} = (\pi, \pi))$   
(no CDW, superconductivity?)

Phonon bandwidth:  $\Delta\omega \equiv \omega_{\max} - \omega_{\min}$ .



No dispersion ( $H_2 = 0$ ) we found  $\beta_c = 6.0 \pm 0.1$ .

Initial effect of  $H_2$ , **checkerboard CDW** still dominant, but shifted  $T_c$ .

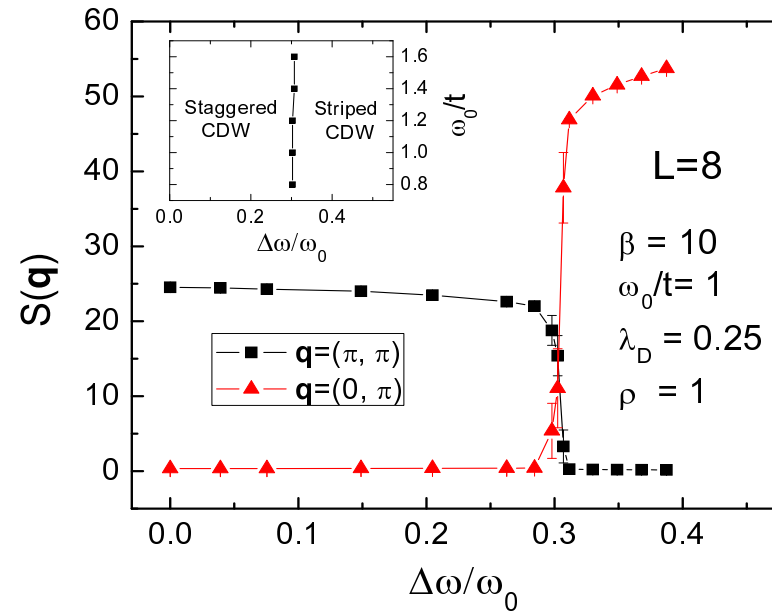
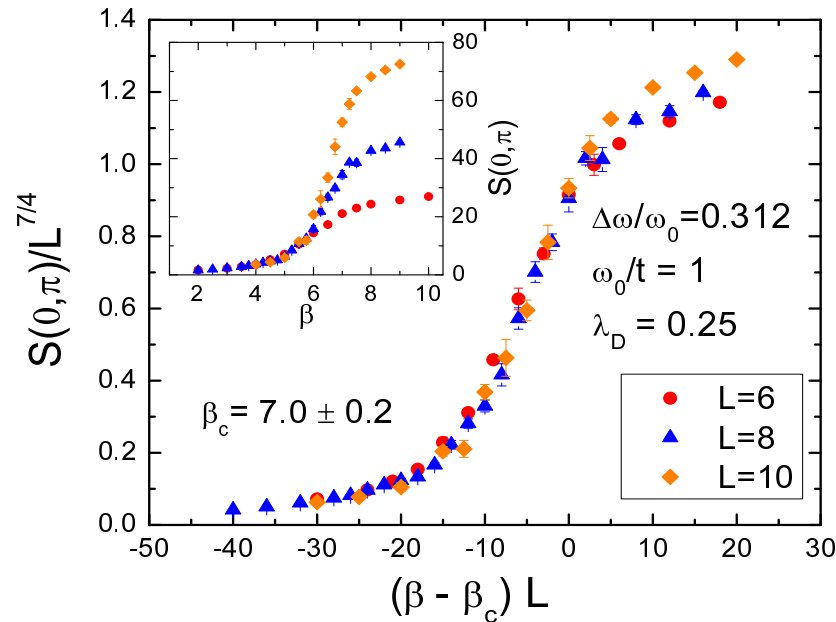


**Top:**  $\hat{X}_i - \hat{X}_j$ : lowers  $\omega(\mathbf{q} = (0, 0))$   
 $\beta_c$  for checkerboard CDW **increases**.

**Bottom:**  $\hat{X}_i + \hat{X}_j$ : lowers  $\omega(\mathbf{q} = (\pi, \pi))$   
 $\beta_c$  for checkerboard CDW **decreases**.

For sufficiently large ‘mixed’  $H_2$ , which favors **stripe** CDW,

Checkerboard to stripe transition:



Key observation here:

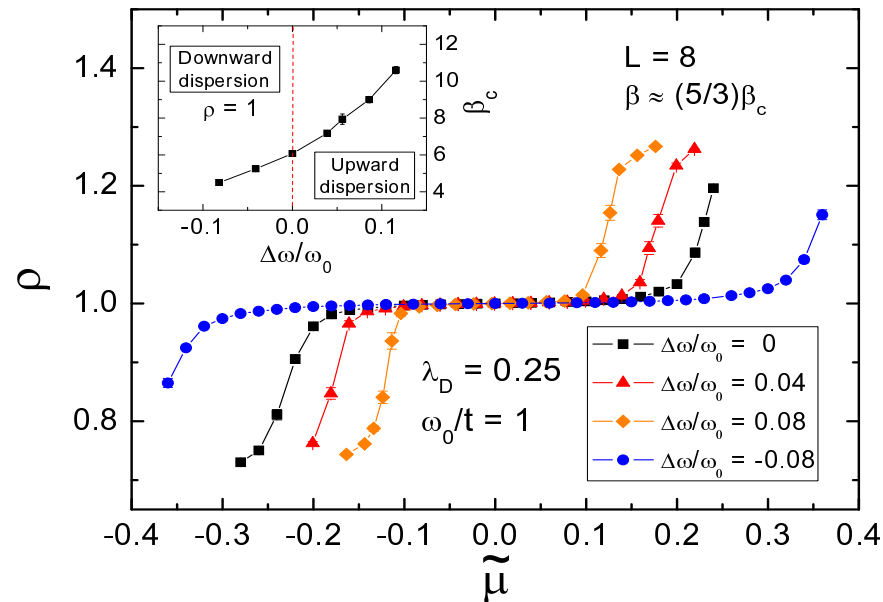
No alteration to electron band structure. Half-filled square lattice.

Fermi surface nesting remains at  $(\pi, \pi)$ .

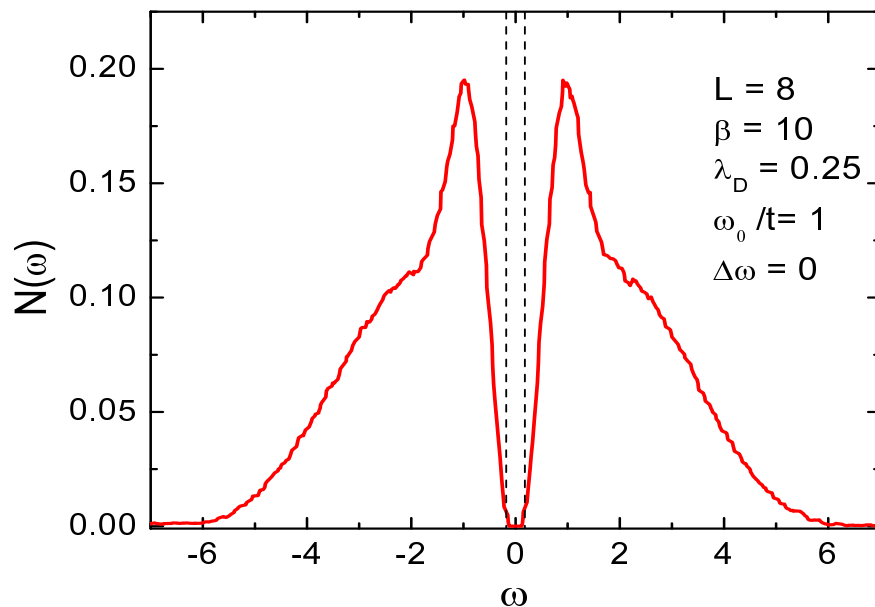
But CDW ordering vector can be elsewhere.

CDW transition outside of canonical Peierls picture.

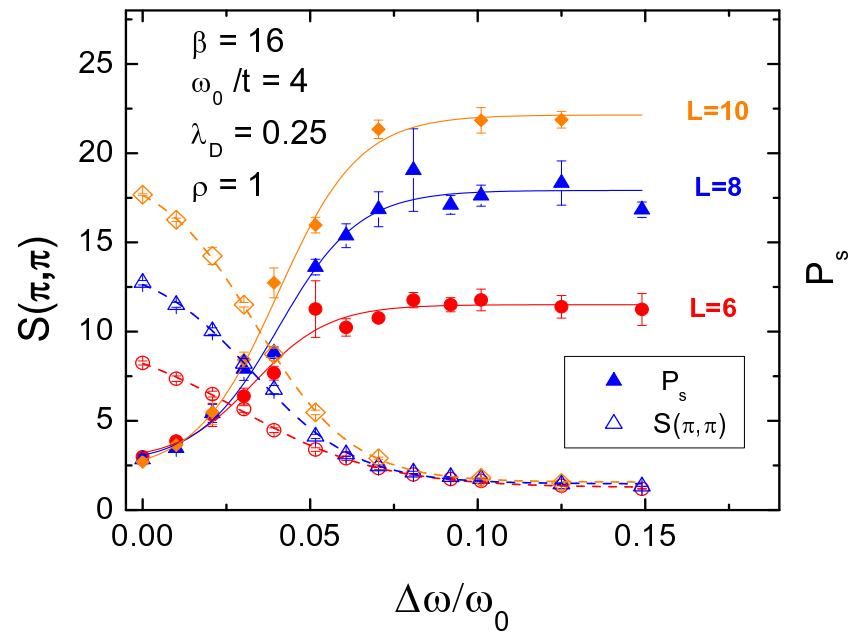
Can also examine these phenomena via CDW gap.



Plateau in  $\rho(\mu)$  shrinks/expands with boson dispersion.

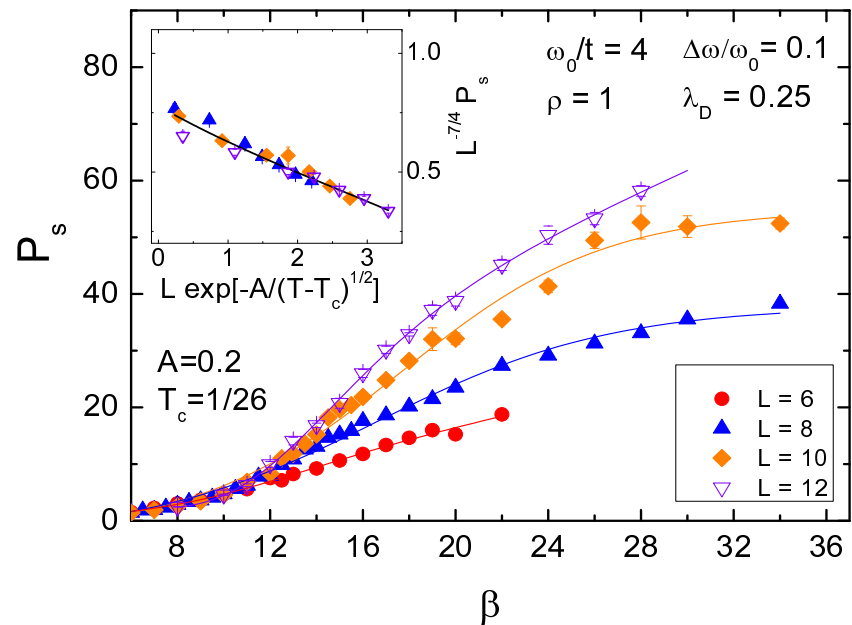


Density of states: gap at Fermi Energy.  
Like AF-Slater gap in  $+U$  Hubbard.  
Mark would have done a much better job at  $N(\omega)$ !



Suppress checkerboard CDW without replacing it with stripes.

Superconducting phase at commensurate filling.



2D superconducting transition (Kosterlitz-Thouless universality).

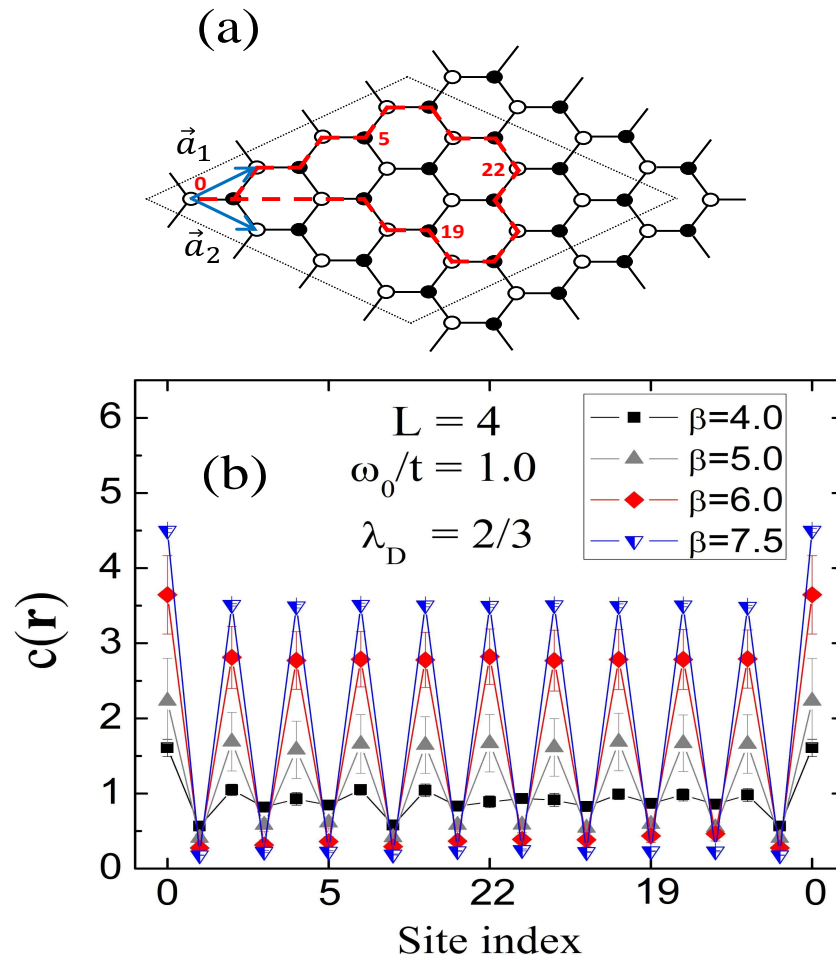
## 4. Holstein Model on Honeycomb Lattice

Dirac spectrum for fermions.

Quantum critical point for Hubbard Model:

Minimal  $U_c/t \gtrsim 3.87$  to induce antiferromagnetic order.

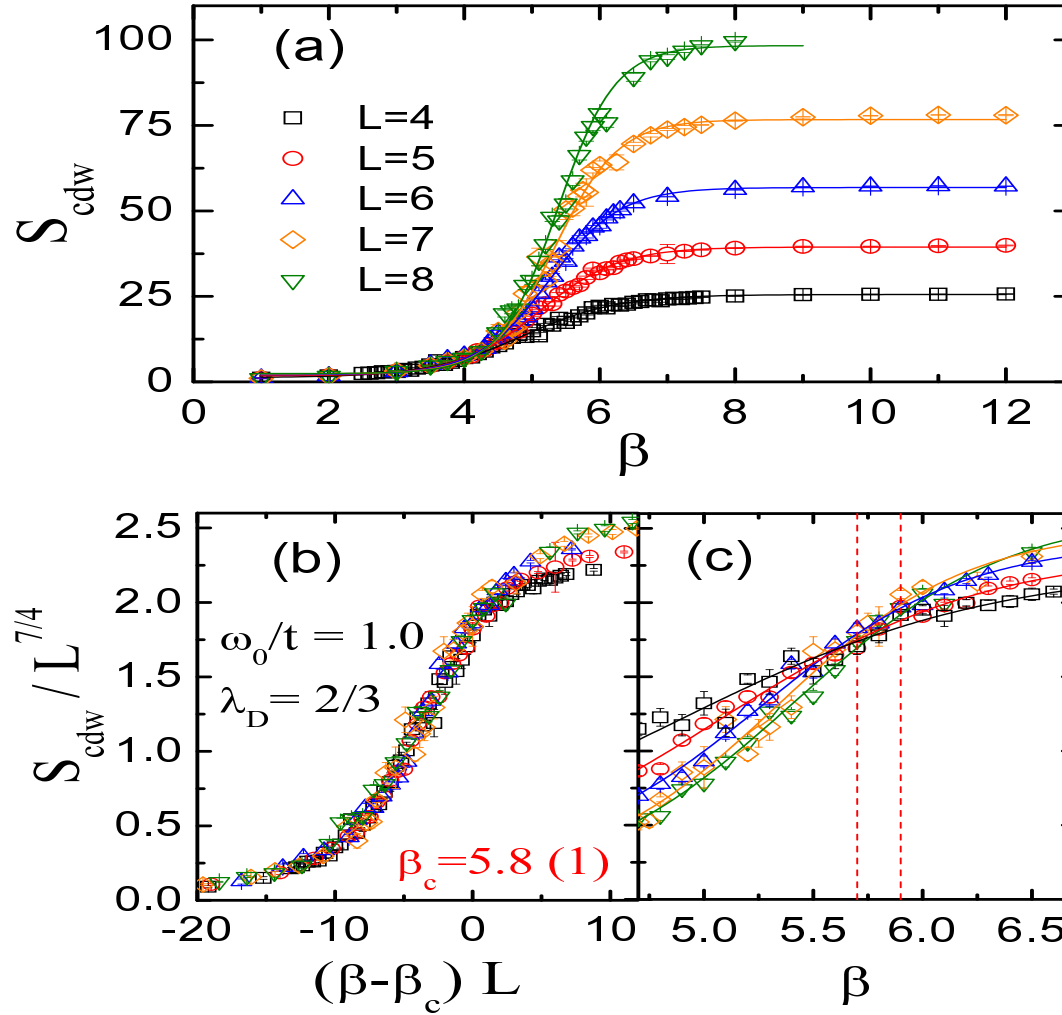
Effect of electron-boson interactions on Dirac fermions and charge order?



Long range real space  
charge correlations develop  
as  $\beta$  increases.

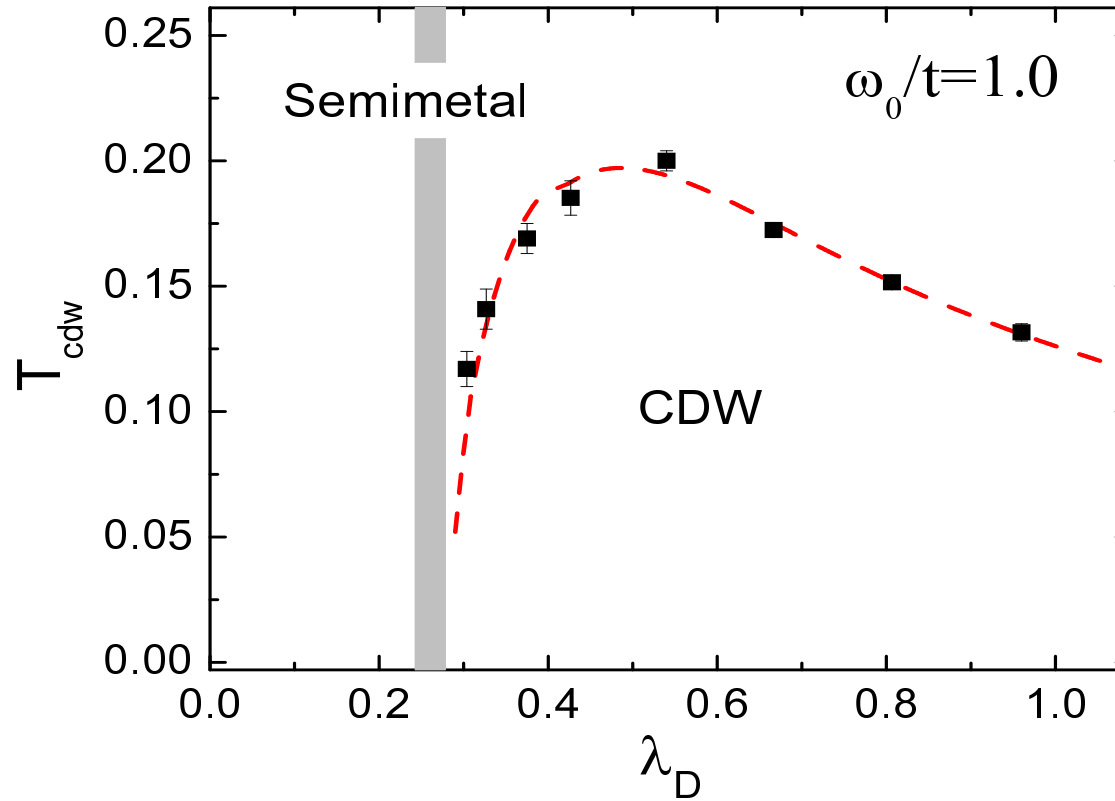
CDW structure  $o(N)$  when charge correlations long range ( $\beta > \beta_c$ ).

Data collapse/crossing yield critical temperature.





## Phase Diagram of Holstein Model on Honeycomb Lattice



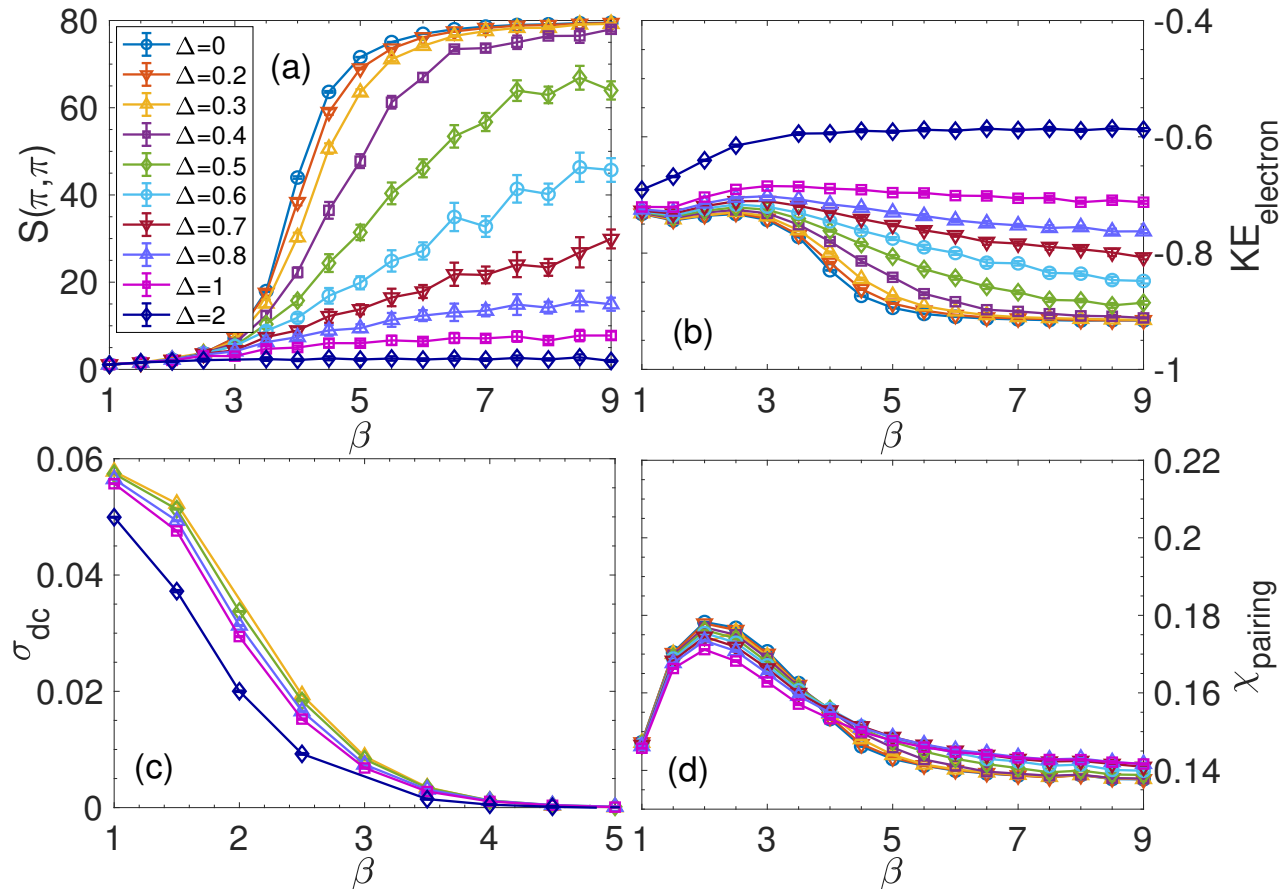
“Charge Order in the Holstein Model on a Honeycomb Lattice,” Y.-X. Zhang, W.-T. Chiu, N.C. Costa, G.G. Batrouni, and RTS, Phys. Rev. Lett. 122, 077602 (2019).

“Charge-Density-Wave Transitions of Dirac Fermions Coupled to Phonons,” C. Chen, X.Y. Xu, Z.Y. Meng, and M. Hohenadler, Phys. Rev. Lett. 122, 077601 (2019).

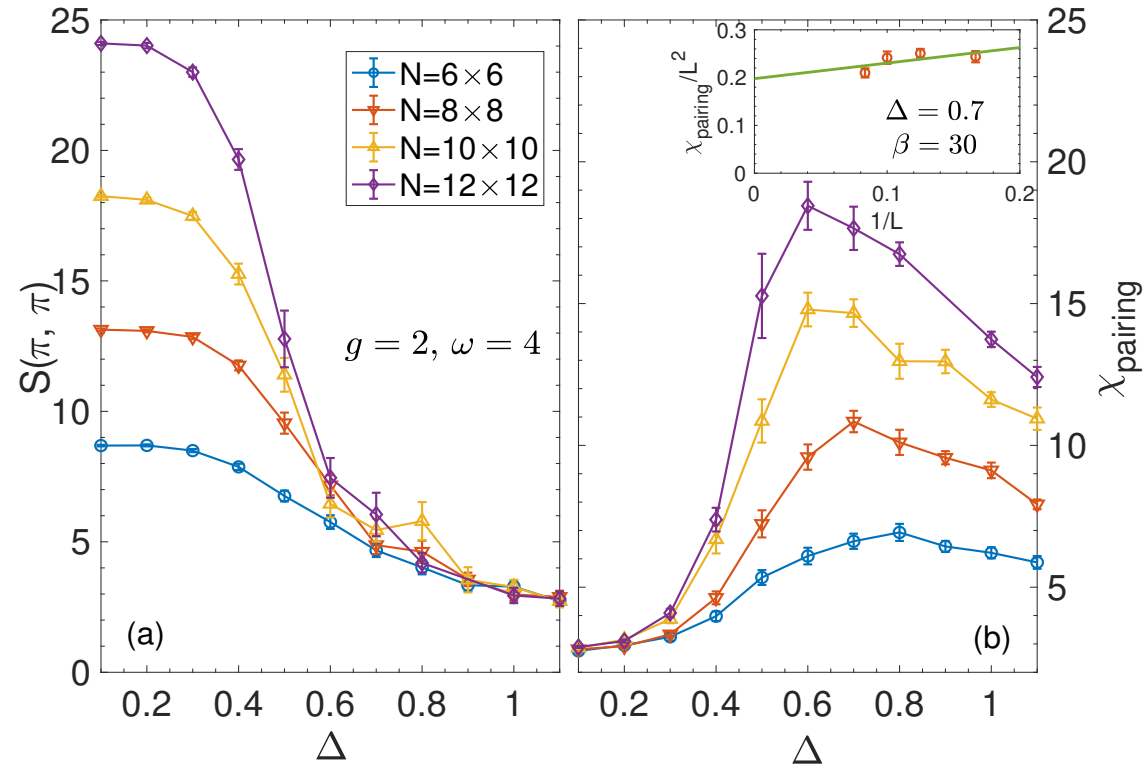
## 5. Phonons and Disorder

What happens when site disorder is added to Holstein Hamiltonian

$$\mathcal{V} = \sum \epsilon_i (n_{i\uparrow} + n_{i\downarrow}) \quad -\Delta < \epsilon_i < +\Delta$$

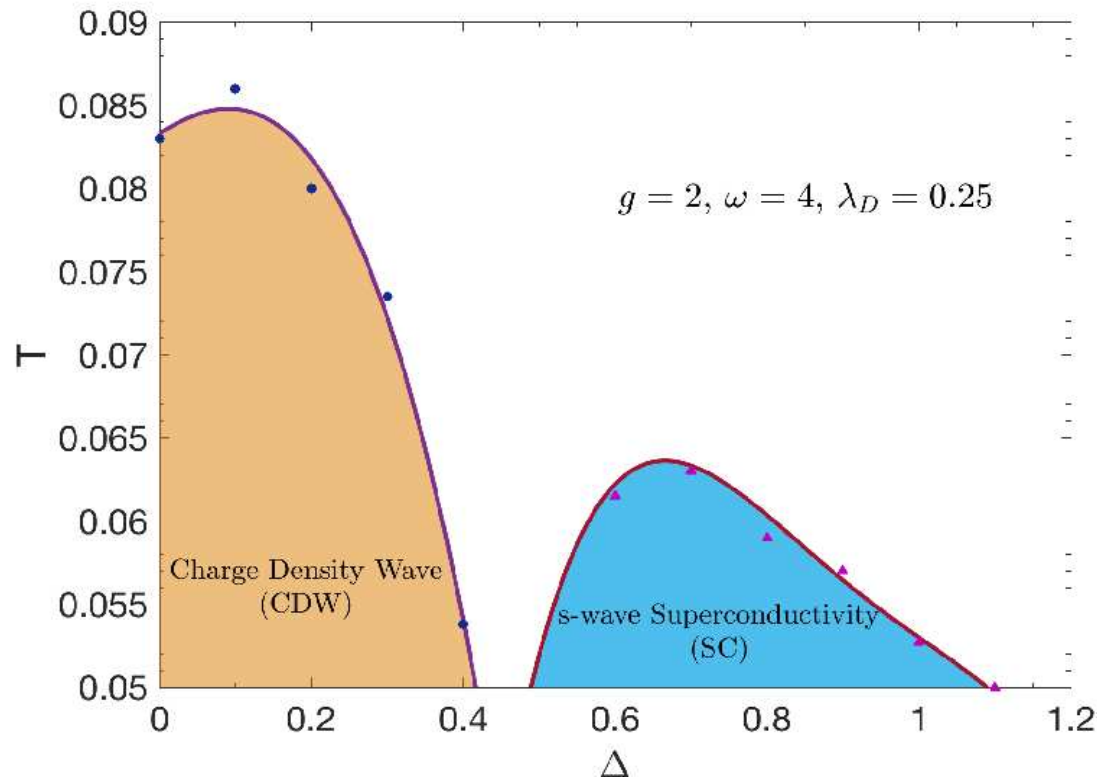


- Charge structure function is suppressed.
- Electron mobility ( $\text{KE}$  and  $\sigma_{\text{dc}}$ ) is reduced.
- Small signal of enhanced superconductivity at intermediate  $\Delta$ .



- Signal of enhanced superconductivity more dramatic at higher  $\omega$ .
- $\chi_{\text{pairing}}$  grows with lattice size.
- Nonzero extrapolation in thermodynamic limit at intermediate  $\Delta$ .

## Phase diagram



“Insensitivity of d-wave pairing to disorder in the high-temperature cuprate superconductors,” A.F. Kemper, D. Doluweera, T.A. Maier, [Mark Jarrell](#), P.J. Hirschfeld, and H.P. Cheng, Physical Review B79, 104502 (2009).

“Study of off-diagonal disorder using the typical medium dynamical cluster approximation,” H. Terletska, C.E. Ekuma, C. Moore, K.M. Tam, J. Moreno, and [Mark Jarrell](#), Physical Review B90, 094208 (2014).

## X. Mark and Janee's Car



A story from **Janee**:

Last year Mark was getting a new set of tires for their car. He made sure he bought a set of snow tires, anticipating Janee's return to Pennsylvania in a few years.

Even facing the challenge of his mortality, he was looking out for the people he loved.