# Quantum Simulation Studies of Charge Patterns in Fermi-Bose Systems

- 1. Hubbard to Holstein
- 2. Peierls Picture of CDW Transition
- 3. Phonons with Dispersion
- 4. Holstein Model on Honeycomb Lattice
- 5. A New Langevin-Based QMC Algorithm
- 6. Conclusions- Potential Applications

Funding:
Department of Energy DE-SC0014671 and DE-NA0002908.

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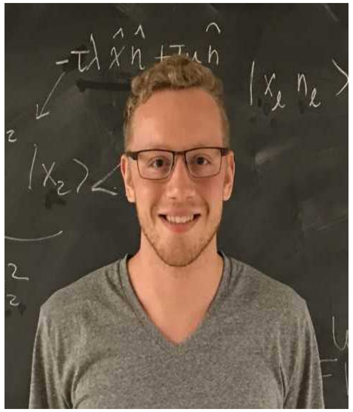

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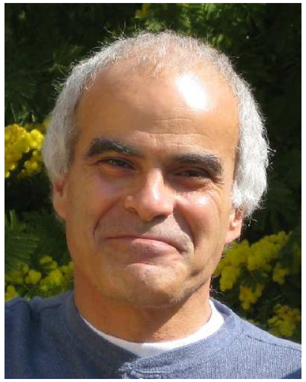

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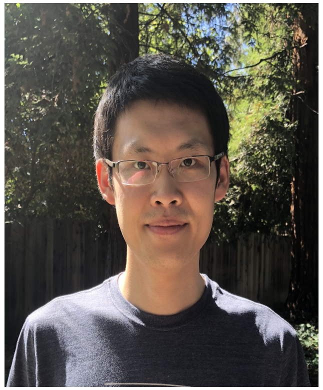

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“Phonon dispersion and the competition between pairing and charge order”, N.C. Costa, T. Blommel, W.-T. Chiu, G.G. Batrouni, and RTS, Phys. Rev. Lett. 120, 187003 (2018).

“Charge Order in the Holstein Model on a Honeycomb Lattice,” Y.-X. Zhang, W.-T. Chiu, N.C. Costa, G.G. Batrouni, and RTS, arXiv:1809.07902.

“Localization, Charge Ordering, and Superfluidity in the Disordered Holstein Model,” B. Xiao, E. Khatami, N. Costa, G. Batrouni, and RTS, in preparation.

Theorists have a reputation for oversimplification:


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

This talk: More realistic 'cows'!

Like the Hubbard Model, the Holstein Model has a considerable lineage:

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

The Holstein model: "Studies of polaron motion: Part II. The 'small' polaron,"
Annals of Physics 8, 343 (1959).

# 1. Hubbard to Holstein

Noninteracting electron kinetic energy:

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

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

$$\hat{H}_{\mathrm{el-el}} = U \sum_{i} \hat{n}_{i\uparrow} \, \hat{n}_{i\downarrow}$$

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

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

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.

Slightly technical: Understanding Hubbard-Holstein Connection

Quantum Monte Carlo at finite temperature- Partition function:

$$Z = \mathrm{Tr}\,[\, e^{-\beta \hat{H}}\,] = \mathrm{Tr}[\, e^{-\Delta\tau \hat{H}} e^{-\Delta\tau \hat{H}} \cdots e^{-\Delta\tau \hat{H}}\,]$$

Path integral: Insert complete sets of boson coordinate states.

$$\frac{1}{2}\omega_0^2\, \hat{X}_i^2 \Rightarrow \frac{1}{2}\omega_0^2\, X_i^2 \qquad\qquad \hat{P}_i^2 \Rightarrow \Big[\, \frac{X_i(\tau+\Delta\tau) - X_i(\tau)}{\Delta\tau}\,\Big]^2$$

Adiabatic approximation (ignore boson kinetic energy).

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

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

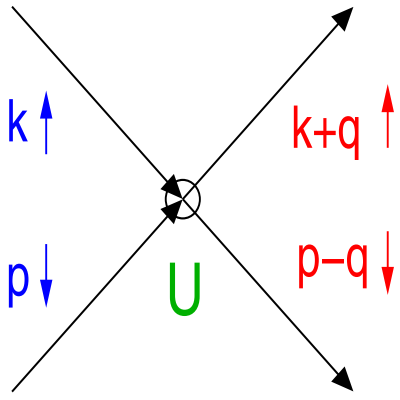
Integrate out bosons: effective on-site interaction *between electrons*.

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

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

Hubbard Model in momentum space:

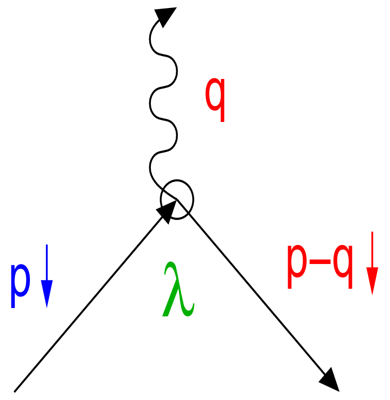
$$\hat{H}_{\mathrm{el-el}} = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{U}{N}\sum_{kpq} \hat{c}^\dagger_{p-q\uparrow}\hat{c}^\dagger_{k+q\downarrow}\hat{c}_{p\uparrow}\hat{c}_{k\downarrow}$$

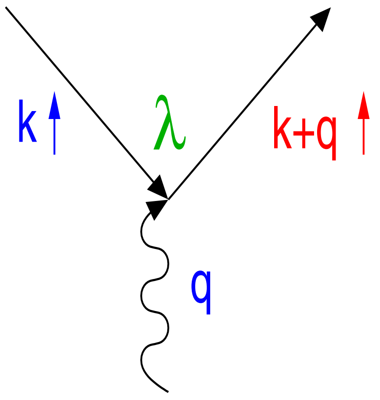



Holstein Model in momentum space:

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

$$\frac{\lambda}{N}\sum_{pq} \left(\hat{a}^\dagger_q + \hat{a}_{-q}\right) \hat{c}^\dagger_{p-q\sigma}\hat{c}_{p\sigma}$$



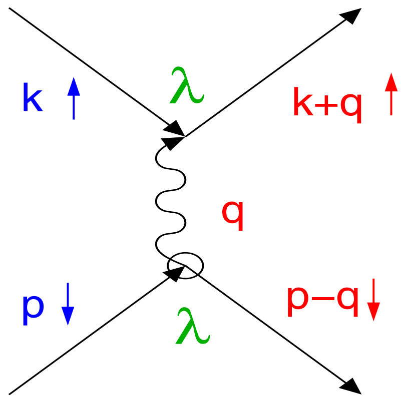




Let's tie the boson lines together...

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 $J$:

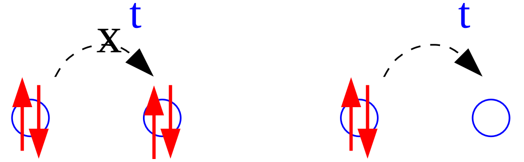
Antiferromagnetism.


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

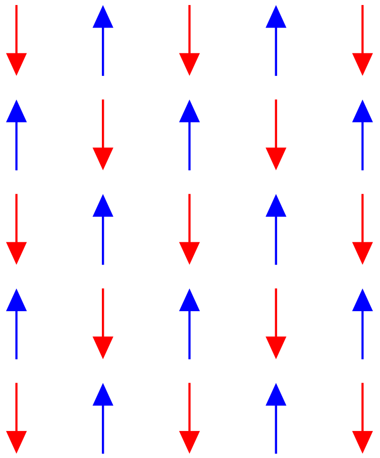
Local pairs form.

Double occupied/empty alternation favored:

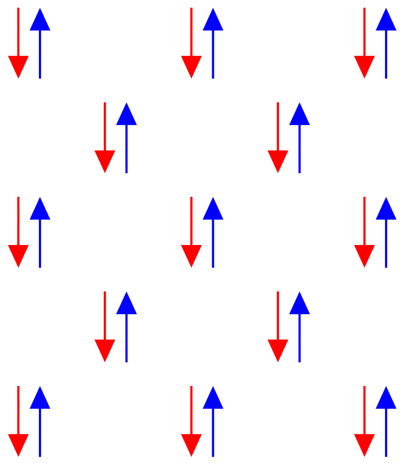
Charge Density Wave.



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).

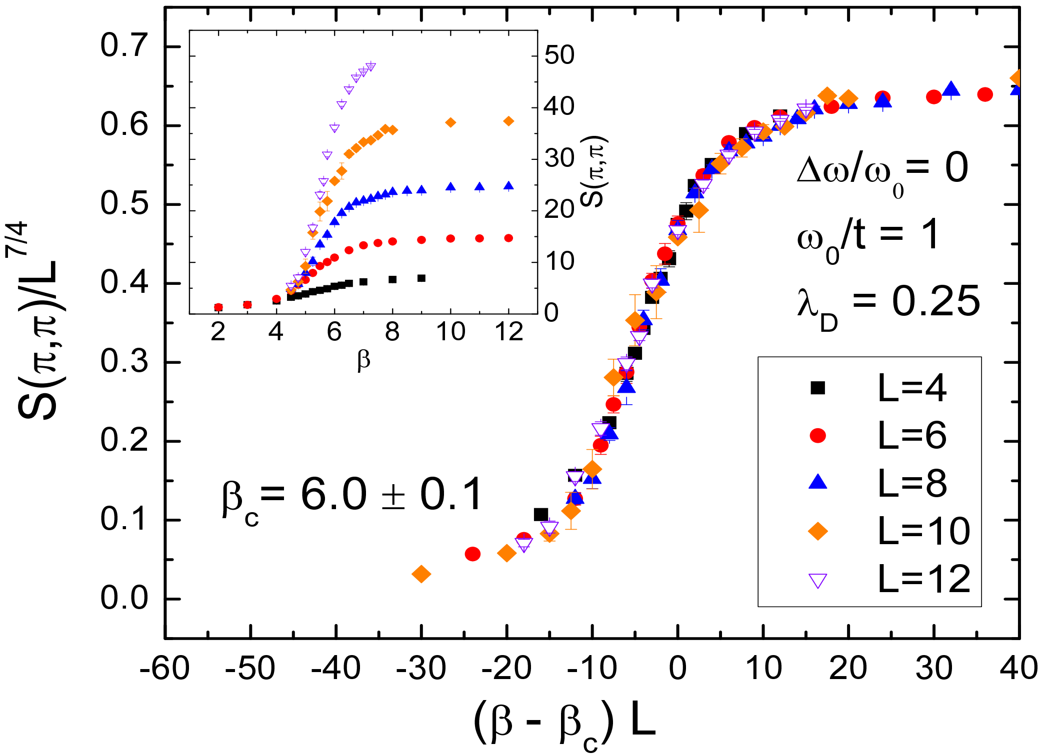
Square Lattice Holstein model

Structure factor

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

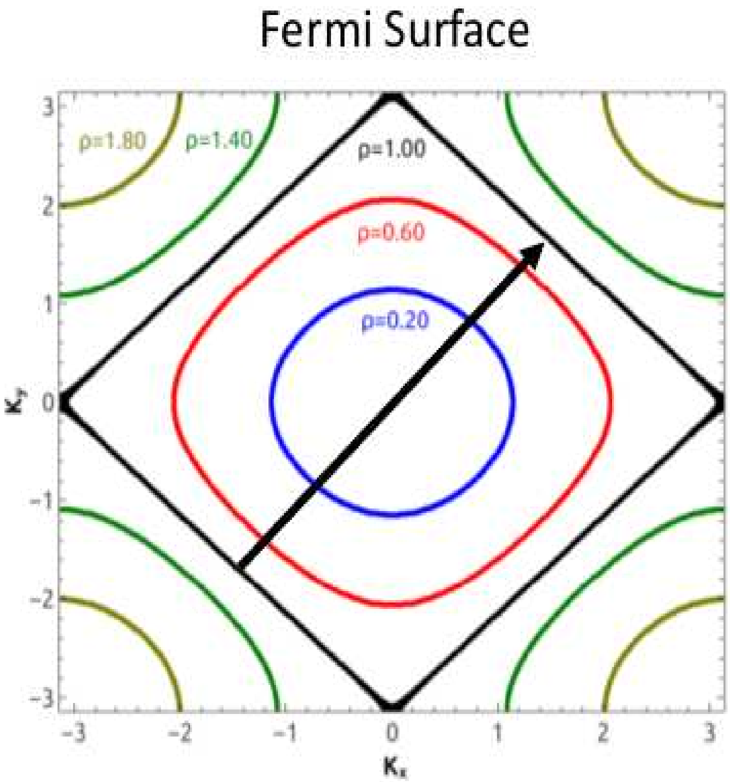
High $T$: $\langle n_i n_j\rangle \sim e^{-|i-j|/\xi} \;\Rightarrow\; S(\pi,\pi)$ independent of $N$.

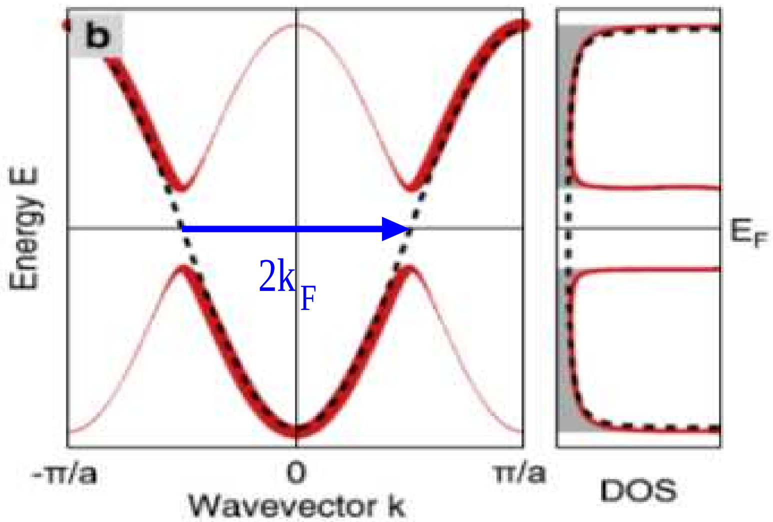
Low $T$: $\langle n_i n_j\rangle \sim$ constant $\;\Rightarrow\; S(\pi,\pi) \propto N$.




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.



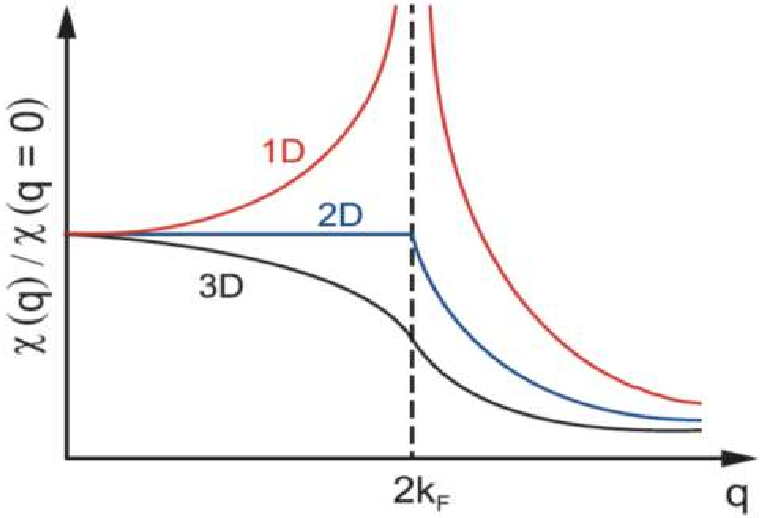

In 1D, always have FSN at $q = 2k_{\mathrm{F}}$.

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 $NbSe_2$: no sign of FSN.

  Attributed instead to momentum dependent electron-boson coupling.

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

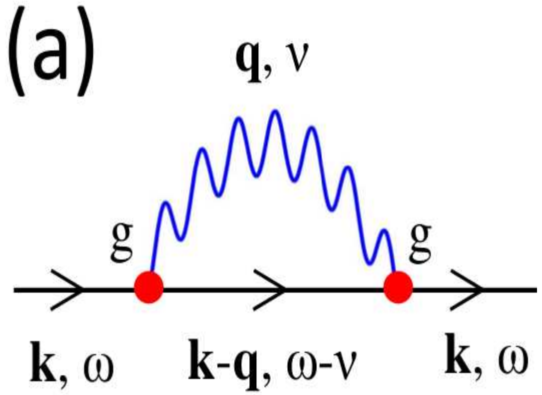
  Attributed instead to electron-electron interactions.

## 3. Phonons with Dispersion

We explored momentum dependence of boson dispersion.

Easy to implement in Determinant QMC.

A ‘close cousin’ of momentum dependent coupling.




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

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

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

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

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

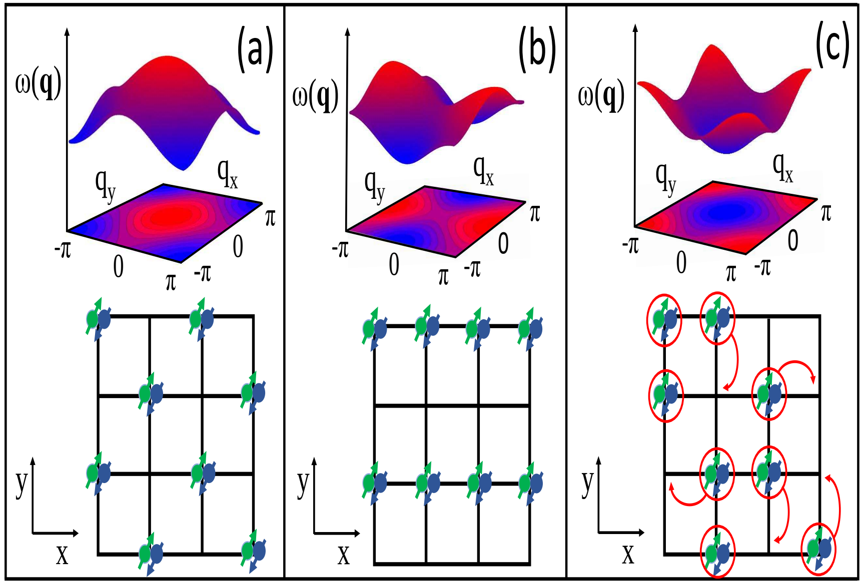
(For nonzero $\nu$ the two self-energies are not equal.)

Conventional Holstein Model:

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

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).

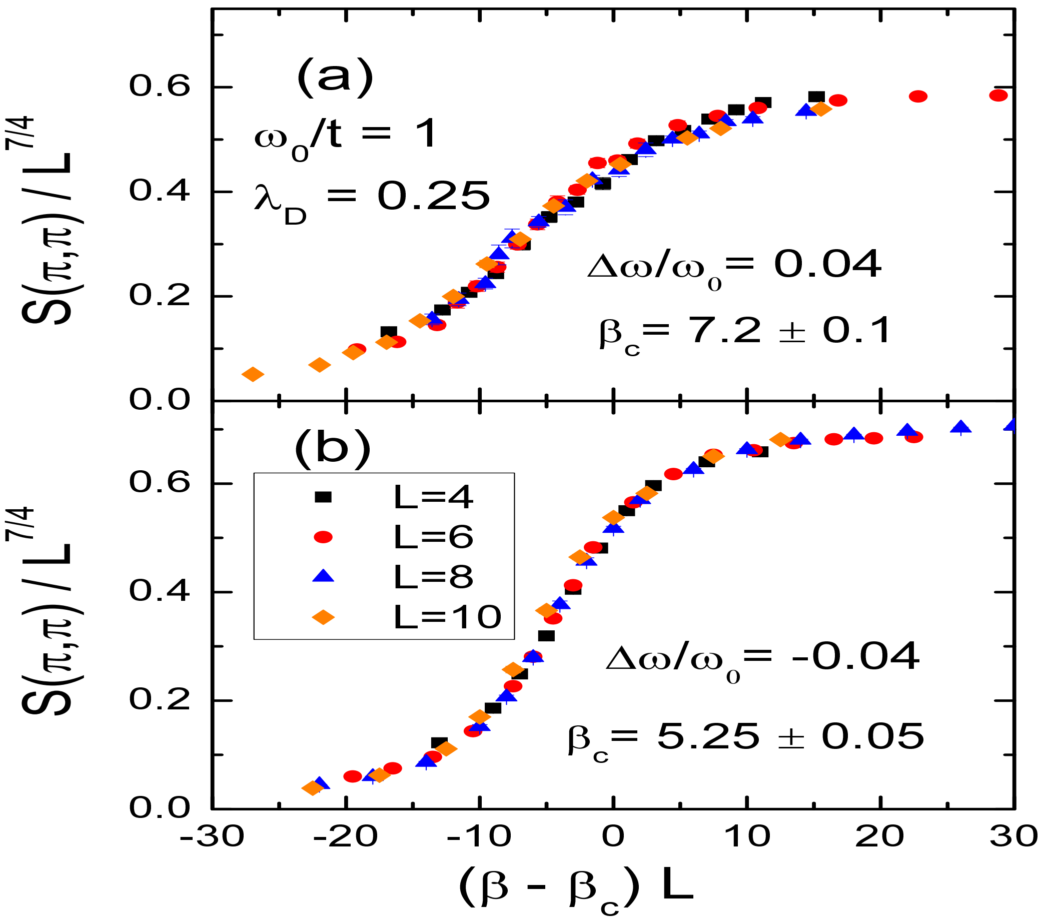
b. Mixed signs in $x, y$ directions: lowers $\omega\big(\mathbf{q} = (0, \pi)\big)$ (Stripe CDW).

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

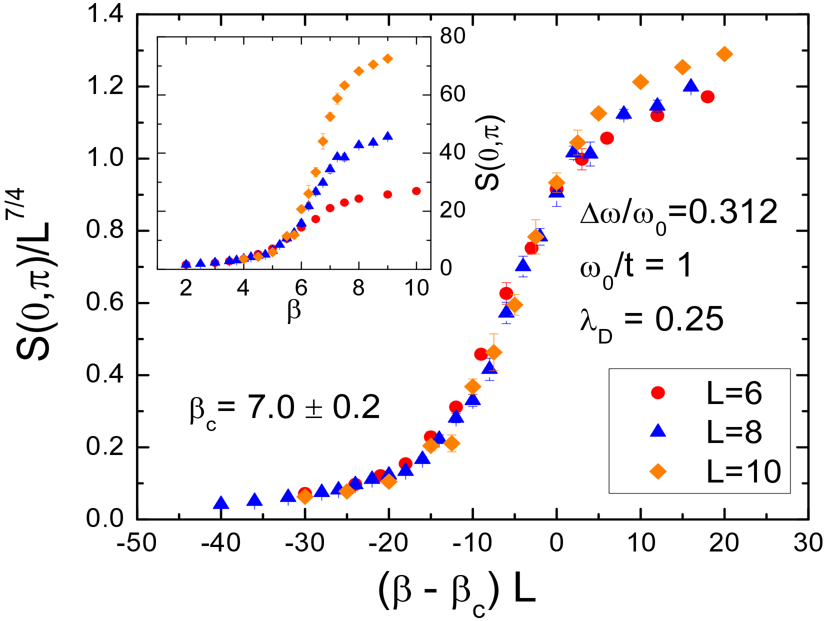
$\beta_c$ for checkerboard CDW increases.

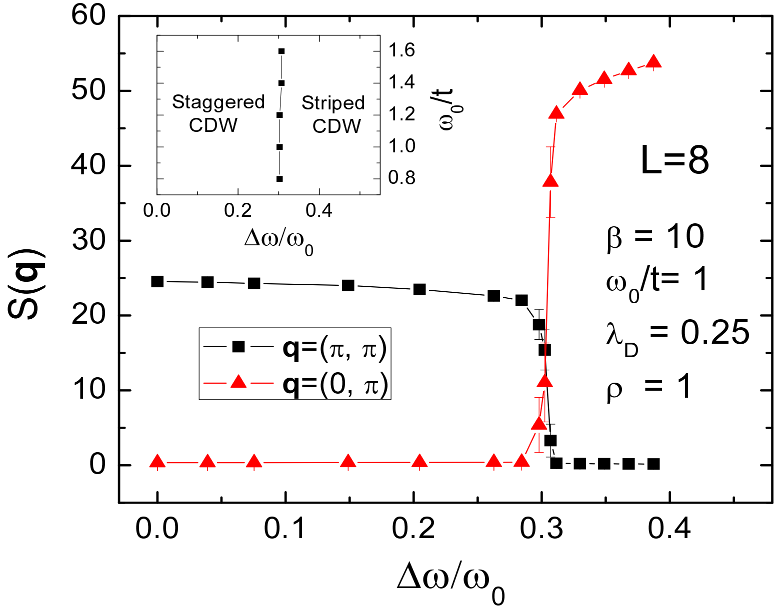
Bottom: $\hat{X}_i + \hat{X}_j$: lowers $\omega\big(\mathbf{q} = (\pi,\pi)\,\big)$

$\beta_c$ for checkerboard CDW decreases.

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

Checkerboard to stripe transition:




Key observation here:

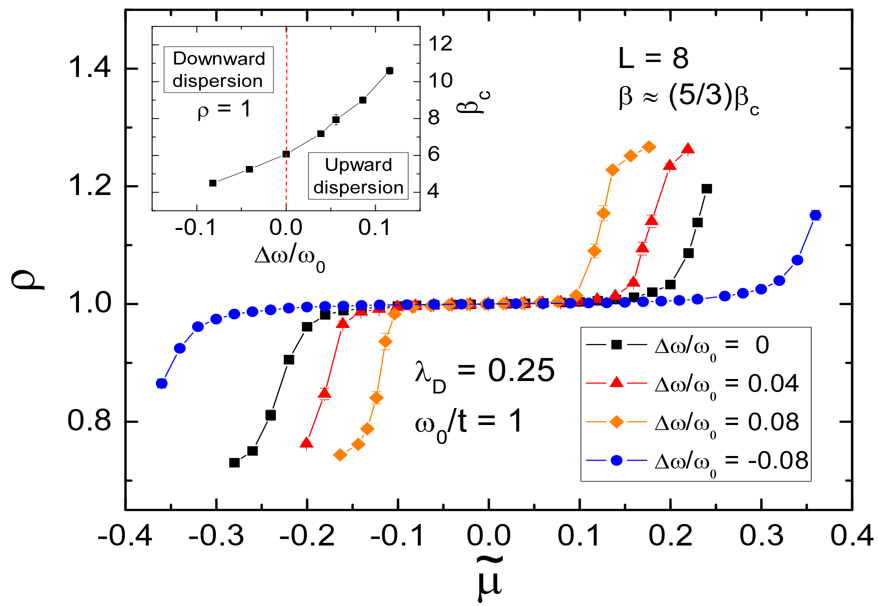
No alteration to electron band structure. Half-filled square lattice.

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

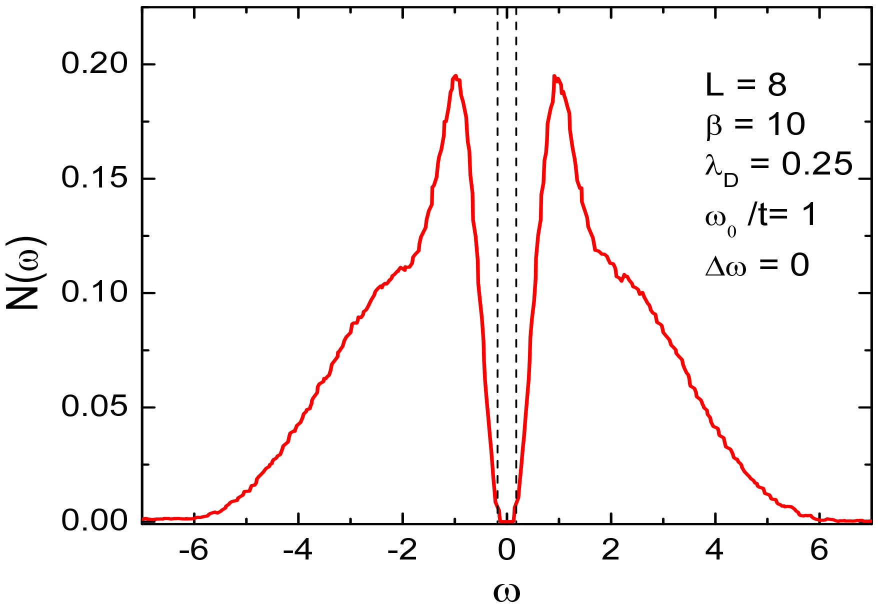
But CDW ordering vector can be elsewhere.

CDW transition outside of canonical Peierls picture.

Can also examine these phenomena via CDW gap.

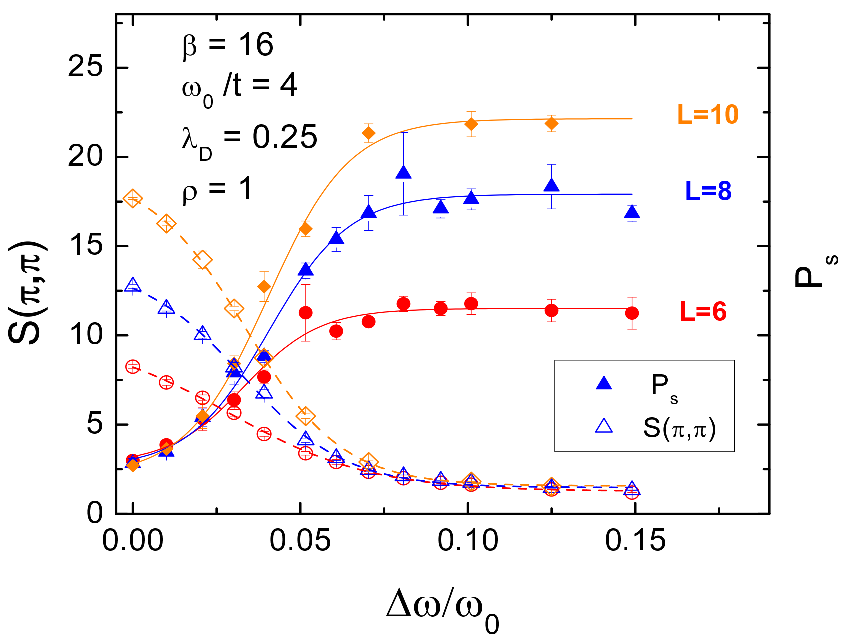



Plateau in $\rho(\mu)$ shrinks/expands with boson dispersion.



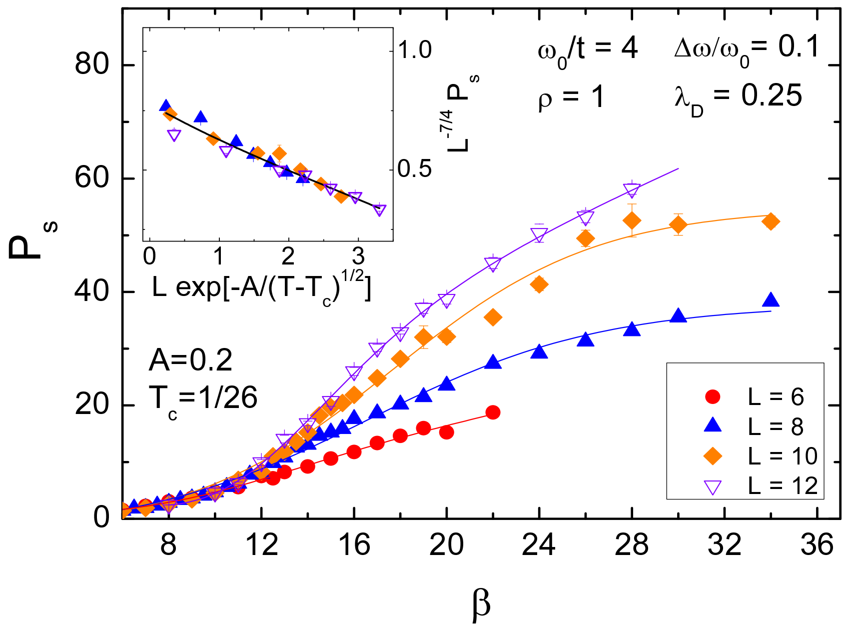

Density of states has a gap at Fermi Energy.

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).

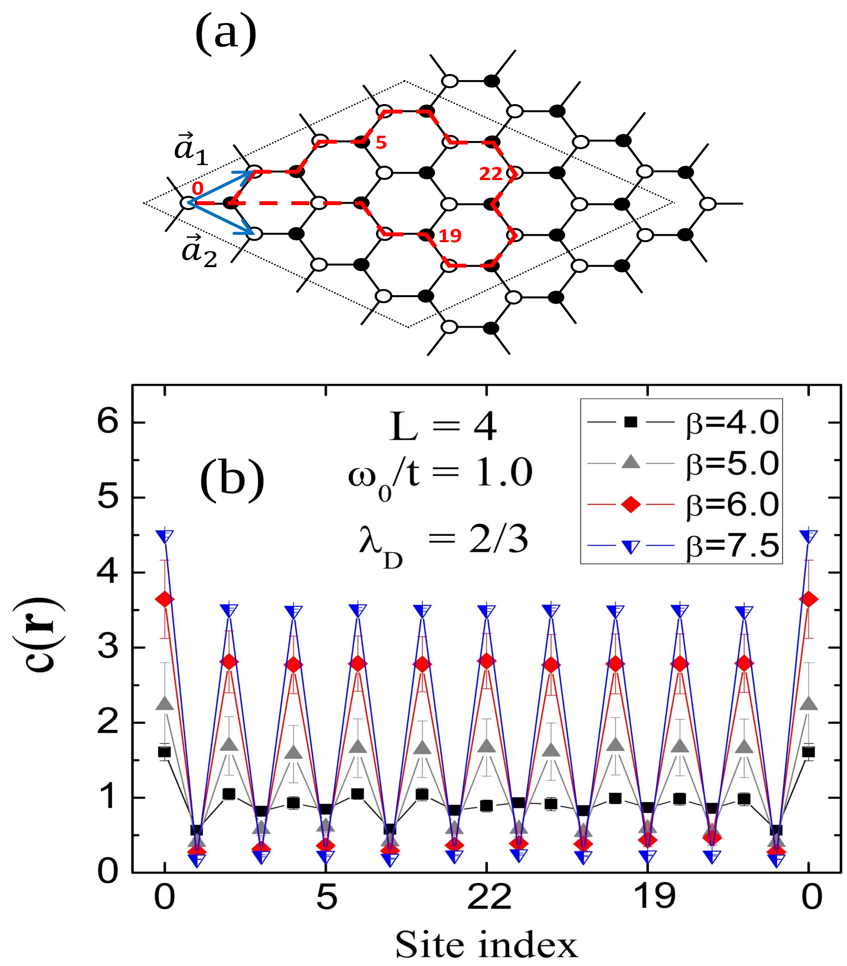
# 4. Holstein Model on Honeycomb Lattice

Dirac spectrum for fermions.

Quantum critical point for Hubbard Model:

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

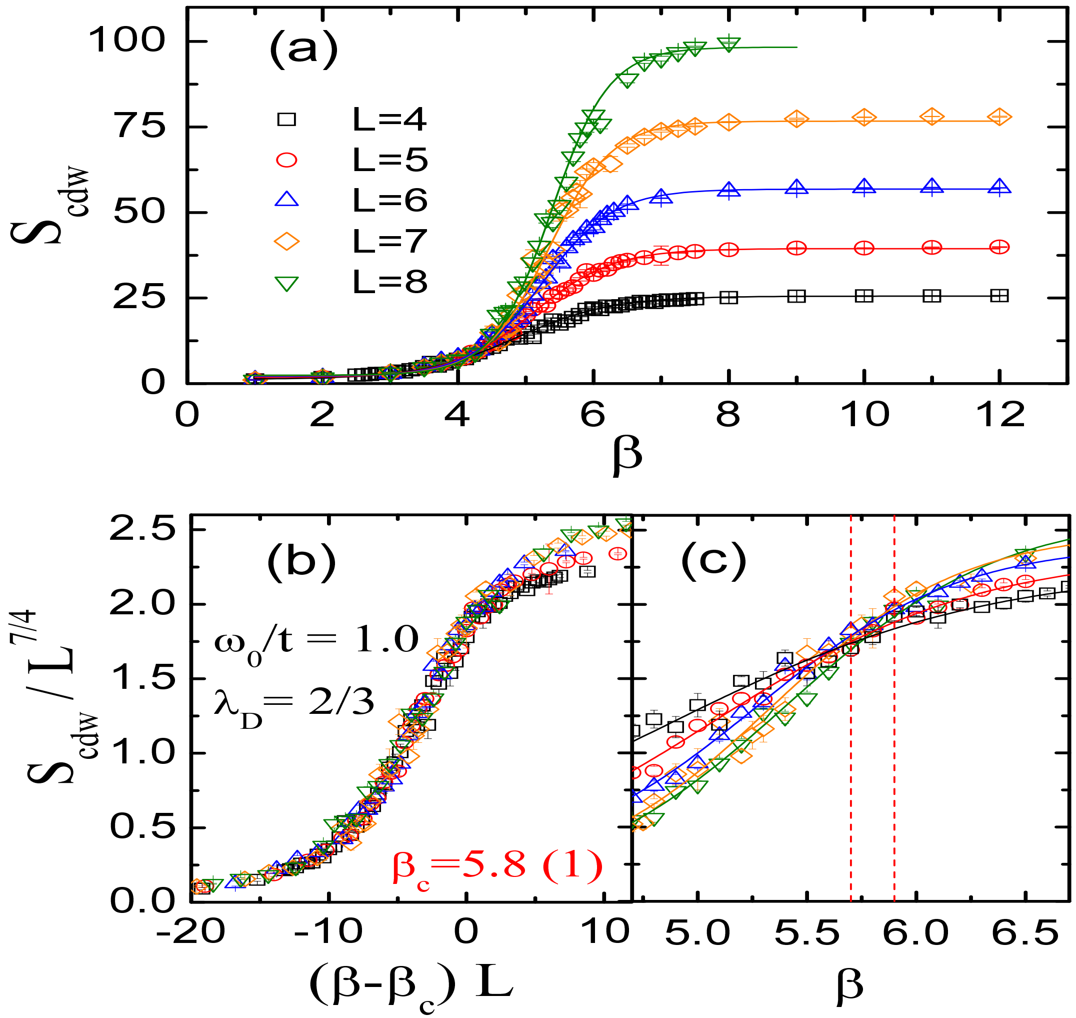
Effect of electron-boson interactions on Dirac fermions and charge order?



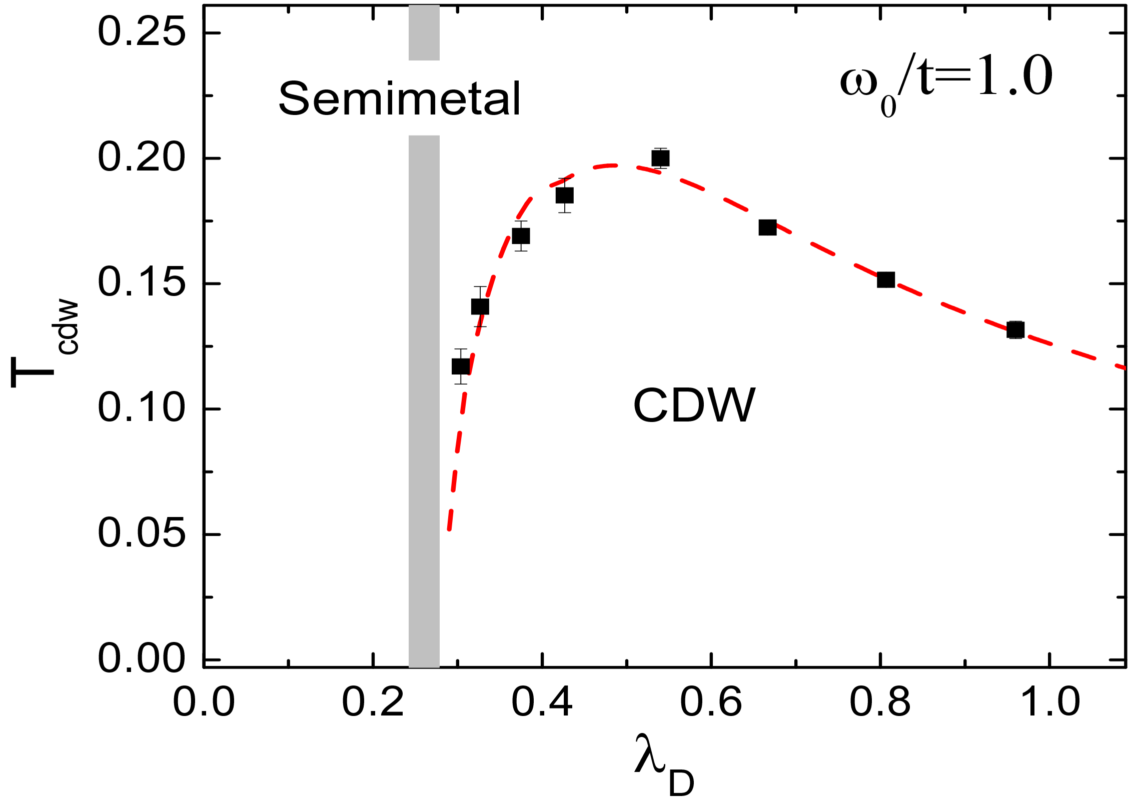

Long range real space charge correlations develop as $\beta$ increases.

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, arXiv:1809.07902.

"Charge-Density-Wave Transitions of Dirac Fermions Coupled to Phonons," C. Chen, X.Y. Xu, Z.Y. Meng, and M. Hohenadler, arXiv:1809.07903

## 5. A New Langevin-Based QMC Algorithm

Many QMC approaches propose local moves.

Inexpensive to evaluate change in action.

In the case of DQMC: $o(N^2)$ to update boson coordinate.

$N\beta$ boson degrees of freedom: Complete scaling is $o(N^3\beta)$.

Alternate approach in Lattice Gauge Theory QMC:

Update all bosonic field variables at same time via Langevin equation.

In principle complete scaling is $o(N\beta)$.

Assumes number of (conjugate gradient) iterations to compute $\mathcal{M}^{-1}\vec{v}$

is independent of system size $N$ and inverse temperature $\beta$.

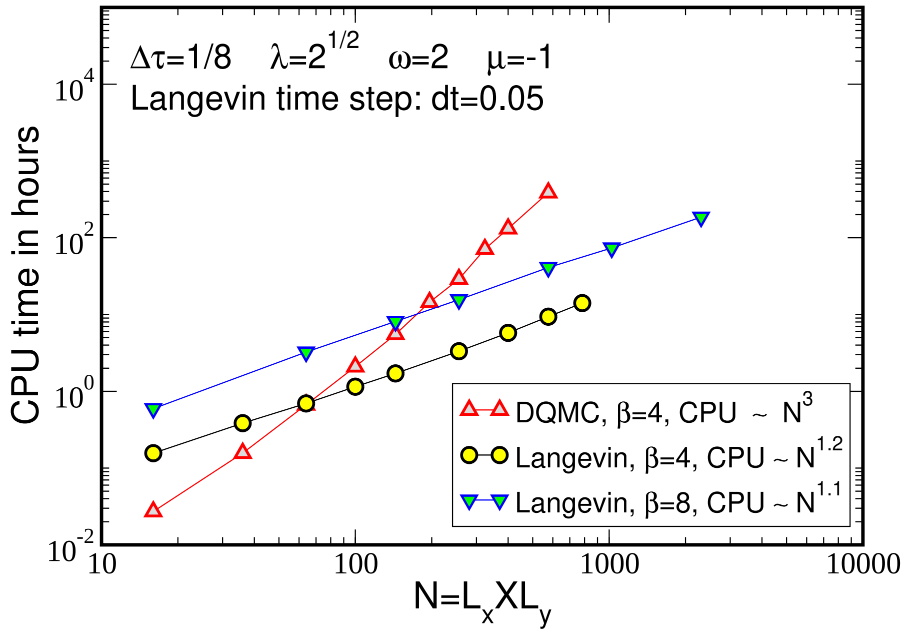
Does not work for Hubbard Model!

Matrix $\mathcal{M}$ is much more ill-conditioned than LGT.

Number of conjugate gradient iterations grows catastrophically with $\beta$.

Key observation: $\hat{P}_i^2 \Rightarrow \left[ \frac{X_i(\tau+\Delta\tau)-X_i(\tau)}{\Delta\tau} \right]^2$ moderates eigenspectrum of $\mathcal{M}$.

(No such term for auxiliary bosonic field in Hubbard model.)

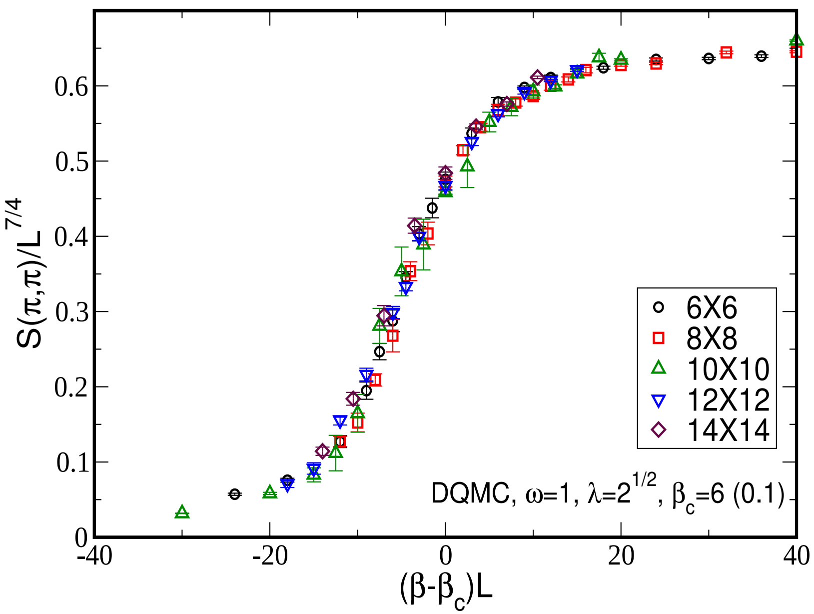


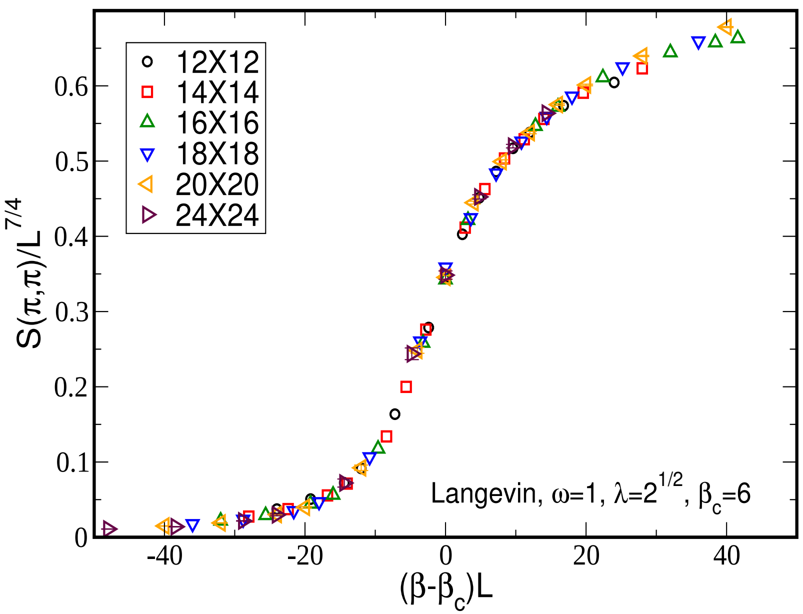

<u>Left:</u> Langevin CPU time is indeed nearly linear in $N$.

<u>Below:</u>

Increase in accessible system size improves scaling collapse.

DQMC (left) vs. Langevin (right).



## 6. Conclusions- Potential Applications

- Phonon dispersion alters CDW wavevector in square lattice Holstein model.

  Non-Peierls CDW Mechanism: order decoupled from Fermi Surface Nesting.

- Honeycomb lattice Holstein model:

  Semi-metal to CDW quantum critical point.

- Langevin approach to updating boson degrees of freedom:

  Greater efficiency for generalizations of Holstein model.

  * Momentum dependent fermion-boson coupling.
  * Interactions of form $n_{\mathbf{i}}^{\rm B}\, n_{\mathbf{i}}^{\rm F}$.

  Both make conventional DQMC $o(N^4)$, i.e. unfeasible.