Charge and Pairing order in the Holstein Hamiltonian

- 1. Holstein Hamiltonian
- 2. Non-Interacting and Strong Coupling Limits
- 3. CDW Order on Square, Honeycomb, and Cubic Lattices
- 4. Superconductivity?
- 5. Phonons with Dispersion
- 6. The Effect of Disorder
- 7. Conclusions

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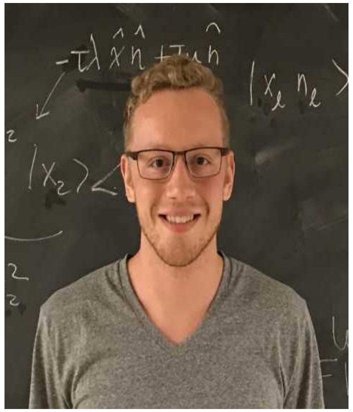

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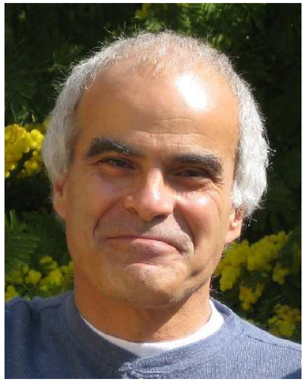

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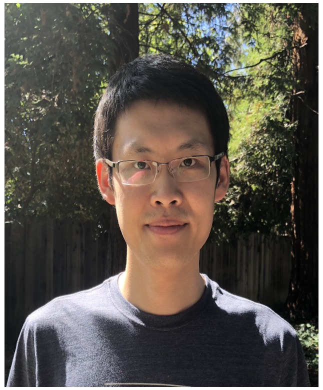

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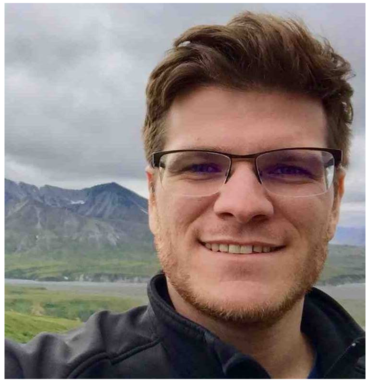

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C. B. Mendl, E. A. Nowadnick, E. W. Huang, S. Johnston, B. Moritz, and T. P. Devereaux
Phys. Rev. B 96, 205141 (2017)

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Zhaoyu Han, Steven A. Kivelson, and Hong Yao
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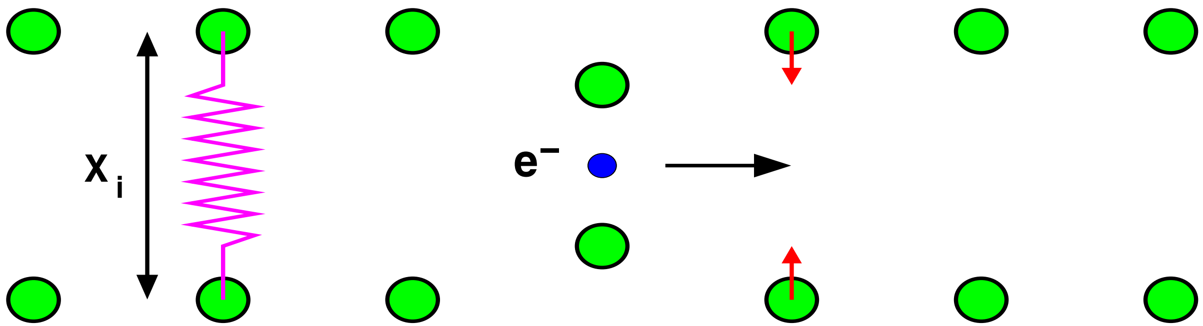
B. Nosarzewski, E. W. Huang, Philip M. Dee, I. Esterlis, B. Moritz, S. A. Kivelson, S. Johnston, T. P. Devereaux,
arXiv:2103.09242

- “Pair-Density-Wave in the Strong Coupling Limit of the Holstein-Hubbard model”
Kevin S. Huang, Zhaoyu Han, Steven A. Kivelson, Hong Yao
arXiv:2103.04984

1. Holstein Hamiltonian



"Studies of polaron motion: Part I. The Molecular-Crystal Model"
T. Holstein, Annals of Physics 8, 325 (1959).

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T. Holstein, Annals of Physics 8, 343 (1959).

Roughly Contemporaneous: "Electron Correlations in Narrow Energy Bands,"
J. Hubbard, Proc. Royal Soc. London 276, 238 (1963).

Linear chain of N identical diatomic molecules.

Inter-nuclear separation on each molecule adjusts if electon is present.

Goal: Describe e^- motion in a solid along with accompanying lattice distortion.

"It is felt that the model, although physically different from the cases encountered in practice, corresponds conceptually to them in sufficient degree, so as to merit investigation."

Holstein: wave function a_i probability amplitude for (*single*) electron on site i.
(Holstein did not use second quantization.)

Modern (many body) notation. Noninteracting electron kinetic energy:

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

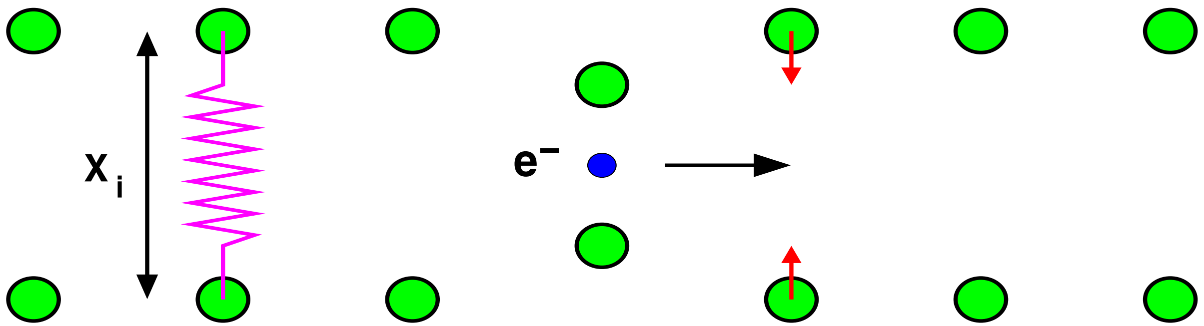
Spin $\uparrow, \downarrow$ electrons interact with boson displacement on site i

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

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.

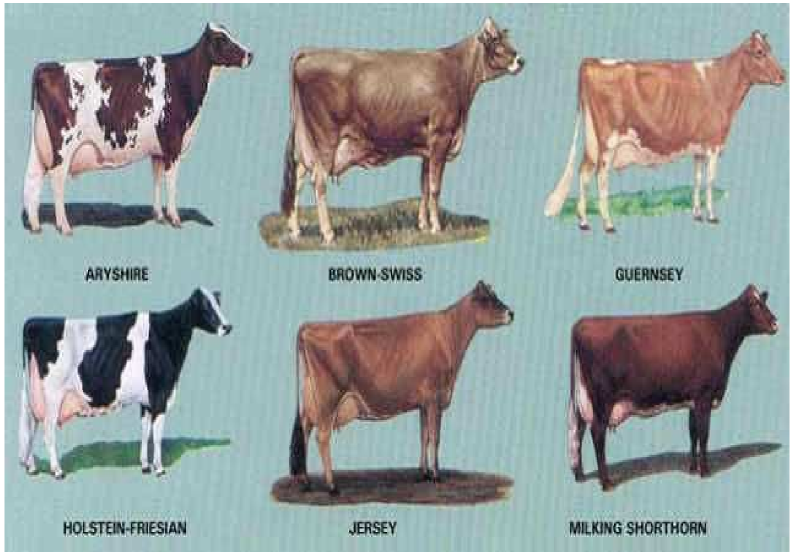


Theorists have a reputation for oversimplification:

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

Today: more real 'cows'?

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



* Higher dimension
* Many electrons: CDW and SC
* Phonon dispersion
* Disorder

If I fail:

circa 1970 Stanford Seminar Notice:

Speaker and Title to be renounced.

Initial insight from $t = 0$ (Independent sites)

Complete the square

$$\frac{1}{2}\omega_0^2 X^2 + \lambda X(n_\uparrow + n_\downarrow) = \frac{1}{2}\omega_0^2\Big(X + \frac{\lambda}{\omega^2}(n_\uparrow + n_\downarrow)\Big)^2 - \frac{\lambda^2}{2\omega_0^2}(n_\uparrow + n_\downarrow)^2$$

Integrate out the phonon coordinate X.

Effective *attraction*

$$-\frac{\lambda^2}{\omega_0^2}\, n_\uparrow n_\downarrow = U_{\rm eff}\, n_\uparrow n_\downarrow \qquad\qquad U_{\rm eff} = -\frac{\lambda^2}{\omega_0^2}$$

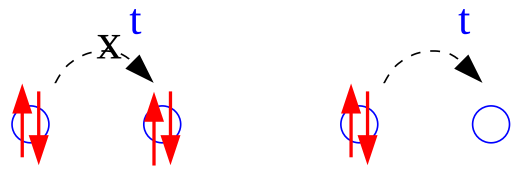
Imagine you are at half-filling. Then turn on t perturbatively.

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

Local pairs form.

Double occupied/empty alternation favored:

Charge Density Wave.

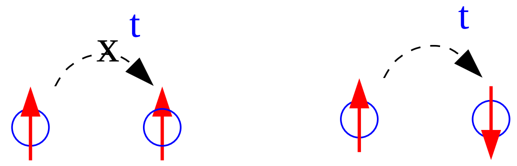


Repulsive interaction ($+U$ Hubbard):

Local moments form.

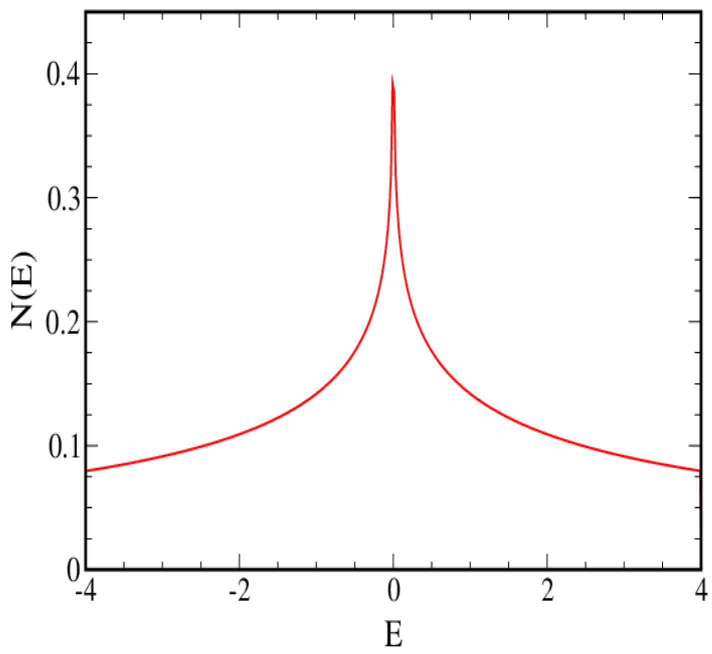
up/down spin alternation favored by J:

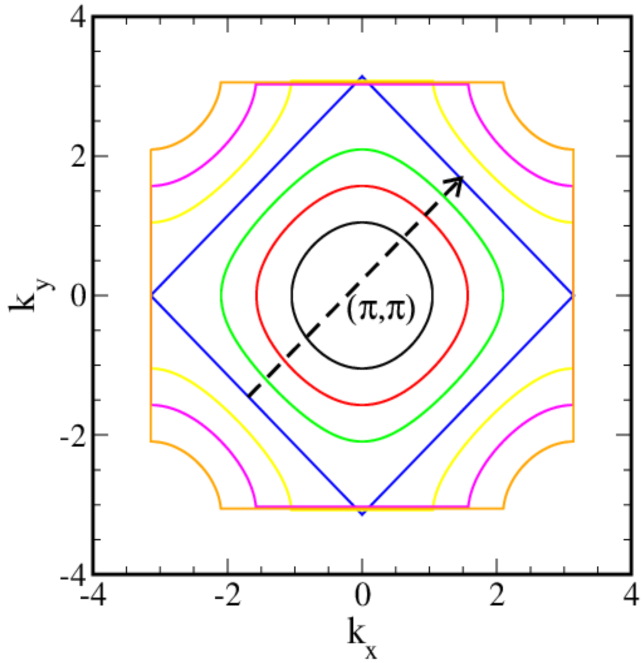
Antiferromagnetism.



The effect of ‘band structure’ (lattice geometry)

Noninteracting $\lambda = 0$ fermions on a lattice (same as Hubbard $U = 0$...)





Square lattice has several interesting features:

- ‘van Hove singularity’ in density of states $N(E = 0)$ at half-filling.
- Perfect ‘nesting’ of Fermi surface, also at half-filling.

Both lead to enhanced ordering tendency when λ (or U) nonzero.

Stoner criterion: $UN(0) = 1$ (Hubbard model language)

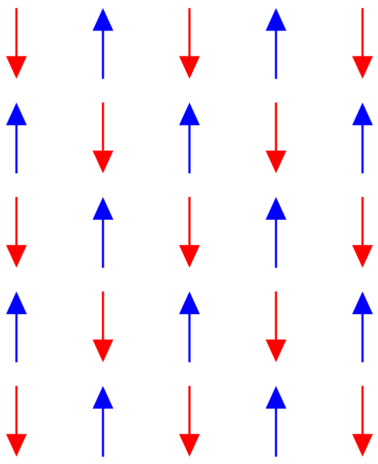
Stoner criterion: $UN(0) = 1$ (Hubbard model language)

On a square lattice $N(0)$ diverges $\Longrightarrow$ long range order at low T for *any* λ or U.

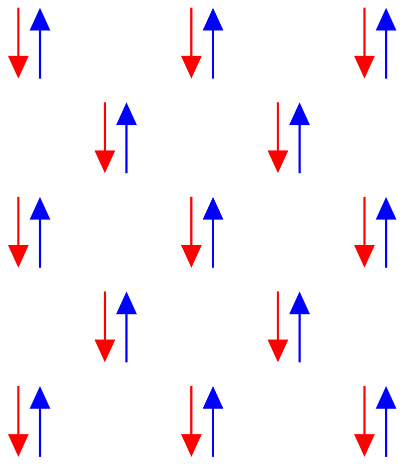
A graduate student enjoys the Stoner Enhancement.

(Courtesy of Dan Arovas.)

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



Repulsive (AF)



Attractive (CDW)

Holstein Model:

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

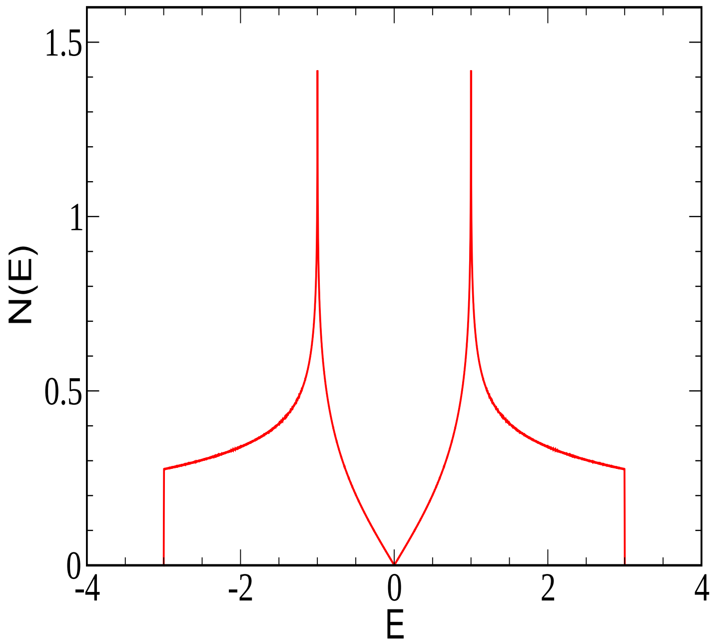
CDW transition at finite T in 2D (Ising universality class).

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).

In contrast, for honeycomb lattice:



Determine λ_c=?? for charge ordering in the Holstein model on a honeycomb lattice.

The Hubbard model $U_c = 3.87t$ for AF order was determined $\sim$ 5 years ago.

Methodology:

- Determinant Quantum Monte Carlo simulations
- Langevin Algorithm (similar to approaches used in lattice gauge theory).

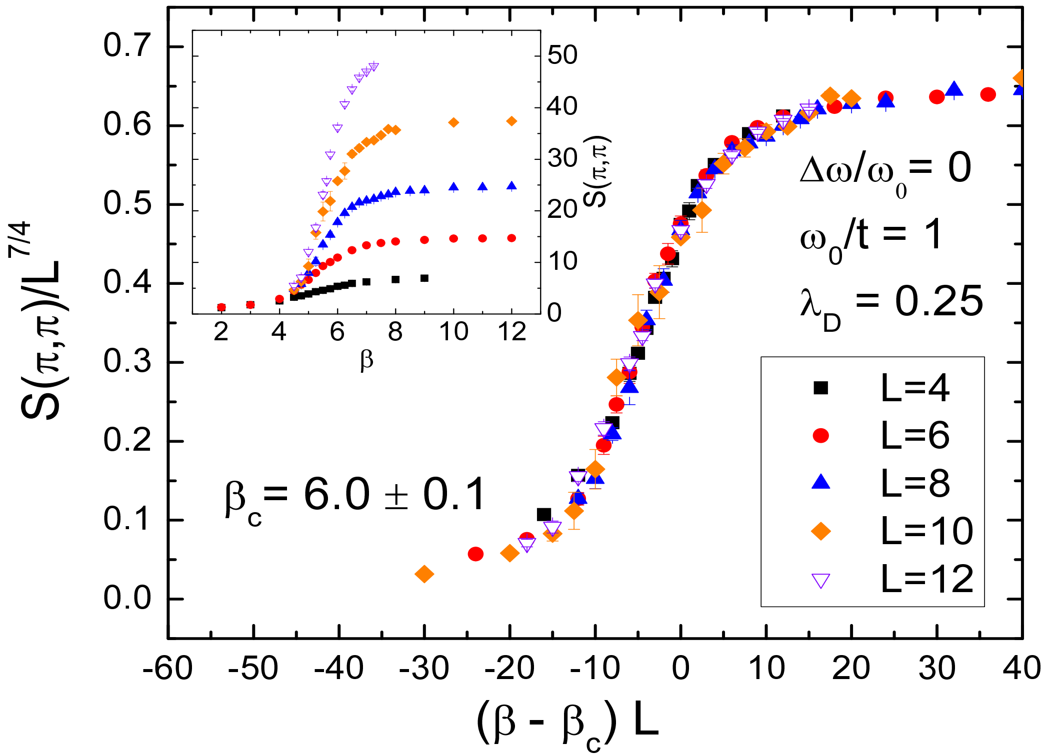
3. CDW Order on Square, Honeycomb, and Cubic Lattices

Structure factor

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

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

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



Square Lattice

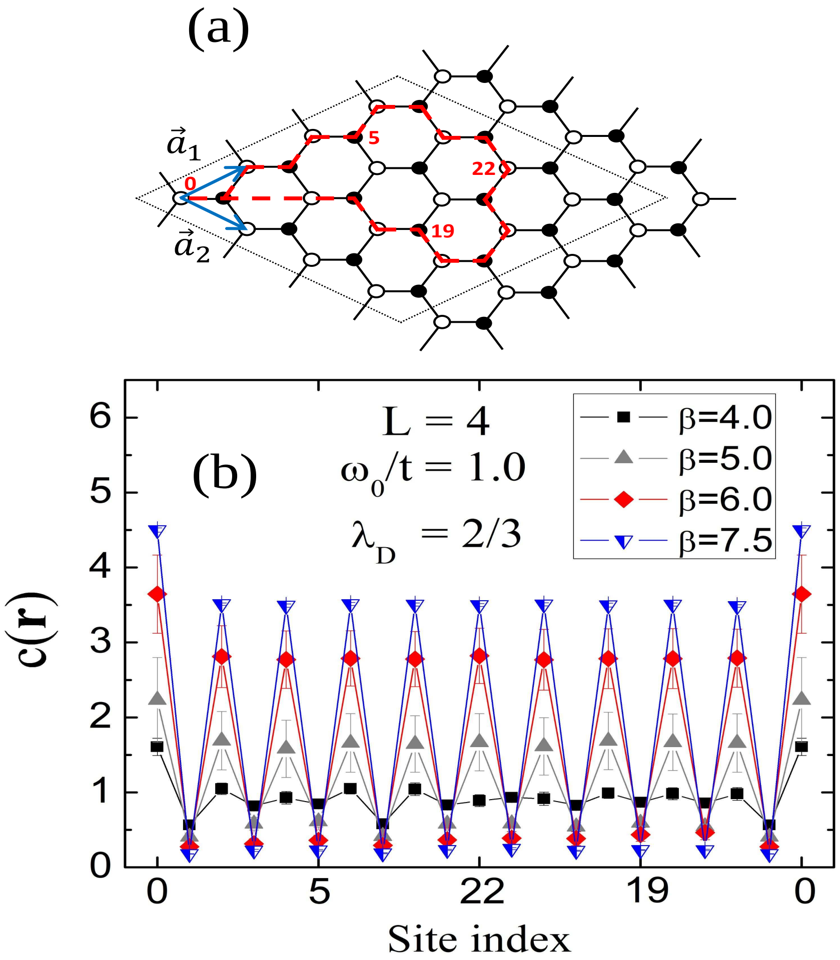
Finite size scaling collapse determines $T_c = 1/\beta_c$.

Honeycomb Lattice:

Dirac spectrum for fermions.

Quantum critical point for Hubbard Model:
Minimal $U_c/t \gtrsim 3.87$ to induce antiferromagnetic order.

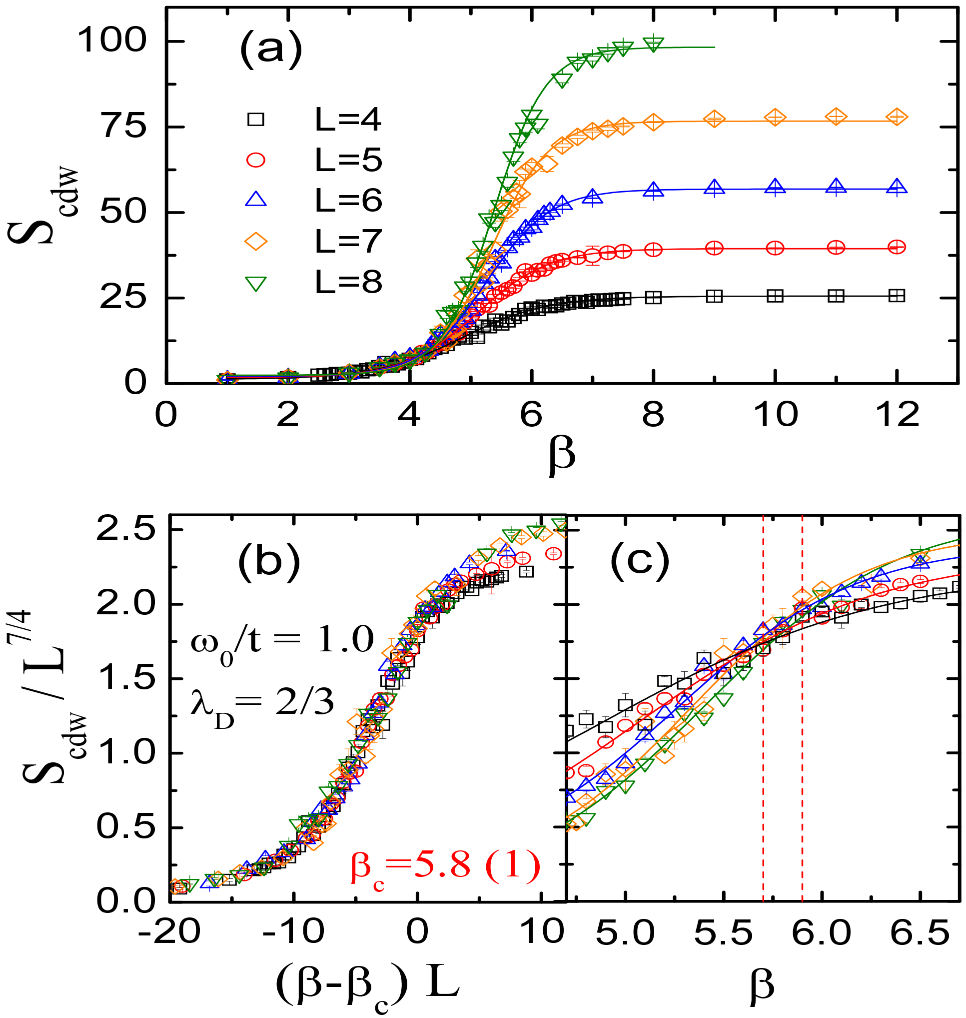
Effect of electron-boson interactions on Dirac fermions and charge order?



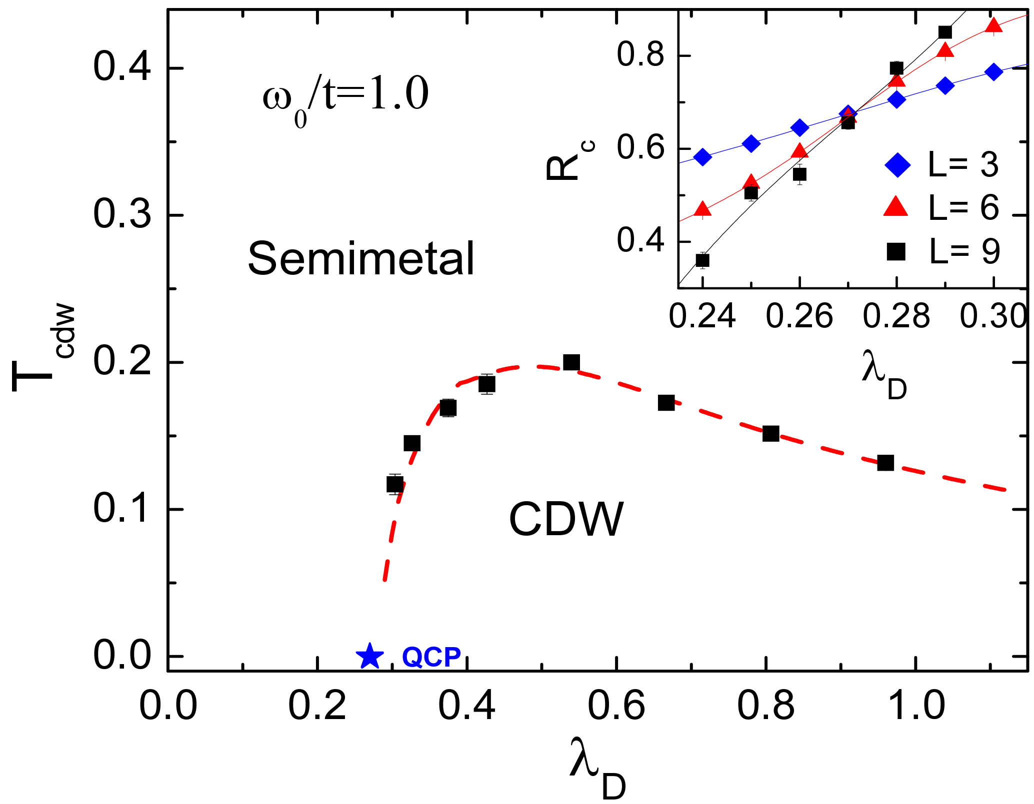
Long range real space charge correlations develop as β increases.

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



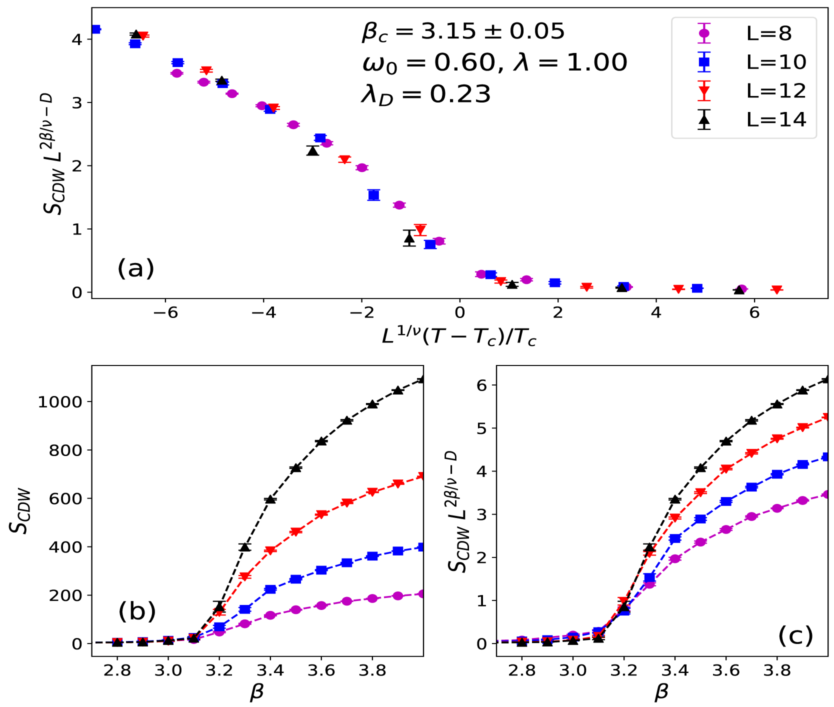
Quantum critical point from $T = 0$
Invariant correlation length crossing

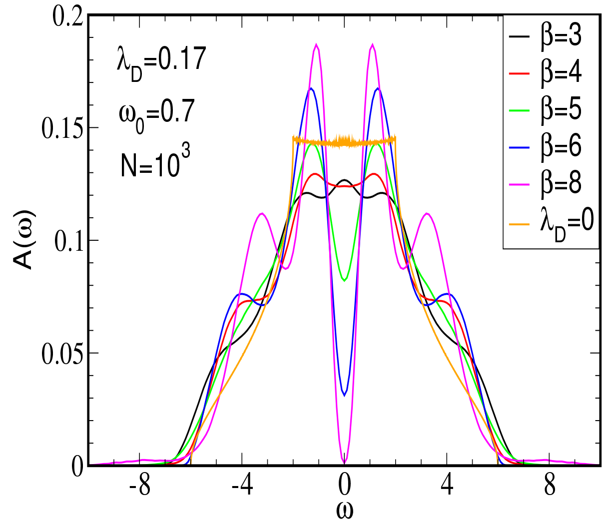
$$R_c \equiv 1 - \frac{S(\mathbf{Q} + \delta\mathbf{q})}{S(\mathbf{Q})}$$

"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).

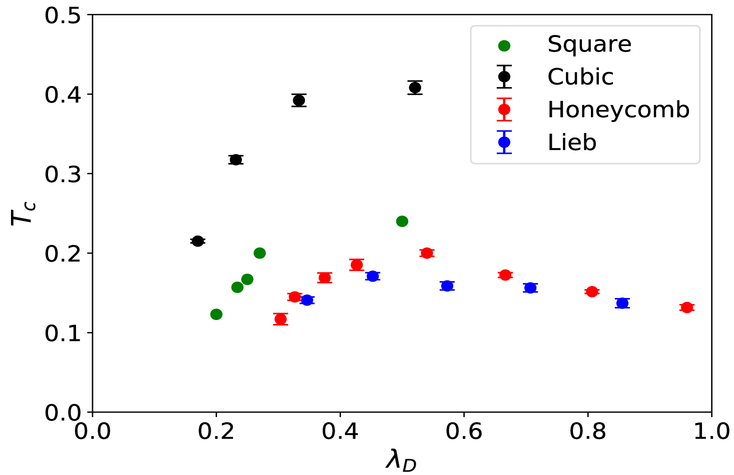
"Charge-Density-Wave Transitions of Dirac Fermions Coupled to Phonons," C. Chen, X.Y. Xu, Z.Y. Meng, and M. Hohenadler, Phys. Rev. Lett. 122, 077601 (2019).

Cubic Holstein





Above Left: Structure factor scaling and Right: Opening of the CDW gap.

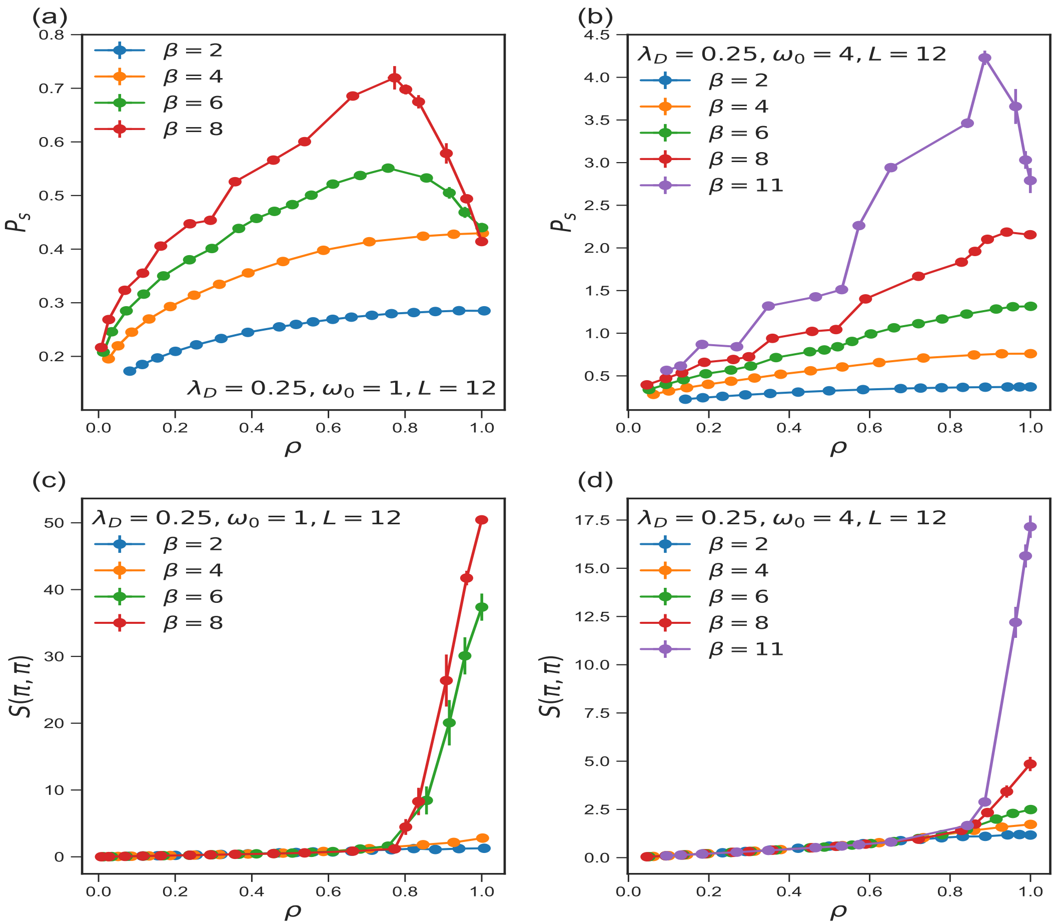


Comparison of Charge Density Wave T_c

Square, cubic, honeycomb, Lieb

4. Superconductivity?

Pairing structure factor $$P_s = \frac{1}{N}\sum_{i,j}\langle \Delta_i \Delta_j^\dagger \rangle$$



CDW structure factor $S(\pi, \pi)$ suppressed rapidly with doping away from half-filling.

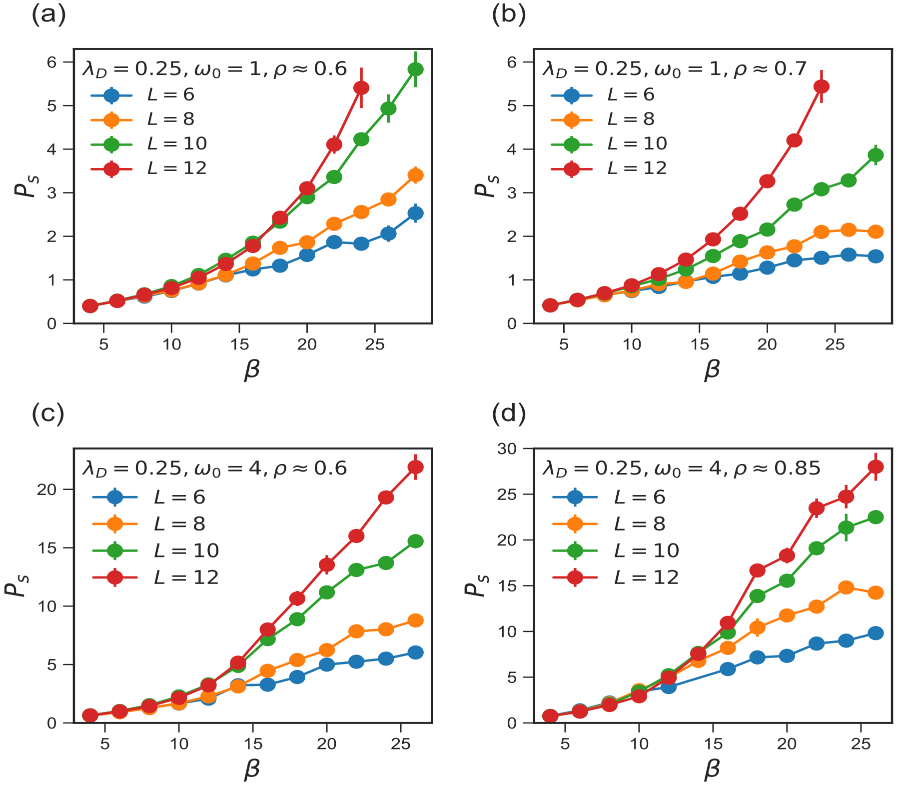
$\omega_0/t = 1$: P_s remains small.

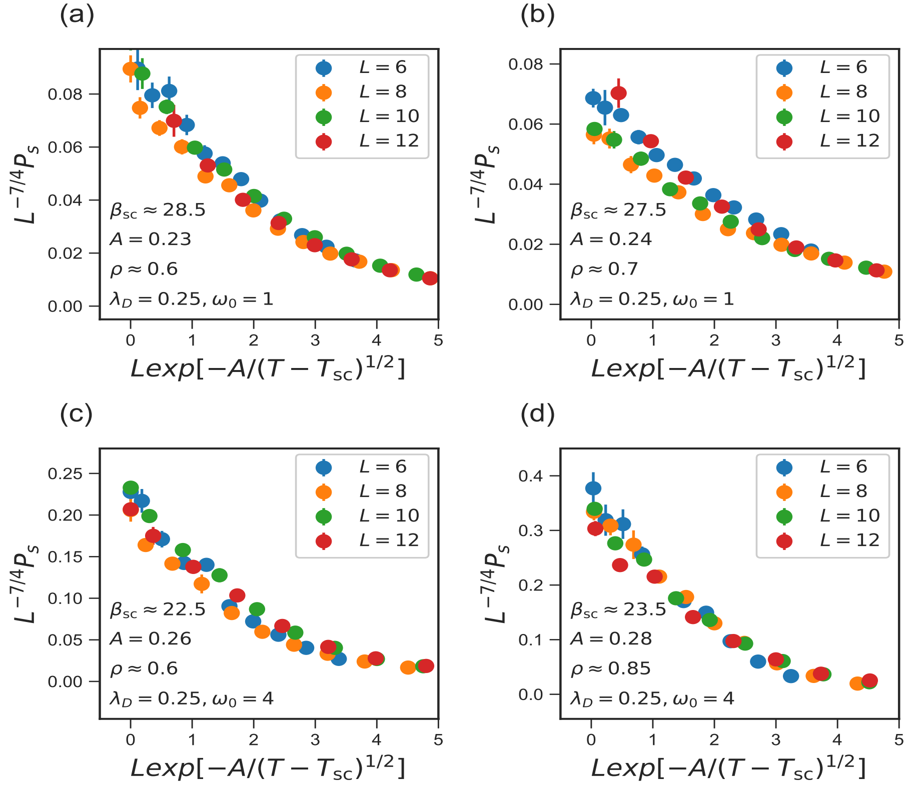
$\omega_0/t = 4$: $P_s \sim \times 10$ larger.

(Quasi-)long range pairing?

(KT univerality class)

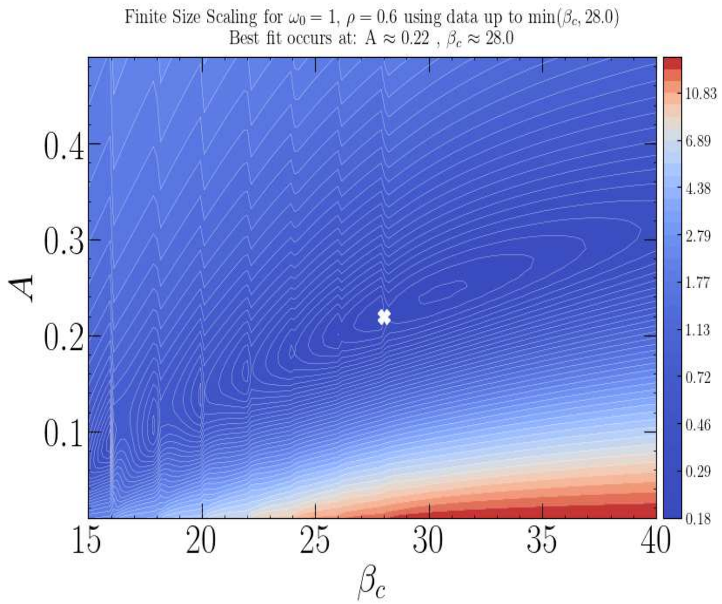
Finite size scaling





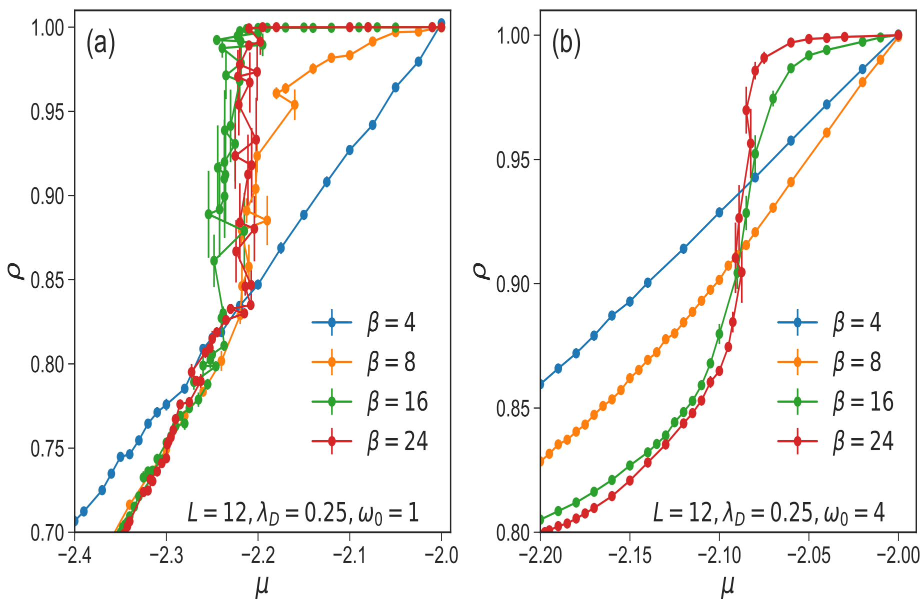
<u>Left:</u> Raw Data

<u>Right:</u> Scaling collapse (not super great...)



Contour plot of best fit to A and β_c.

$\omega_0/ = t$: $T_c = \beta_c^{-1} \sim t/28 = W/224$:



An unexpected feature.

First order phase transition?

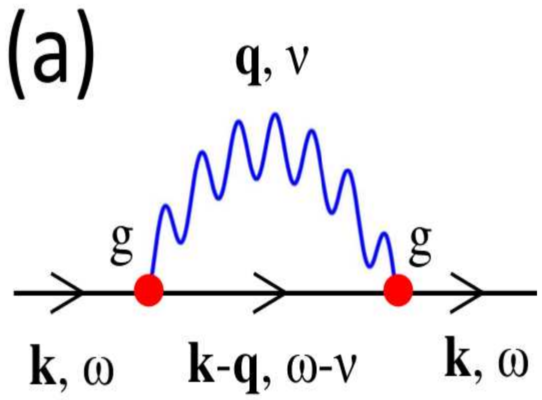
Density ρ takes a discontinuous jump with chemical potential μ.

5. Phonons with Dispersion

We explored momentum dependence of boson dispersion.

Easy to implement in Determinant QMC.

A 'close cousin' of momentum dependent coupling $g = \lambda/\sqrt{2\omega_0}$.



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

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

Σ^g: momentum dependent electron-boson coupling.

Σ^ω: momentum dependent boson dispersion.

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

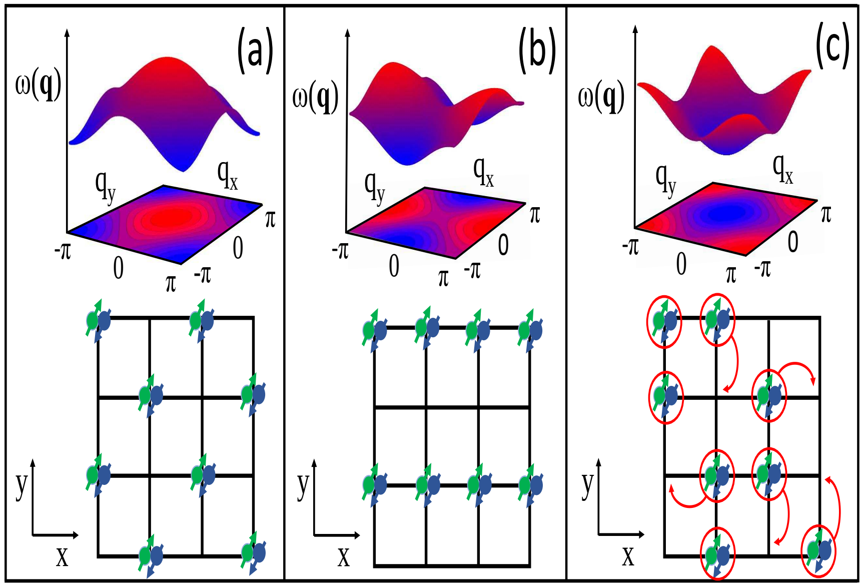
(For nonzero ν the two self-energies are not equal.)

Conventional Holstein Model:

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

An intersite boson coupling introduces **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).

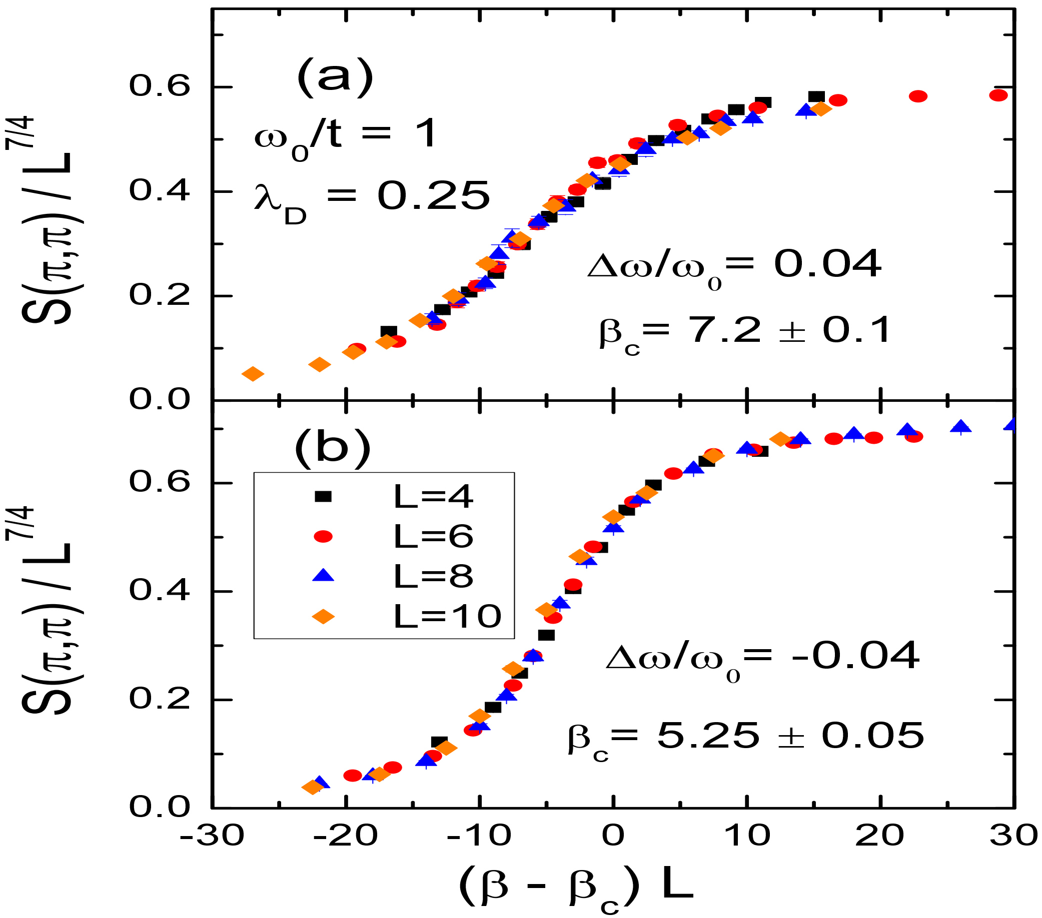
b. Mixed signs in x, y directions: lowers $\omega\big(\mathbf{q} = (0, \pi)\big)$ (Stripe CDW).

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 $\omega\big(\mathbf{q} = (0,0)\,\big)$

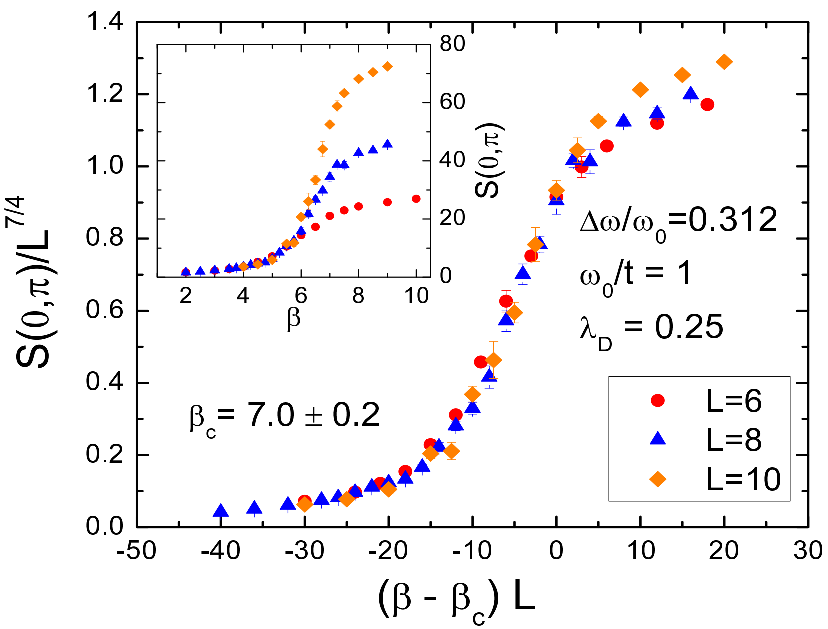
β_c for checkerboard CDW increases.

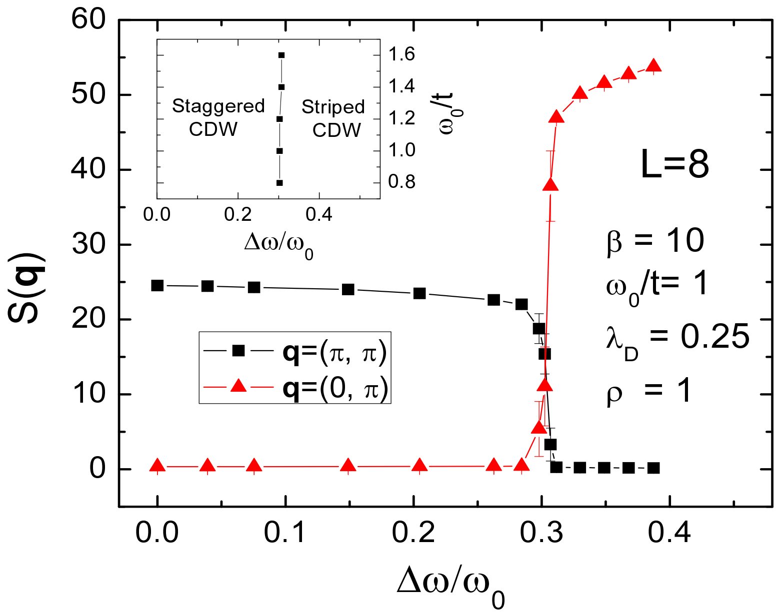
Bottom: $\hat{X}_i + \hat{X}_j$: lowers $\omega\big(\mathbf{q} = (\pi,\pi)\,\big)$

β_c for checkerboard CDW decreases.

For sufficiently large 'mixed' H_2, which favors stripe CDW,

Checkerboard to stripe transition:





Key observation here:

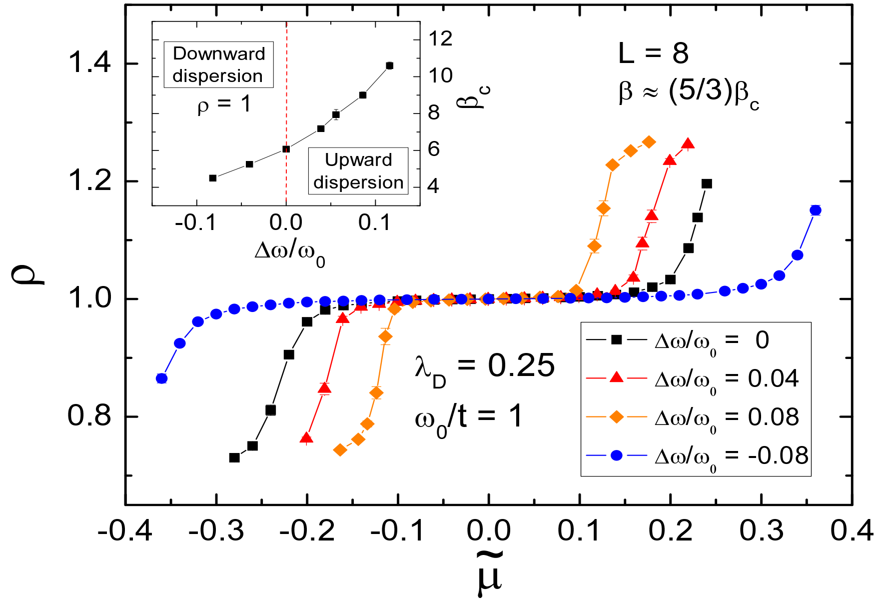
No alteration to electron band structure. Half-filled square lattice.

Fermi surface nesting remains at (π, π).

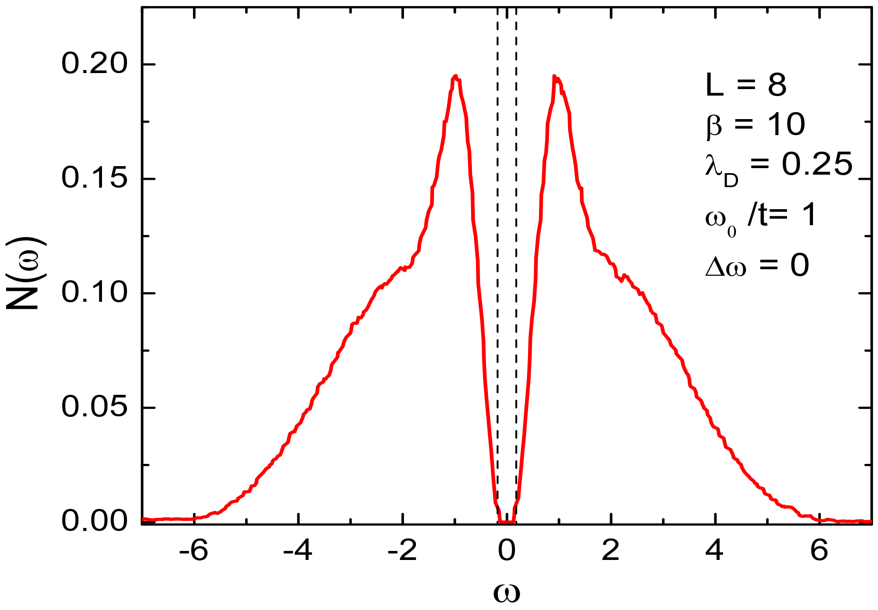
But CDW ordering vector can be elsewhere.

CDW transition outside of canonical Peierls picture.

Can also examine these phenomena via CDW gap.

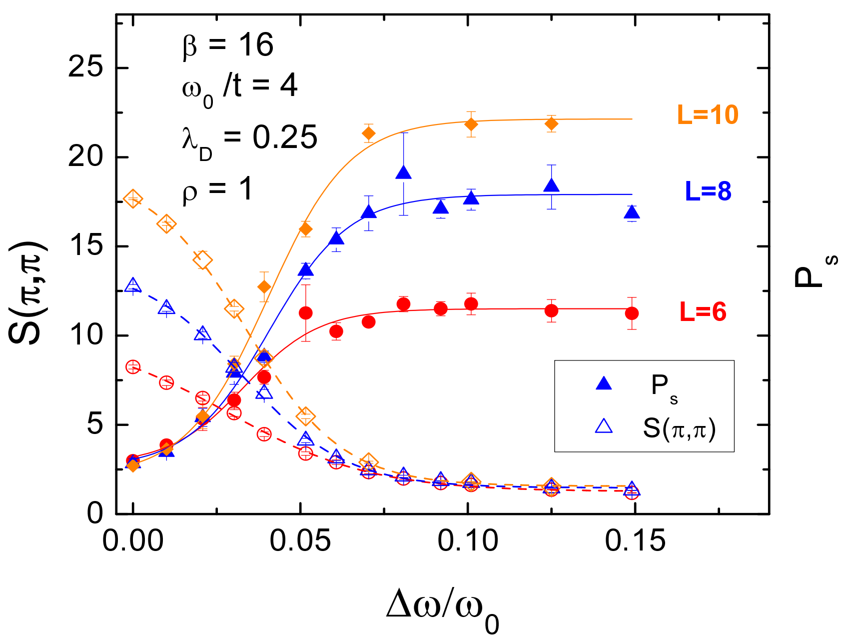


Plateau in $\rho(\mu)$ shrinks/expands with boson dispersion.



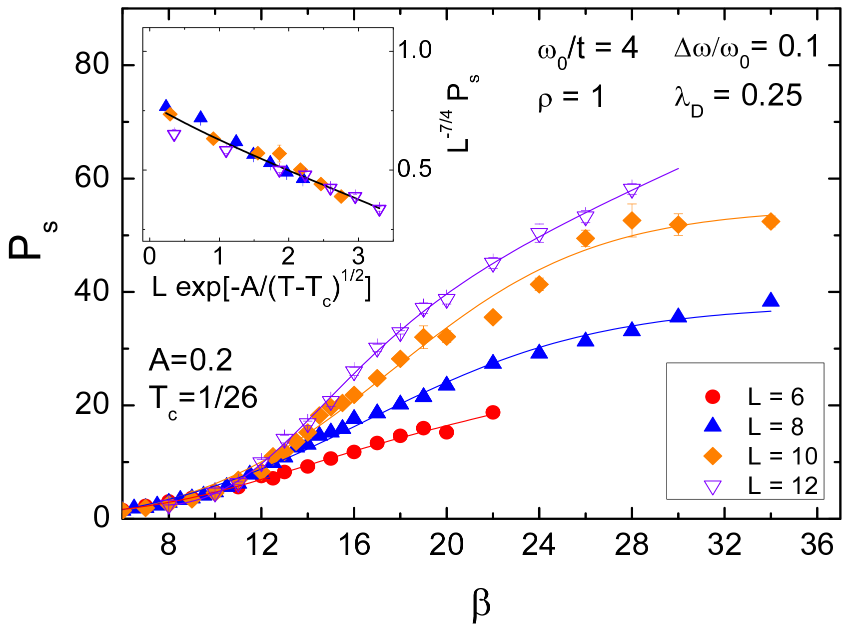
Density of states has a gap at Fermi Energy.

Like AF-Slater gap in $+U$ Hubbard.



Suppress checkerboard CDW without replacing it with stripes.

Superconducting phase at commensurate filling.

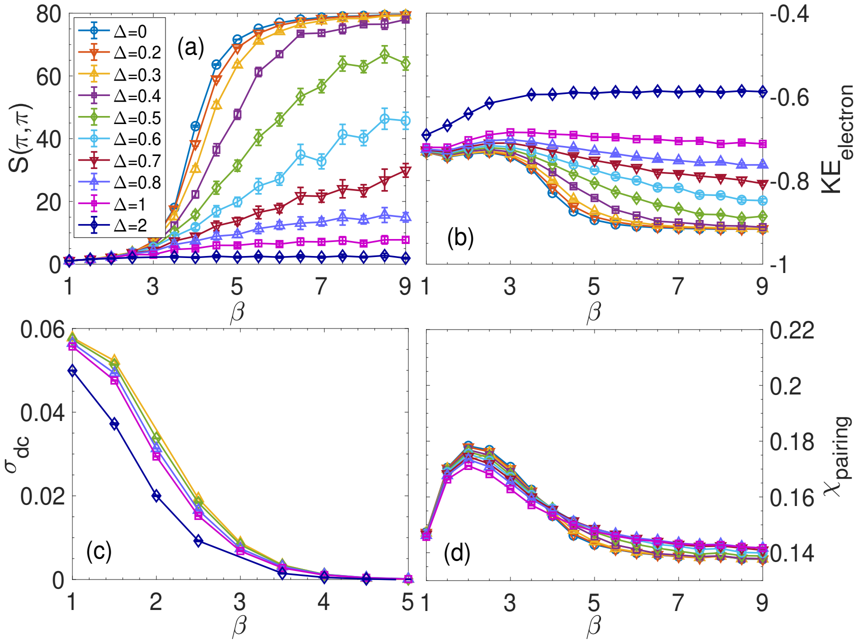


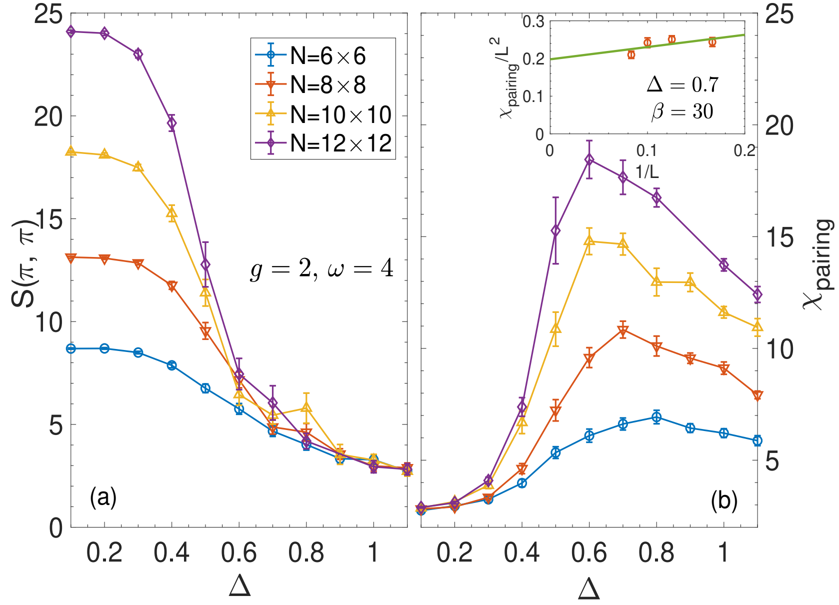
2D superconducting transition (Kosterlitz-Thouless universality). Again, $T_c = \beta_c^{-1} \sim t/26 = W/208$:

6. Effect of Disorder

Random site energies

$$\mathcal{H}_\Delta = \sum_{i\,\sigma} \mu_i n_{i\,\sigma} \qquad -\Delta \le \mu_i \le +\Delta$$





<u>Left:</u> $\omega_0 = 1$: Δ suppresses CDW, no SC signature.

<u>Right:</u> $\omega_0 = 4$: Δ suppresses CDW, large $\chi_{\rm pairing}$.

7. Conclusions

- Holstein Hamiltonian hosts finite-T CDW at half-filling.

  Four bipartite lattices: square, Lieb, honeycomb, cubic.

  Honeycomb lattice quantum phase transition λ_c.

- Introduce phonon dispersion: 'Non-Peierls' CDW Mechanism

  Order at $Q = (\pi, 0)$ decoupled from Fermi surface nesting at $Q = (\pi, \pi)$.

- Superconductivity away from half-filling is difficult to establish: $\beta_c \gtrsim 25/t$.

  Suppression of CDW by phonon dispersion $\Rightarrow$ pairing.

  Suppression of CDW by disorder $\Rightarrow$ pairing.