Quantum Monte Carlo Study of the Doped Holstein Model

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Introduction

- Condensed matter physics: Interested in phases of matter in many-body systems
- E.g. ferromagnetism, charge ordering, superconductivity
- Electron-phonon interaction: CDW order, superconductivity (SC)
- What is the interplay between competing phases (CDW and SC)?
- Simulate a model Hamiltonian which describes the essential physics

Holstein Model: $\hat{H} = \hat{K} + \hat{U} + \hat{V}$

Electron Kinetic energy:

$$\hat{K} = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \right) - \mu \sum_{i\sigma} \hat{n}_{i,\sigma}$$

Phonon KE and PE:

$$\hat{U} = \frac{1}{2} \sum_i \hat{P}_i^2 + \frac{\omega_0^2}{2} \sum_i \hat{X}_i^2$$

Electron-Phonon Interaction:

$$\hat{V} = \lambda \sum_{i,\sigma} \hat{n}_{i,\sigma} \hat{X}_i$$

- $\hat{c}^{\dagger}_{i\sigma}$ and $\hat{c}_{j\sigma}$ are electron creation/annihilation operators
- $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$ is the number operator
- t is the nearest-neighbor hopping term

- $\hat{X}_i$ and $\hat{P}_i$ are position and momentum operators for independent harmonic oscillators on each site of the lattice

- On-site electron-phonon coupling with interaction strength λ
- Electron-phonon coupling also expressed as: $g = \frac{\lambda}{\sqrt{2\omega_0}}$

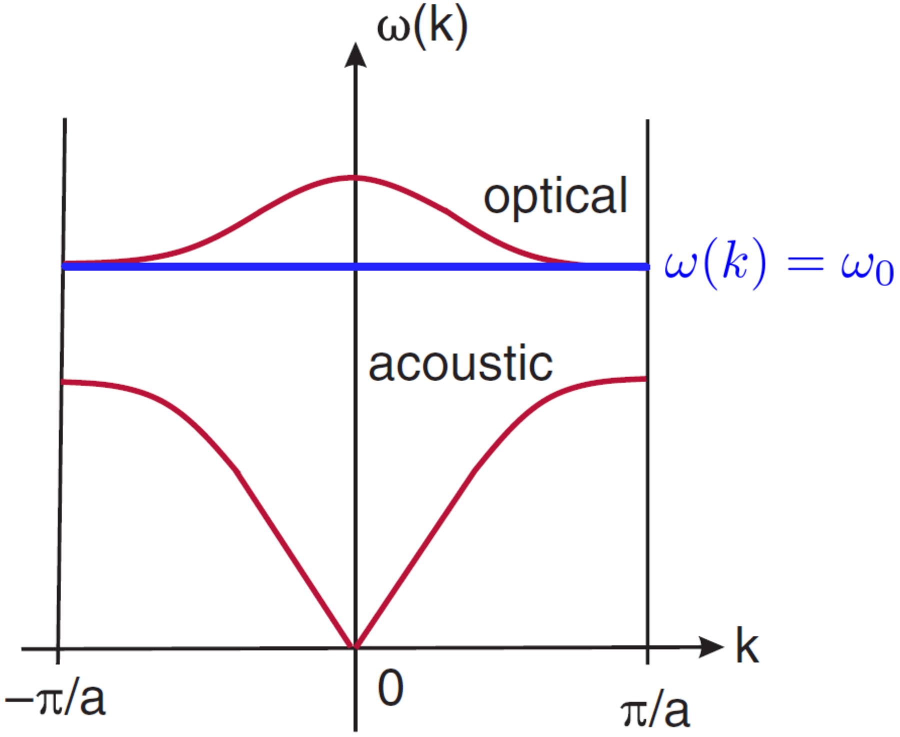
Holstein Model: $\hat{H} = \hat{K} + \hat{U} + \hat{V}$

- Simple model of electron-phonon interactions on a lattice:
- Nearest neighbor hopping only
- Fixed on-site electron phonon coupling λ
- Fixed dispersionless phonon frequency ω_0

$$\hat{K} = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \right) - \mu \sum_{i\sigma} \hat{n}_{i,\sigma}$$

$$\hat{U} = \frac{1}{2} \sum_i \hat{P}_i^2 + \frac{\omega_0^2}{2} \sum_i \hat{X}_i^2$$

$$\hat{V} = \lambda \sum_{i,\sigma} \hat{n}_{i,\sigma} \hat{X}_i$$



"Field Guide to Solid State Physics", M. S. Wartak, C. Y. Fong

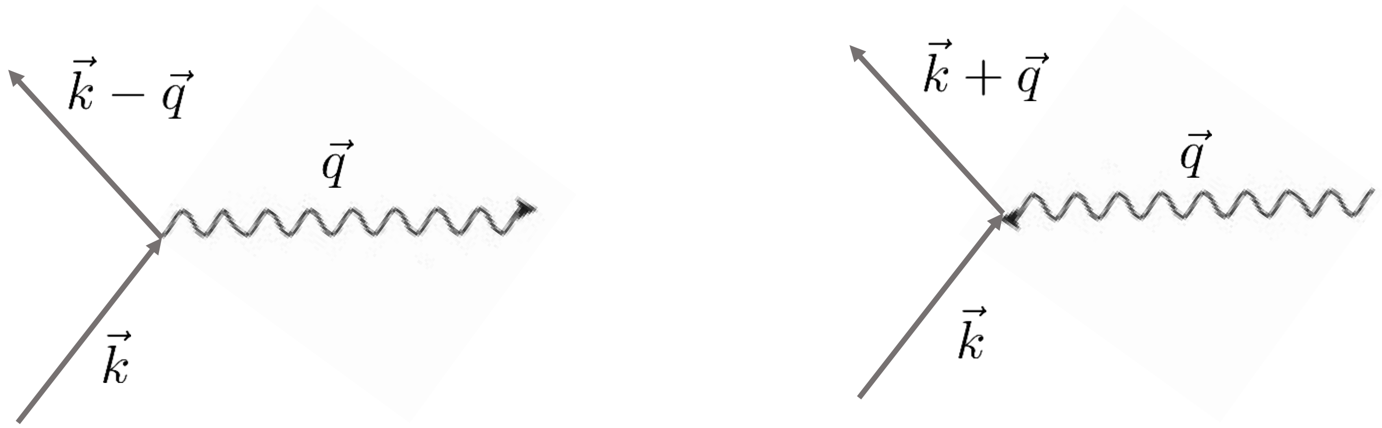
Holstein Model:

$$\hat{c}_{\mathbf{j}\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{j}} \qquad \hat{c}^{\dagger}_{\mathbf{j}\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} e^{-i\mathbf{k}\cdot\mathbf{j}}$$

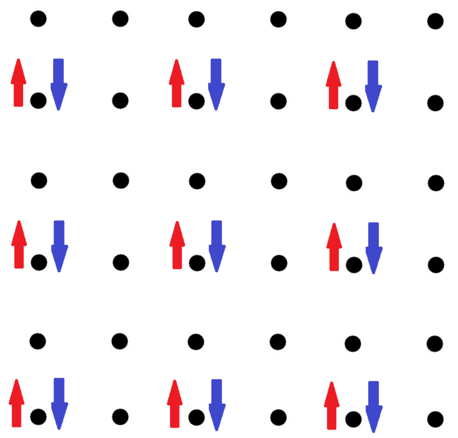
- Fourier transform: Electron-Phonon interaction in momentum space

$$\hat{V} = \frac{\lambda}{\sqrt{2\omega_0}} \frac{1}{\sqrt{N}} \sum_{q,k,\sigma} \left[\hat{b}^{\dagger}_q \hat{c}^{\dagger}_{k-q,\sigma} \hat{c}_{k,\sigma} + \hat{b}_q \hat{c}^{\dagger}_{k+q,\sigma} \hat{c}_{k,\sigma} \right]$$

- Describes phonon emission and absorption:



Holstein Model:



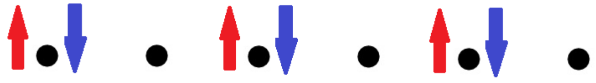
- Single site (t=0) limit:

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

$$\hat{H} = \frac{1}{2}\hat{P}^2 + \frac{1}{2}\omega_0\left[\hat{X}^2 + \frac{\lambda}{\omega_0^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)\right]^2 \underbrace{-\frac{1}{2}\frac{\lambda^2}{\omega_0^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)^2} - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow)$$

Attractive electron-electron interaction: $U_{eff} = -\frac{\lambda^2}{\omega_0^2}$

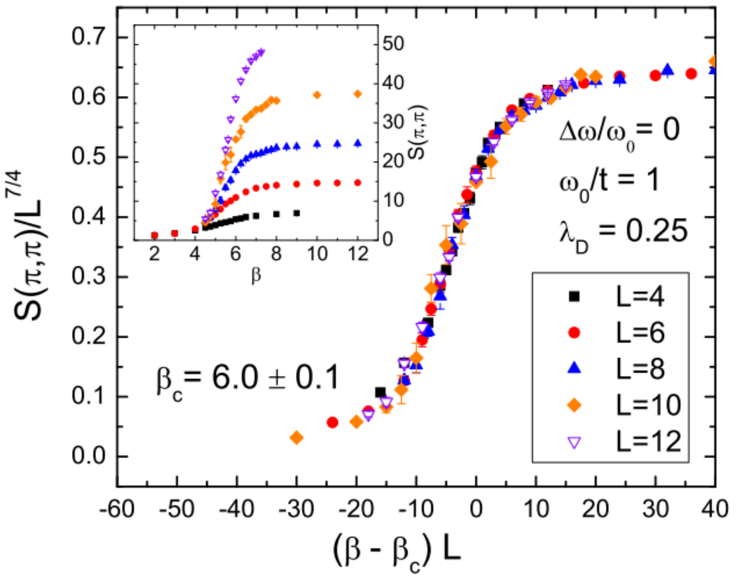
- Attractive electron-electron coupling causes local pairs to form
- Alternating doubly-occupied and empty sites favored



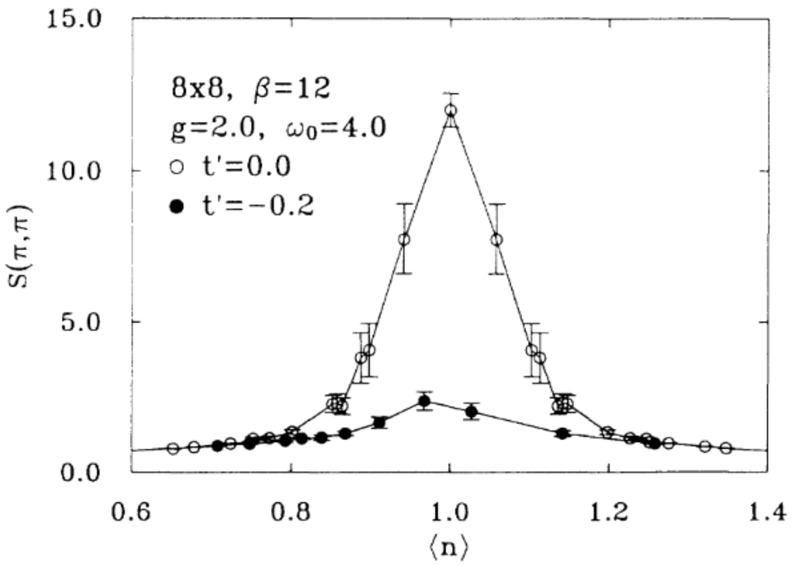
- At half-filling: one electron on average per lattice site charge ordering on bipartite lattice
- Charge density wave (CDW) at half-filling

Motivation

- Holstein model well-studied at **half-filling**. CDW order on square lattice below T_{CDW}
- But when doped away from half-filling, it is known that CDW order is reduced and SC order increases.
- Some attempts to find T_{SC} for the doped Holstein model in literature but not fully understood, and not computationally feasible in the past.
- **Goal**: Study the interplay between CDW and SC order in the **doped** Holstein model and try to find some estimates of T_{SC}

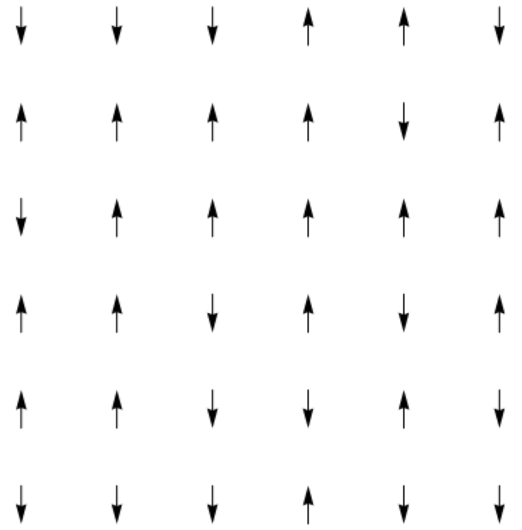


N.C. Costa, T. Blommel, W.-T. Chiu, G. Batrouni, R. T. Scalettar, Phys. Rev. Lett. **120**, 187003 (2018)



M. Vekić, R. M. Noack, S. R White, Phys. Rev. B. **46** 271 (1992)

Monte Carlo (Classical):



N spins

2^N possible configurations

- Simple example: Ising Model $$H = -J \sum_{\langle i,j \rangle} S_i S_j$$

- Probability of a configuration C is given by the Boltzmann distribution:

$$p(C) = \frac{e^{-\beta E_C}}{Z} \qquad Z = \sum_C e^{-\beta E_C} \qquad \beta = \frac{1}{T}$$

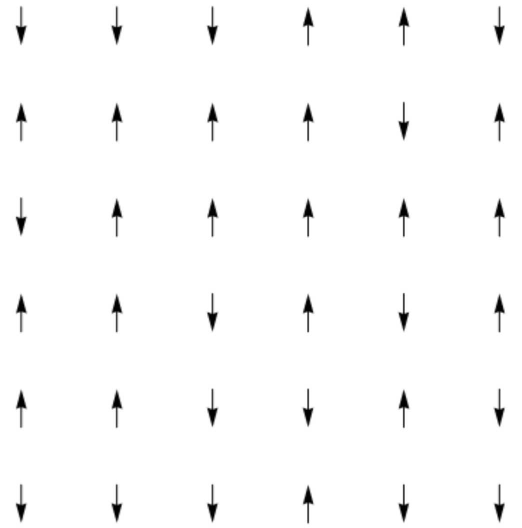
- Importance sampling: Goal is to generate configurations with desired probability distribution

- Markov process: Generate a sequence of configurations according to some transition probability:

  $P(a \to b)$ is the probability to generate configuration *b* from configuration *a*

- The algorithm we use to do this should ensure convergence to the desired distribution

Monte Carlo (Classical):



Detailed balance condition: $p(a)P(a \to b) = p(b)P(b \to a)$

Satisfied by the Metropolis algorithm: $P(a \to b) = \min\left[1, \frac{p(b)}{p(a)}\right]$

E.g. for Ising model:

1. Start with an initial configuration *a* of spins
2. Propose a change to a new configuration *b*: "Glauber update" ⟶ flip a randomly chosen spin
3. Calculate energy difference $\Delta E = E_b - E_a$
4. Choose random number $R \in [0, 1]$
5. Accept move if: $R < e^{\beta \Delta E}$
6. Repeat steps 2-5

$$\frac{p(b)}{p(a)} = \frac{e^{-\beta E_b}}{e^{-\beta E_a}} = e^{-\beta(E_b - E_a)}$$

Determinant Quantum Monte Carlo

- Partition function of the Holstein Hamiltonian: $Z = Tr\left(e^{-\beta\hat{H}}\right) = Tr\left(e^{-\beta(\hat{K}+\hat{U}+\hat{V})}\right)$
- We write $\beta = L_T\Delta\tau$ and use Suzuki-Trotter approximation: $e^{-\Delta\tau(\hat{A}+\hat{B})} = e^{\Delta\tau\hat{A}}e^{-\Delta\tau\hat{B}} + \underbrace{O(\Delta\tau^2)}_{\text{“Trotter error”}}$

$$Z = Tr\left[e^{-\Delta\tau(\hat{K}+\hat{U}+\hat{V})}e^{-\Delta\tau(\hat{K}+\hat{U}+\hat{V})}\dots e^{-\Delta\tau(\hat{K}+\hat{U}+\hat{V})}\right]$$

$$\approx Tr\left[(e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{U}}e^{-\Delta\tau\hat{V}})(e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{U}}e^{-\Delta\tau\hat{V}})\dots(e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{U}}e^{-\Delta\tau\hat{V}})\right]$$

- We have introduced an imaginary time axis which adds an additional dimension.
- To proceed we perform the trace over both phonon degrees of freedom $\{x_{il}\}$ and electron degrees of freedom $\{n_{i\sigma}\}$. Phonon field is displacement of phonons at each spatial site and time $(l = 1, 2, \dots, L_T)$
- First, we insert an identity operator at each imaginary time slice:

$$Z = \int_{-\infty}^{\infty}\prod_{i,\tau}dx_{i\tau}\,\underset{\{n_{i\sigma}\}}{Tr}\langle x_{i,1}|e^{\Delta\tau\hat{K}}e^{\Delta\tau\hat{U}}e^{\Delta\tau\hat{V}}|x_{i,2}\rangle\langle x_{i,2}|e^{\Delta\tau\hat{K}}e^{\Delta\tau\hat{U}}e^{\Delta\tau\hat{V}}|x_{i,3}\rangle\dots\langle x_{i,L}|e^{\Delta\tau\hat{K}}e^{\Delta\tau\hat{U}}e^{\Delta\tau\hat{V}}|x_{i,1}\rangle$$

$$= \int_{-\infty}^{\infty}\prod_{i,\tau}dx_{i\tau}\langle x_{i,1}|e^{\Delta\tau\hat{U}}|x_{i,2}\rangle\langle x_{i,2}|e^{\Delta\tau\hat{U}}|x_{i,3}\rangle\dots\langle x_{i,L}|e^{\Delta\tau\hat{U}}|x_{i,1}\rangle\,\underset{\{n_{i\sigma}\}}{Tr}\left[e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,1})}e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,2})}\dots e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,L})}\right]$$

Determinant Quantum Monte Carlo

- A single contraction between imaginary time slices has the form:

$$\langle x_{i,\tau}|e^{-\Delta\tau\hat{U}}|x_{i,\tau+1}\rangle = \exp\left(-\Delta\tau\left[\frac{\omega_0}{2}\sum_i x_{i,\tau}^2 - \frac{1}{2}\sum_i\left(\frac{x_{i,\tau+1}-x_{i,\tau}}{\Delta\tau}\right)^2\right]\right)$$

- The partition function can then be written as:

$$Z = \int_{-\infty}^{\infty}\prod_{i,\tau} dx_{i,\tau}e^{-S}\prod_{\sigma}\underset{\{n_i\}}{Tr}\left[e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,1})}e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,2})}\dots e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,L})}\right]$$

where $S = \Delta\tau\left[\frac{\omega_0^2}{2}\sum_{i,\tau}x_{i,\tau}^2 - \frac{1}{2}\sum i,\tau\left(\frac{x_{i,\tau+1}-x_{i,\tau}}{\Delta\tau}\right)^2\right]$ is the "phonon action"

- Now, K and V are quadratic in fermion creation and annihilation operators, so they can be written in matrix form:

$$\hat{K} = \underline{\hat{c}}^\dagger\bar{K}\underline{\hat{c}} \qquad \hat{V}(x_{i,\tau}) = \underline{\hat{c}}^\dagger\bar{V}(x_{i,\tau})\underline{\hat{c}}$$

- Theorem:

$$Tr\left[e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(1)}e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(2)}\dots e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(L)}\right] = \det\left[1+e^{-\Delta\tau\bar{K}}e^{-\Delta\tau\bar{V}(1)}e^{-\Delta\tau\bar{K}}e^{-\Delta\tau\bar{V}(2)}\dots e^{-\Delta\tau\bar{K}}e^{-\Delta\tau\bar{V}(L)}\right]$$

Determinant Quantum Monte Carlo

$$Z = \int_{-\infty}^{\infty} \prod_{i,\tau} dx_{i,\tau} e^{-S} \prod_{\sigma} \det \left[1 + e^{-\Delta\tau \bar{K}} e^{-\Delta\tau \bar{V}(1)} e^{-\Delta\tau \bar{K}} e^{-\Delta\tau \bar{V}(2)} \ldots e^{-\Delta\tau \bar{K}} e^{-\Delta\tau \bar{V}(L)} \right]$$

$$Z = \int_{-\infty}^{\infty} \prod_{i,\tau} dx_{i,\tau} e^{-S} \det(\bar{M}_{\uparrow}) \det(\bar{M}_{\downarrow})$$

$$Z = \int_{-\infty}^{\infty} \prod_{i,\tau} dx_{i,\tau} e^{-S} [\det(\bar{M})]^2 = \int_{-\infty}^{\infty} \prod_{i,\tau} dx_{i,\tau} W(\{x_{i,\tau}\})$$

- Partition function is now a function of the phonon field $\{x_{i\tau}\}$ only
- Use Metropolis algorithm to update phonon field: $P(\{x_{i,\tau}\} \rightarrow \{x'_{i,\tau}\}) = \min \left[1, \frac{W(\{x'_{i,\tau}\})}{W(\{x_{i,\tau}\})} \right]$

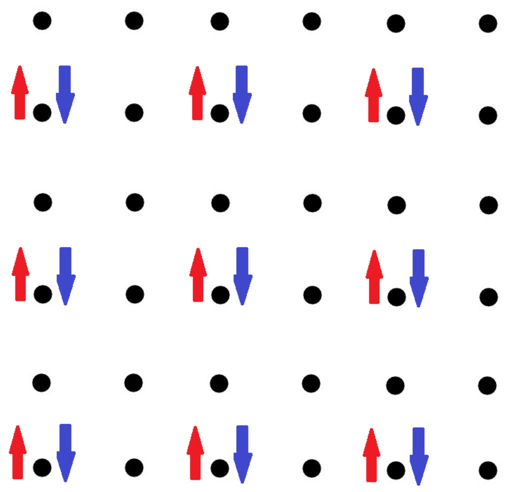
- Physical quantities of interest come from measuring fermion Green's function, e.g.:

$$G_{ij} = \langle c_i c_j^{\dagger} \rangle = \left[1 + e^{-\Delta\tau \bar{K}} e^{-\Delta\tau \bar{V}(1)} e^{-\Delta\tau \bar{K}} e^{-\Delta\tau \bar{V}(2)} \ldots e^{-\Delta\tau \bar{K}} e^{-\Delta\tau \bar{V}(L)} \right]^{-1} = \bar{M}_{ij}^{-1}$$

DQMC Measurements:

- Density-Density Correlation: $C(\mathbf{r}) = \langle n_{\mathbf{i}} n_{\mathbf{i+r}} \rangle = \langle (n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow})(n_{\mathbf{i+r}\uparrow} + n_{\mathbf{i+r}\downarrow}) \rangle$

- CDW structure factor: $S(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{i},\mathbf{j}} e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})} \langle n_{\mathbf{i}} n_{\mathbf{j}} \rangle$



$$S(\pi,\pi) = \frac{1}{N} \sum_{\mathbf{i},\mathbf{j}} (-1)^{([i_x - j_x) + (i_y - j_y)]} \langle n_{\mathbf{i}} n_{\mathbf{j}} \rangle$$

Detects charge ordering (checkerboard CDW)

- S-wave pair susceptibility:

$$P_s = \frac{1}{N} \int_0^\beta \langle \Delta(\tau) \Delta^\dagger(0) \rangle \quad \text{where: } \Delta(\tau) = \sum_{\mathbf{i}} c_{\mathbf{i}\downarrow}(\tau) c_{\mathbf{i}\uparrow}(\tau)$$

Results:

- Electron-phonon coupling: $g = \dfrac{\lambda}{\sqrt{2\omega_0}}$

- Dimensionless coupling constant: $\lambda_D = \dfrac{\lambda^2}{\omega_0 W}$ $\quad W = 8t$

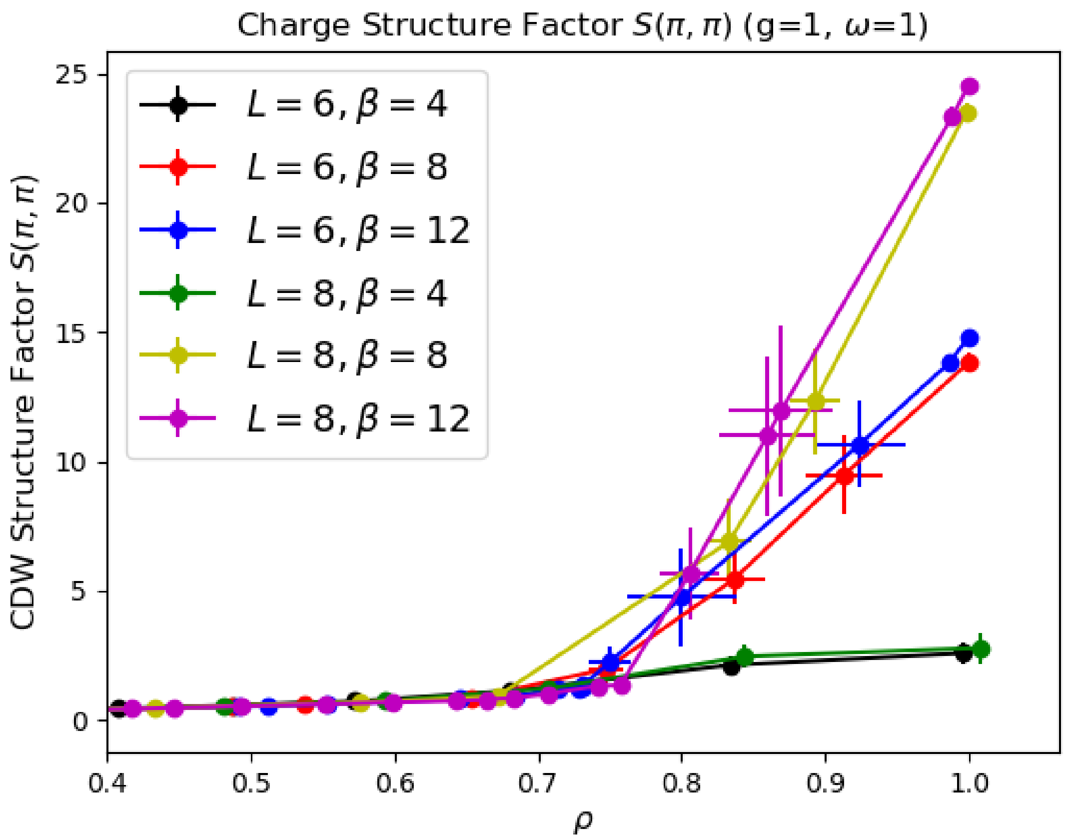
- Half-filling occurs when: $\mu = \dfrac{-\lambda^2}{\omega_0^2}$ $\quad \langle n \rangle \equiv \rho = 1$

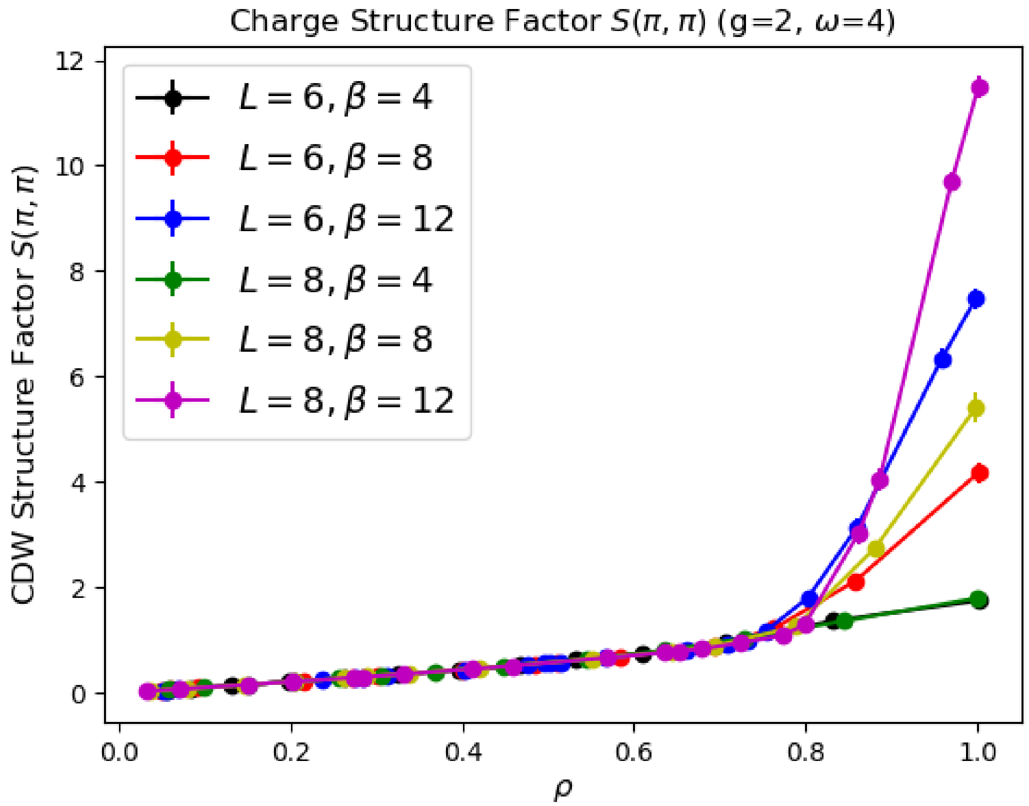
- Dope away from half-filling by varying chemical potential

- Study the competition between CDW order and SC order as system is doped away from half-filling. Focus on two parameter sets: $g = 1,\ \omega_0 = 1$ and $g = 2,\ \omega_0 = 4$

- Lattice sizes: $L = 6,\ 8,\ 10,\ 12$ Temperatures: $\beta = 1\text{–}28$

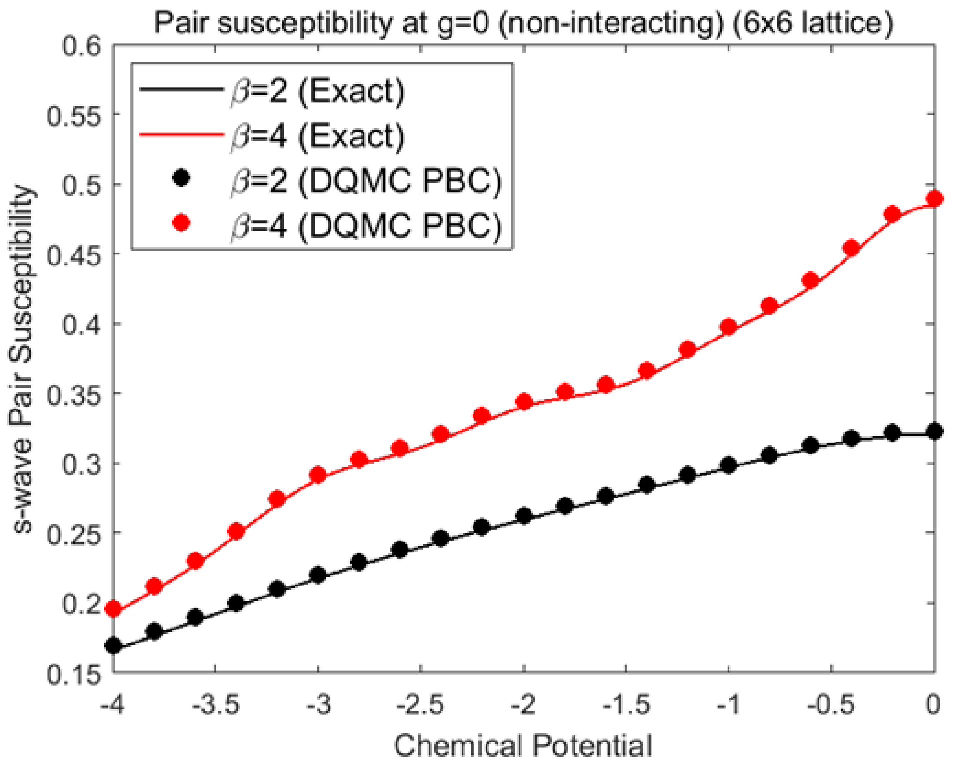
CDW structure factor vs density

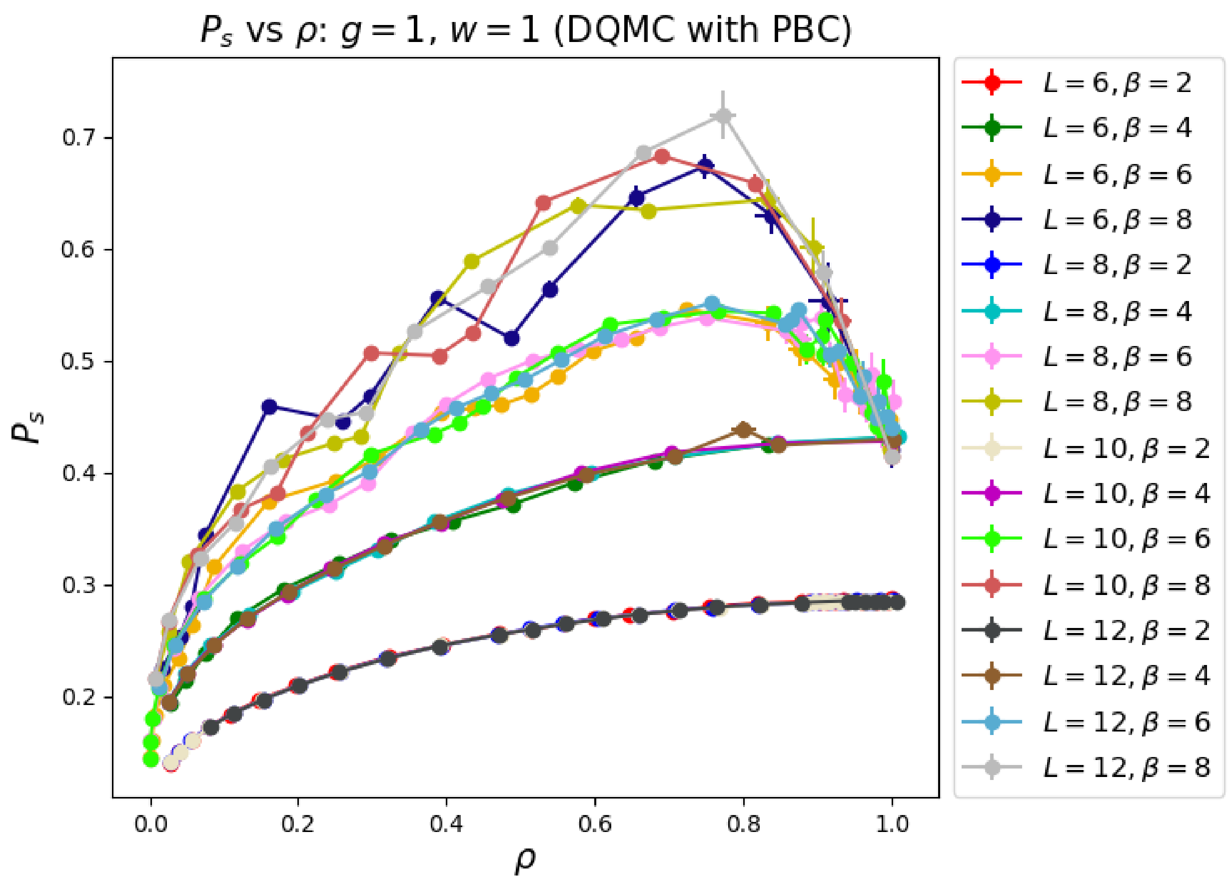




- $S(\pi, \pi)$ measures charge order on the square lattice (checkerboard CDW)
- CDW correlations decrease when doped away from half-filling
- CDW structure factor strongly suppressed for $\rho \lesssim 0.75–0.85$

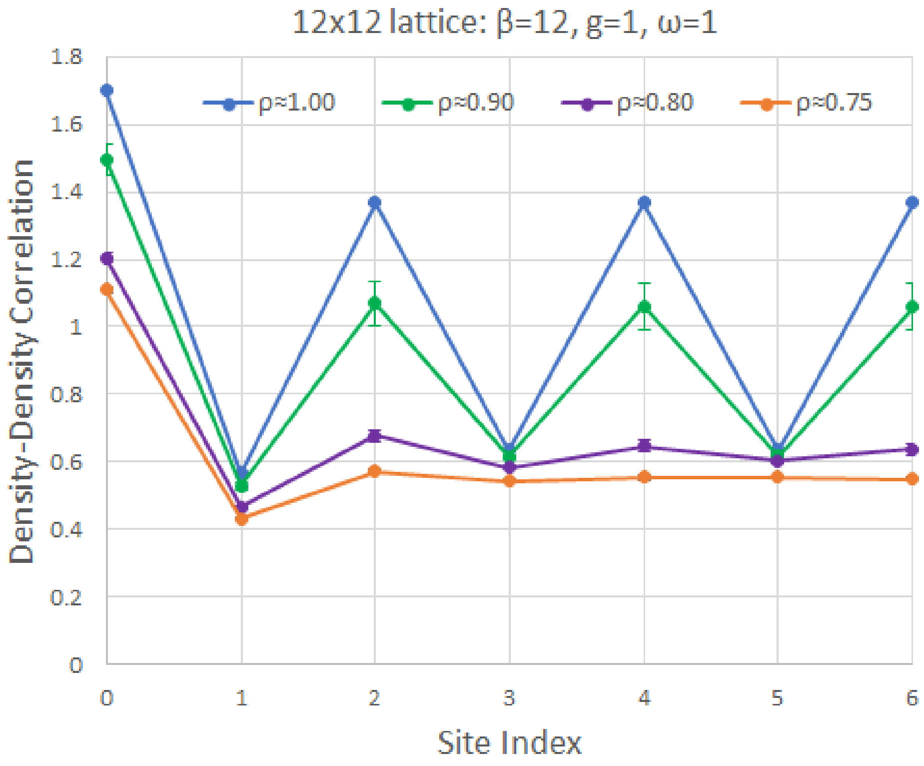
S-wave pair susceptibility vs density

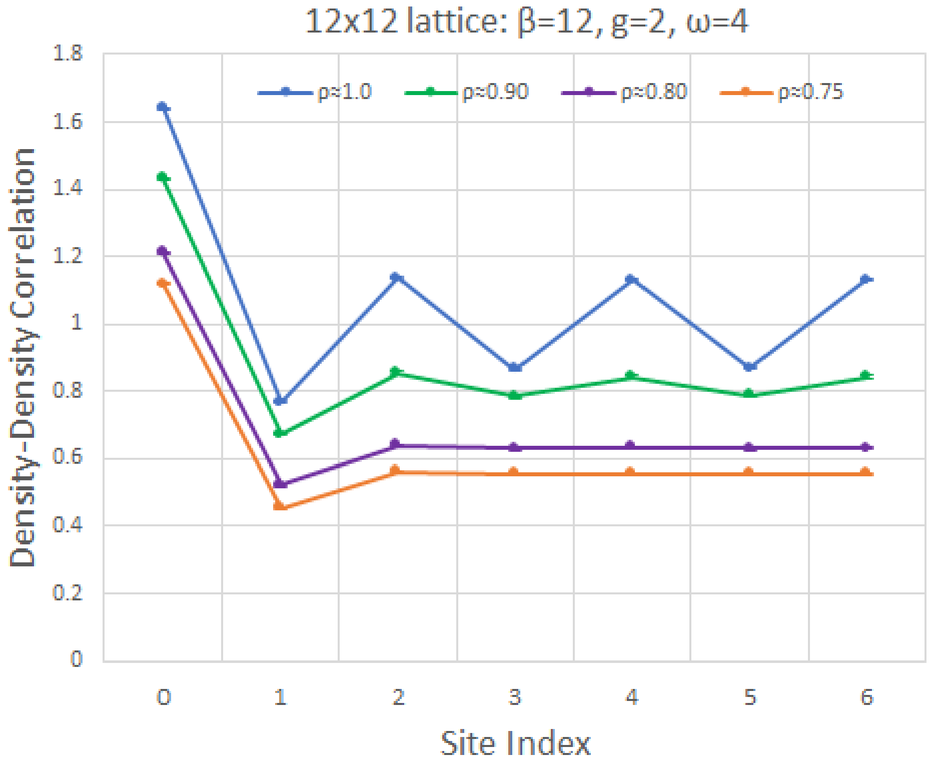




- Simultaneously, the pair susceptibility increases when doped away from half-filling. No longer suppressed by CDW.
- E.g. for g=1, ω=1 pair susceptibility peaks for $\rho \approx 0.6$–0.7
- Non-interacting (g=0) pair susceptibility agrees with DQMC data

Density-density correlations vs site index





- In checkerboard CDW phase at ρ=1 (half-filling)
- Away from half-filling, the CDW ordering weakens
- Increasing phonon frequency: Doping away from half-filling, CDW correlations become suppressed more quickly.
- Decreasing ω strengthens CDW correlations and weakens SC correlations.

SC Phase Transition:

$$P_s = \frac{1}{N}\int_0^\beta \langle \Delta(\tau)\Delta^\dagger(0)\rangle \qquad \Delta(\tau) = \sum_{\mathbf{i}} c_{\mathbf{i}\downarrow}(\tau)c_{\mathbf{i}\uparrow}(\tau)$$

- SC order parameter has a U(1) symmetry putting it in the same universality class as the 2D XY model
- The 2D superconducting transition should be in Kosterlitz-Thouless universality class:

$$T \to T_c^+ : \quad P_s \sim \xi^{2-\eta} \quad \eta = 1/4 \qquad \xi \sim \exp\left(At^{-1/2}\right) \qquad t \equiv \frac{T - T_c}{T_c}$$

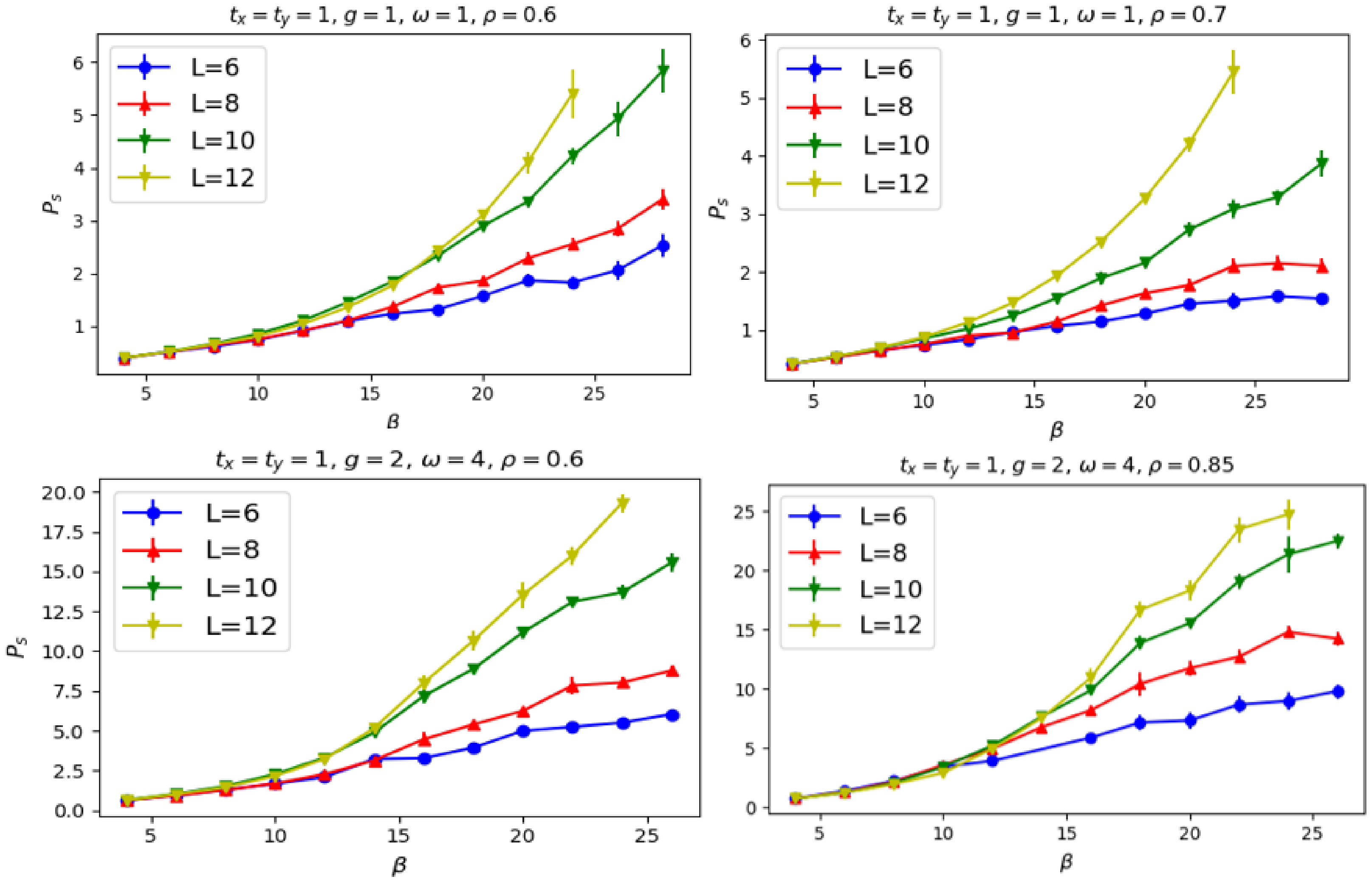
- Scaling hypothesis: For finite size system of size *L*, an observable which diverges at *Tc* (in the thermodynamic limit) should scale as a power of *L* multiplied by a function of *L/ξ*

$$P_s = L^{2-\eta} f\left(\frac{L}{\xi}\right) \Longrightarrow P_s = L^{7/4} f\left(L\exp[-A(T-T_c)^{-1/2}]\right) \Longrightarrow P_s L^{-7/4} = f\left(L\exp[-A(T-T_c)^{-1/2}]\right)$$

- Finite-size scaling: For different lattice sizes L, plotting $P_s L^{-7/4}$ as a function of $L\exp[-A(T-T_c)^{-1/2}]$ should result in data collapse onto a single curve. Can find estimate of T_c.

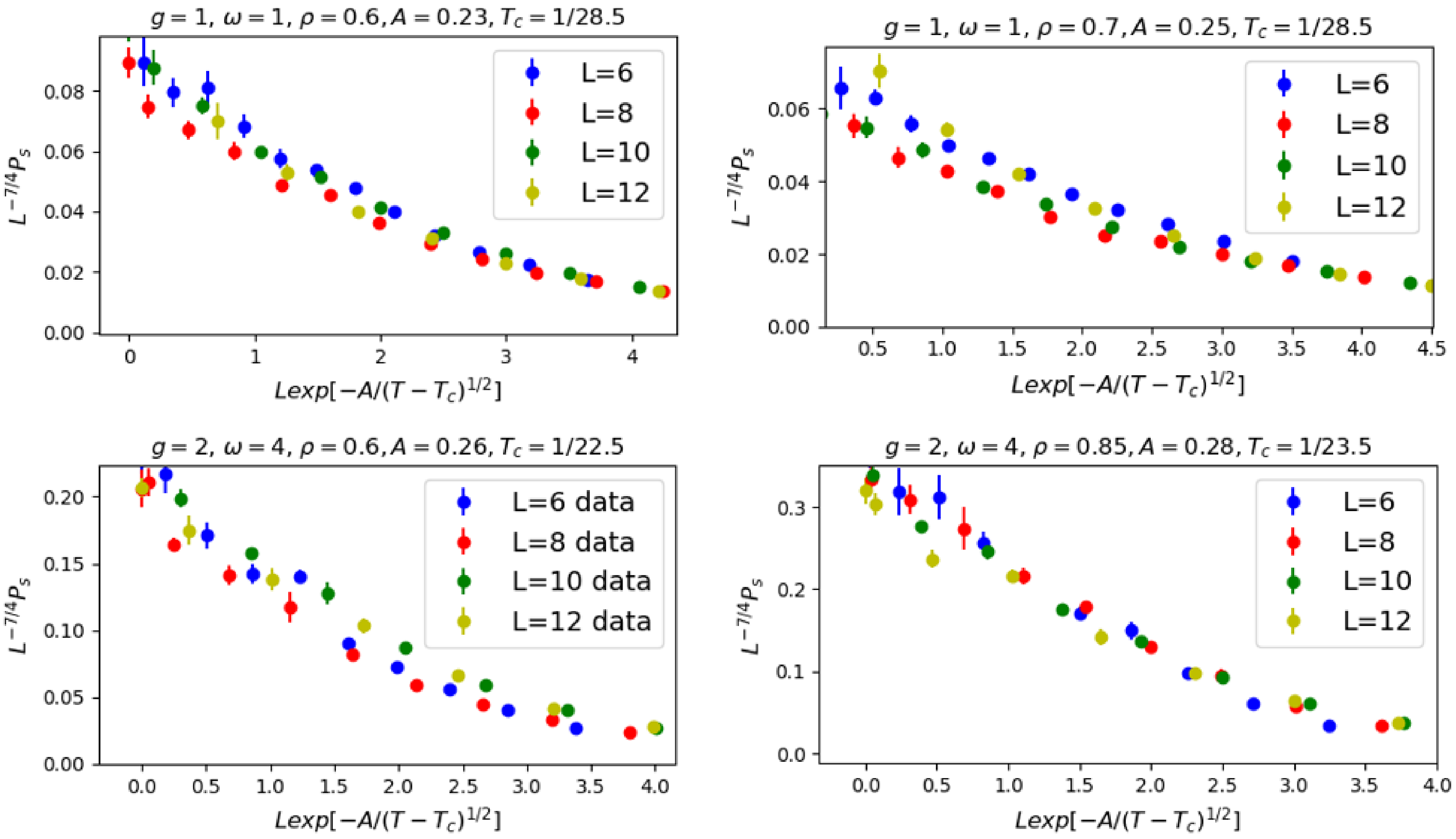
- Note: Below T_c, ξ diverges but is limited by *L* in a finite-size system. Expect: $P_s \sim L^{2-\eta}$

S-wave pair susceptibility vs temperature



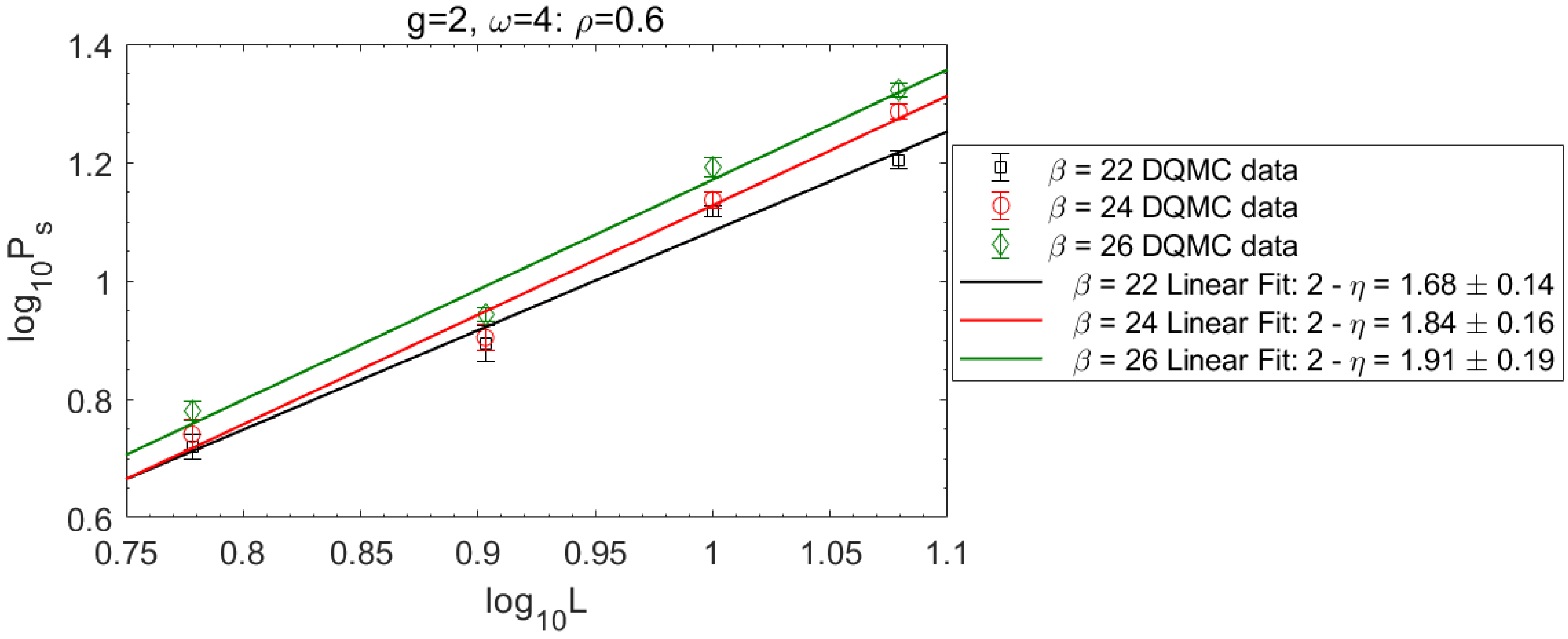
- S-wave pair susceptibility versus beta for g=1, ω=1 (top) and g=2, ω=4 (bottom), at fixed density.
- For g=1, ω =1 the density is fixed at ρ=0.6 and ρ=0.7, and for g=2, omega=4 the density is fixed at ρ=0.6 and ρ=0.85.
- Plots show size-independence at high temperature, and size-dependence at low temperature suggesting that a scaling analysis can be applied to find *Tc*.

S-wave pair susceptibility data collapse



- For the two densities at g=1, ω=1 the data collapses at around $T_c \approx 1/28.5$
- For the two densities at g=2, ω=4 the data collapses for $T_c \approx 1/22.5 - 1/23.5$
- These values of T_c are only approximate as we are quite limited by the range of lattice sizes we can study.

For $T < T_c$: $P_s \sim L^{2-\eta} \Longrightarrow \log(P_s) \sim (2-\eta)\log(L)$



- Plot is linear: confirms system is in SC phase
- However studying larger system sizes (*L* > *12*) is not feasible at such low temperatures using DQMC

Summary:

- Finding estimates of T_c for superconducting transition in the Holstein model is difficult, but possible with DQMC
- Obtained estimates of T_c for different values of electron-phonon coupling and phonon frequency, at fixed densities away from half-filling. Previous studies unable to perform scaling analysis!
- Increasing phonon frequency enhances SC response, lowers T_c

Future work:

- Doped Holstein model on square lattice: Estimates of T_c for $\omega < t$
- Newly developed algorithms for Holstein model on cubic lattice.
  Possible to find SC transition when doped away from half-filling?

Thank you!