UCDAVIS

Langevin simulations of the Half-Filled Cubic Holstein Model

- Holstein Hamiltonian- Polarons and Pairing
- Holstein Hamiltonian- Charge Density Wave Order
- Langevin-based Quantum Monte Carlo Algorithm
- Honeycomb Lattice
- Cubic Lattice
- Conclusions

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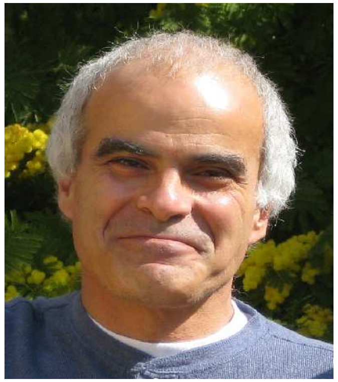
Ben
Cohen-Stead

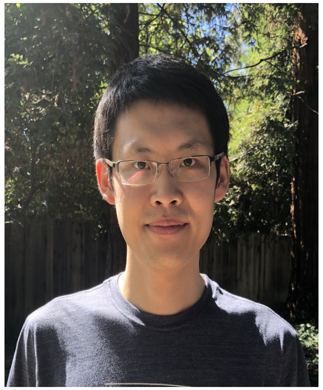
Kipton
Barros

Zi Yang
Meng

Chuang
Chen



George
Batrouni



Bo
Xiao

Yuxi
Zhang

WeiTing
Chiu

Natanael
Costa

Chunhan
Feng

Holstein Hamiltonian- Polarons and Pairing

Holstein: wave function a_i probability amplitude for (*single*) electron on site i.

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

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

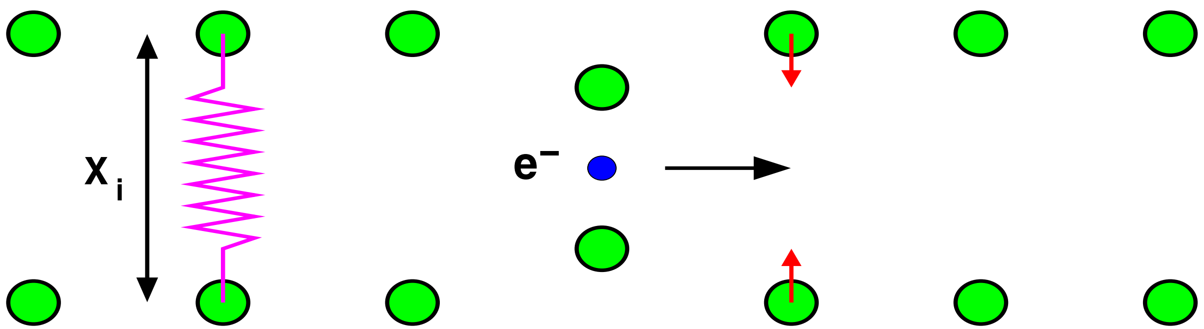
Spin $\uparrow, \downarrow$ electrons interact with boson displacement on site i

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

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.



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*

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

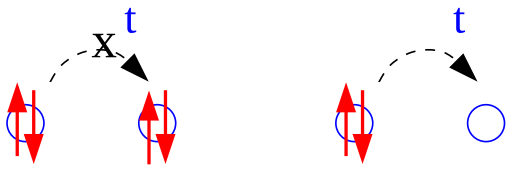
Imagine you are at half-filling. Then turn on t perturbatively.

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

Local pairs form.

Double occupied/empty alternation favored:

Charge Density Wave.

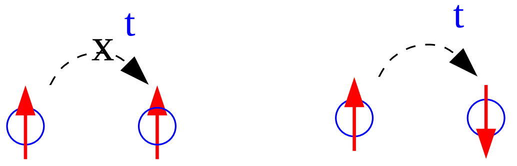


Repulsive interaction ($+U$ Hubbard):

Local moments form.

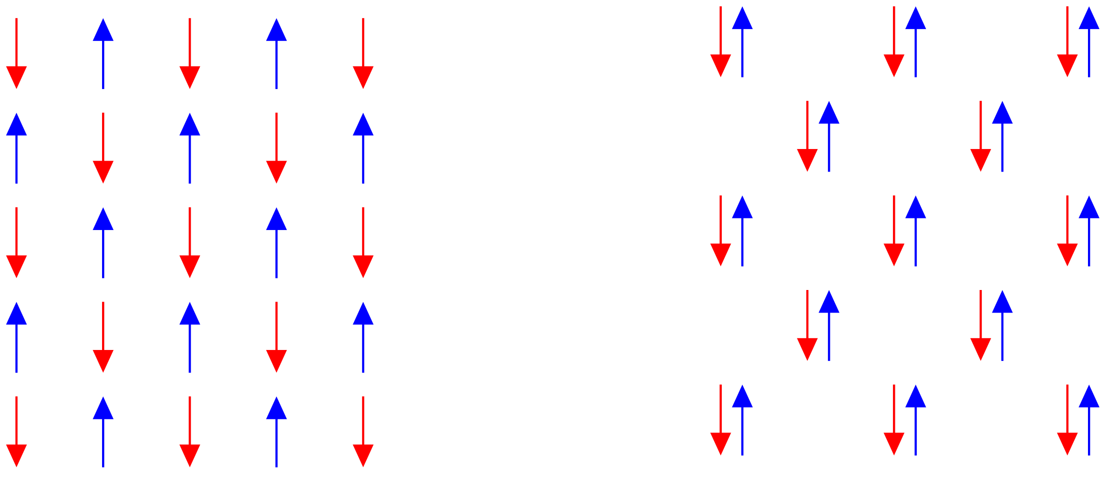
up/down spin alternation favored by J:

Antiferromagnetism.



Holstein Hamiltonian- Charge Density Wave Order

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 rerlatively recently!

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

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 β.

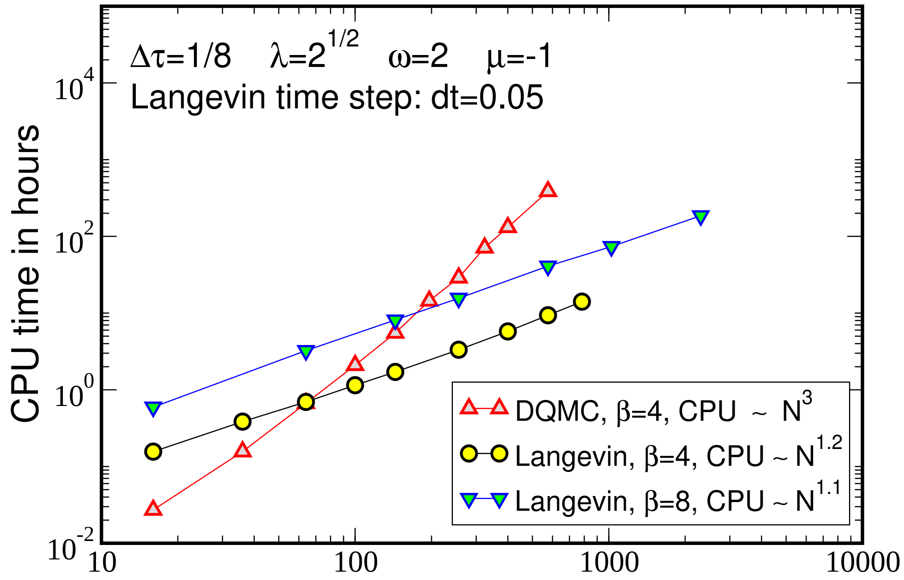
Does not work for Hubbard Model!

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

Number of conjugate gradient iterations grows catastrophically with β.

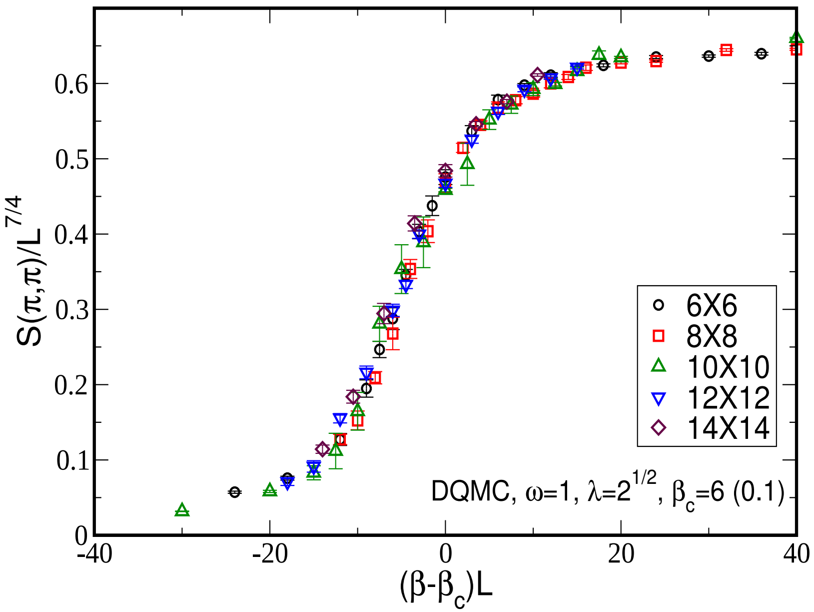
Key observation: $\hat{P}_i^2 \Rightarrow \left[\frac{X_i(\tau+\Delta\tau)-X_i(\tau)}{\Delta\tau} \right]^2$ moderates eigenspectrum of $\mathcal{M}$.

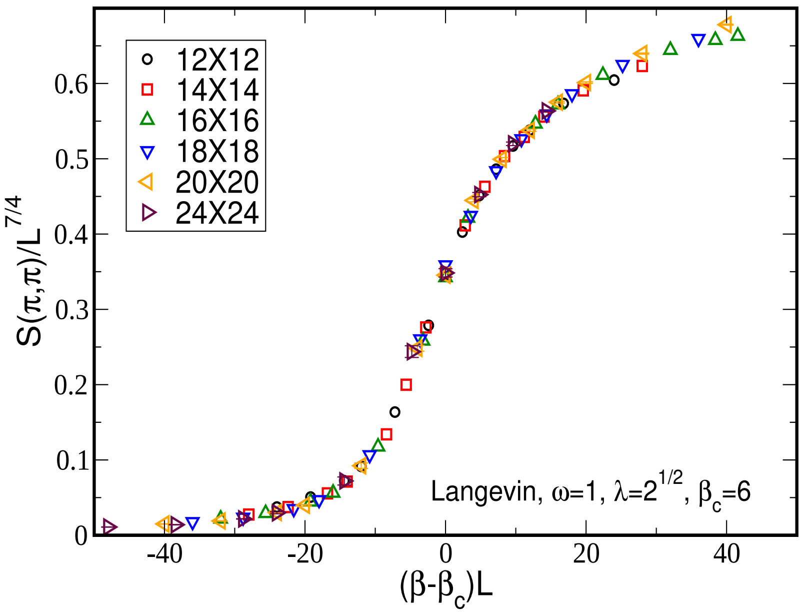
(No such term for auxiliary bosonic field in Hubbard model.)



<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).





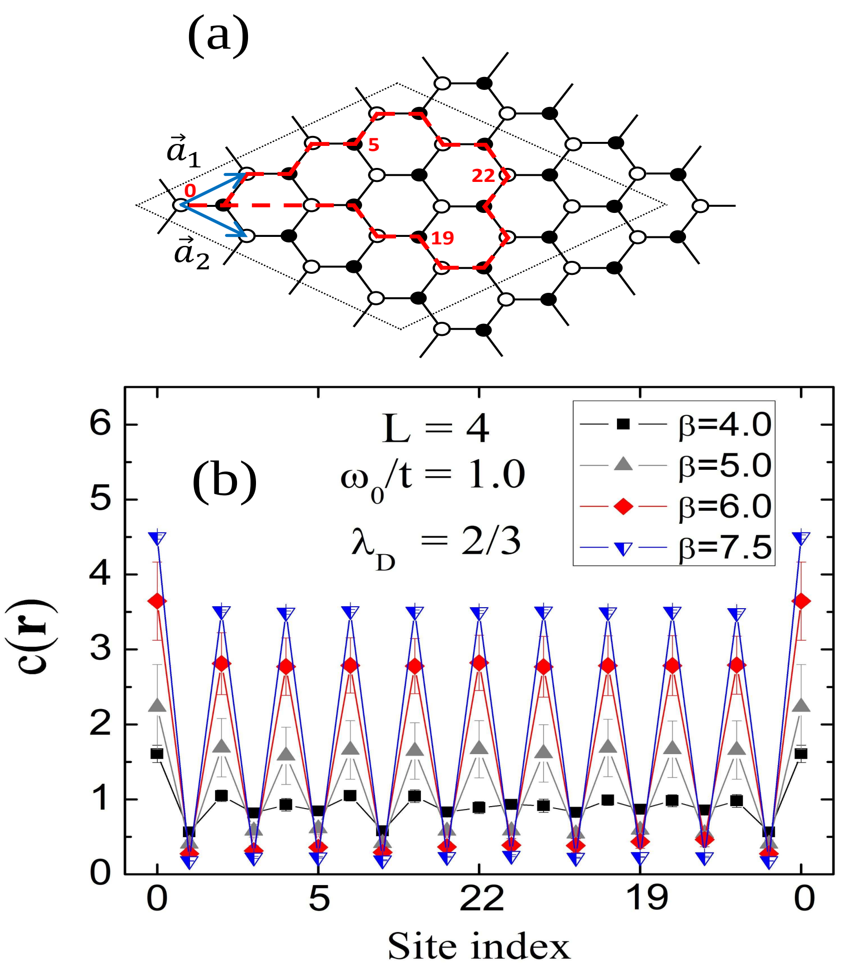
Honeycomb Lattice

Dirac spectrum for fermions.

Quantum critical point for Hubbard Model:

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

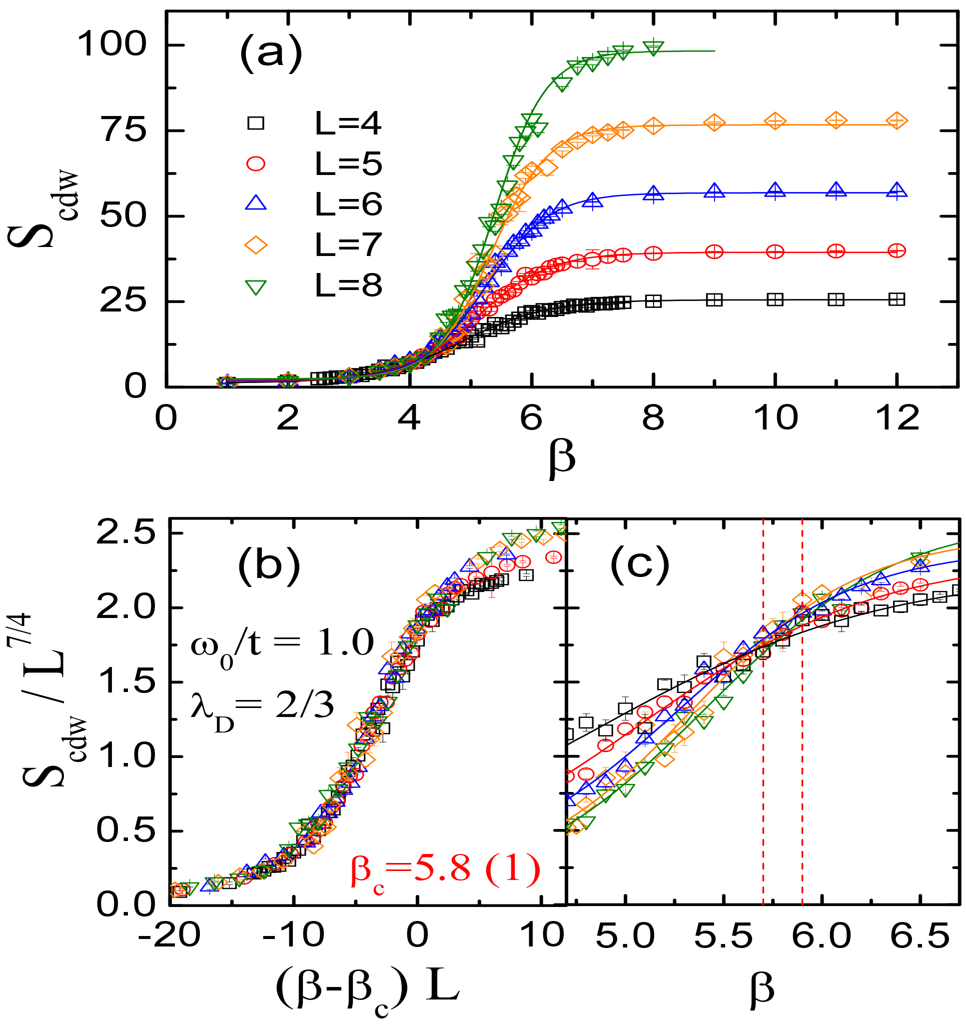
Effect of electron-boson interactions on Dirac fermions and charge order?



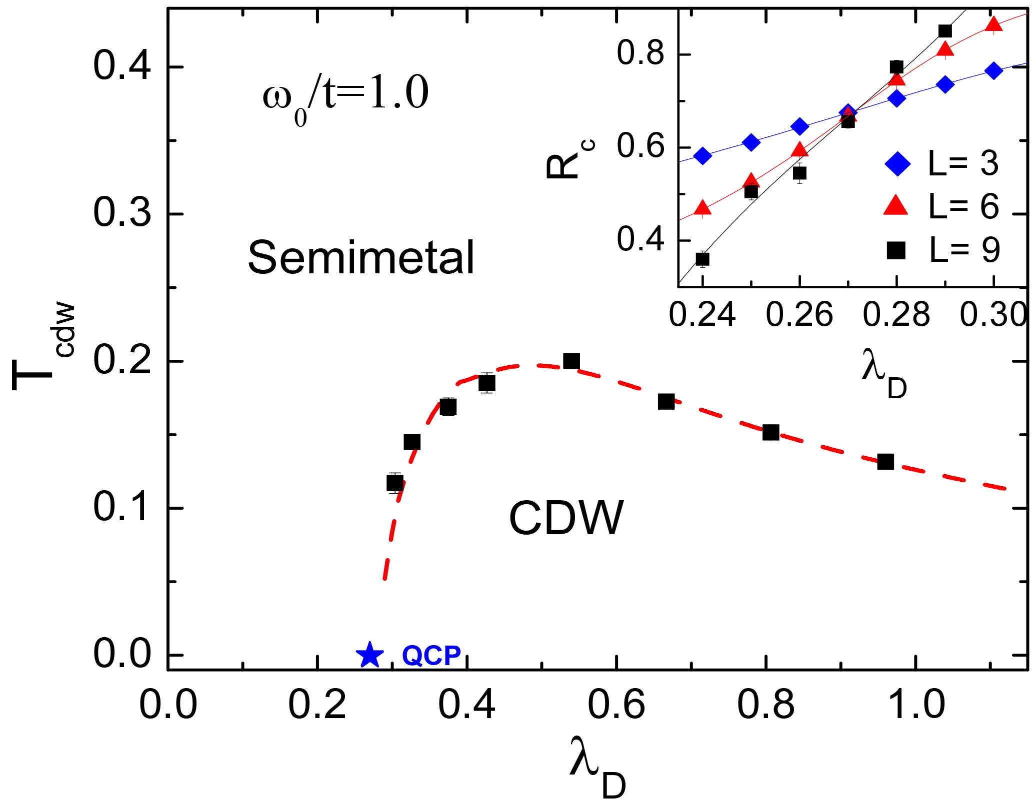
Long range real space charge correlations develop as β increases.

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

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

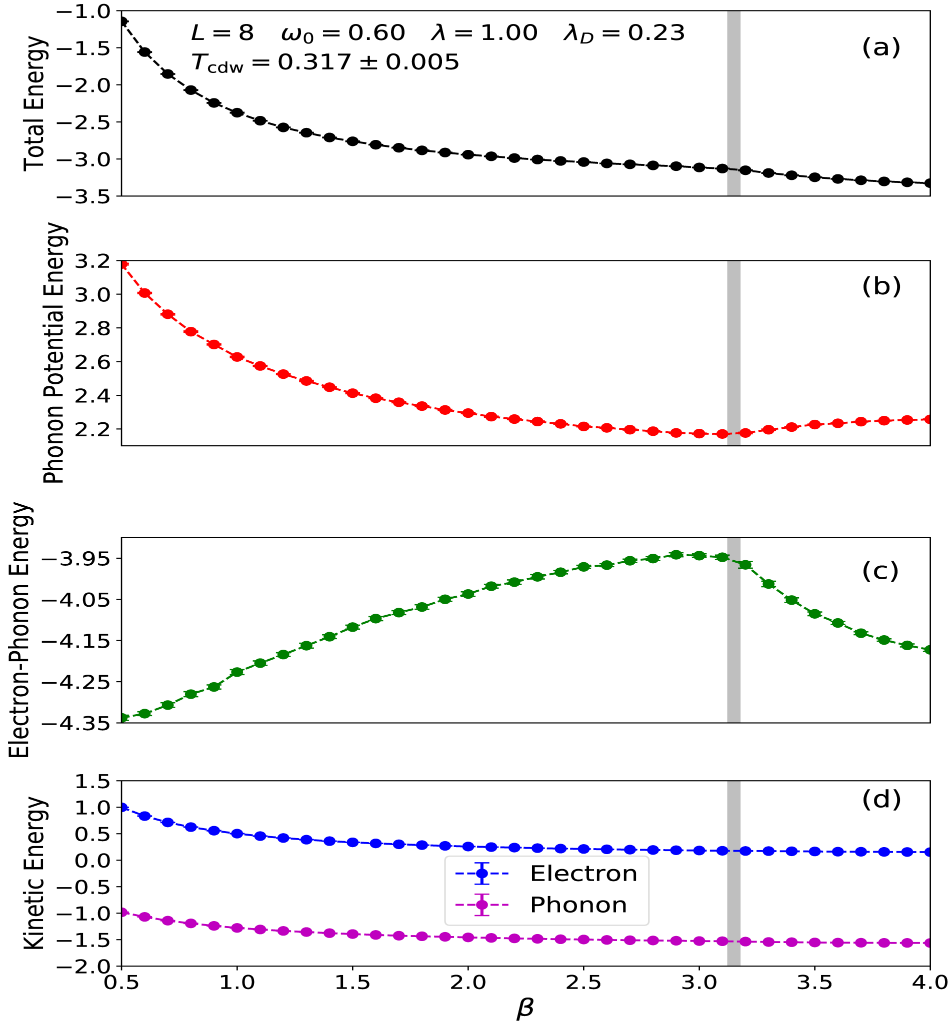
"Charge Order in the Holstein Model on a Honeycomb Lattice," Y.-X. Zhang, W.-T. Chiu, N.C. Costa, G.G. Batrouni, and RTS, Phys. Rev. Lett. 122, 077602 (2019).

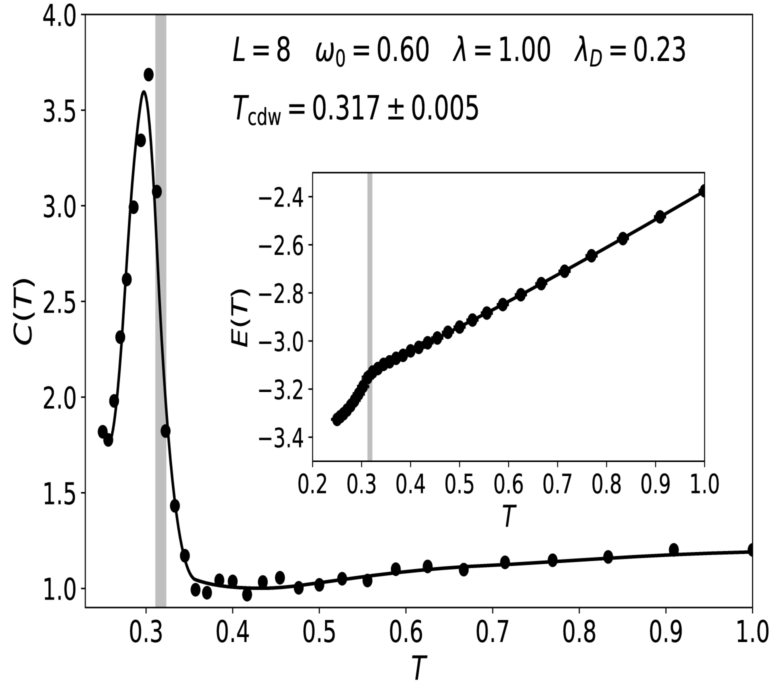
"Charge-Density-Wave Transitions of Dirac Fermions Coupled to Phonons," C. Chen, X.Y. Xu, Z.Y. Meng, and M. Hohenadler, Phys. Rev. Lett. 122, 077601 (2019).

Cubic Lattice

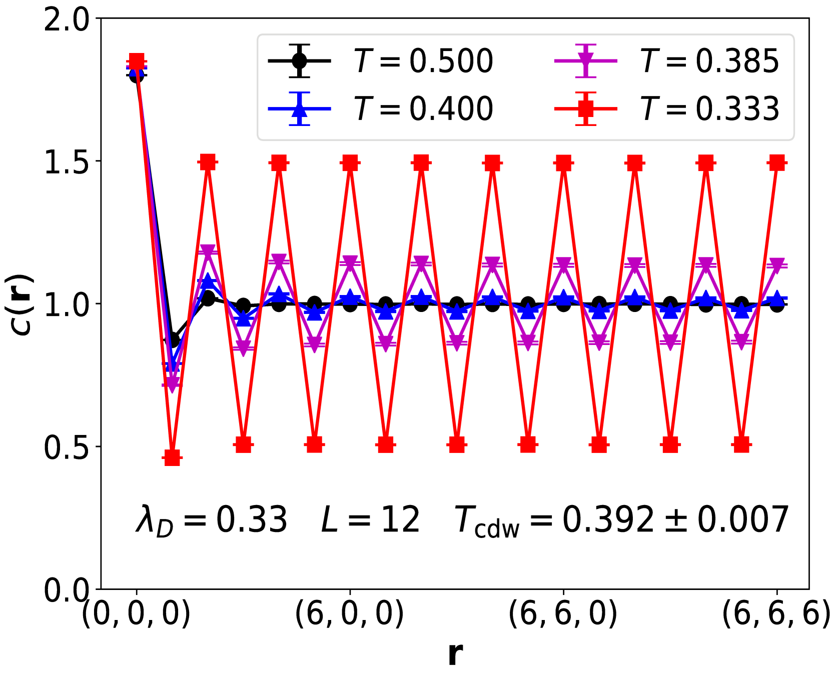
Thermodynamics

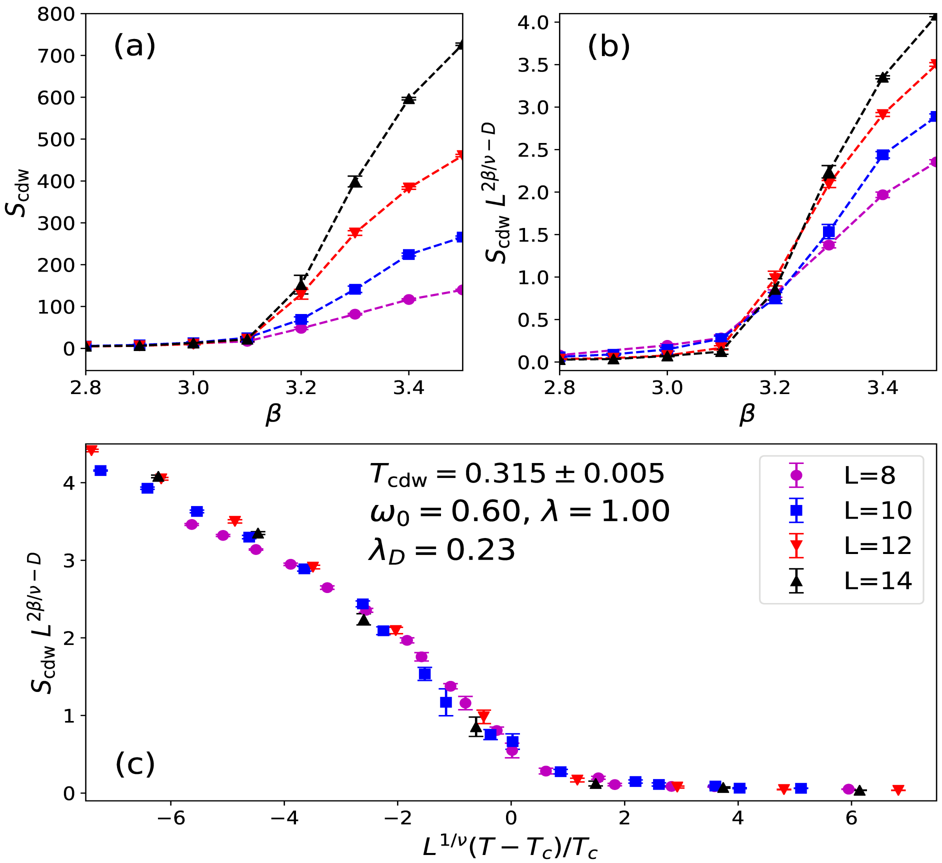
Structure in Energies $\rightarrow$ peak in specific heat



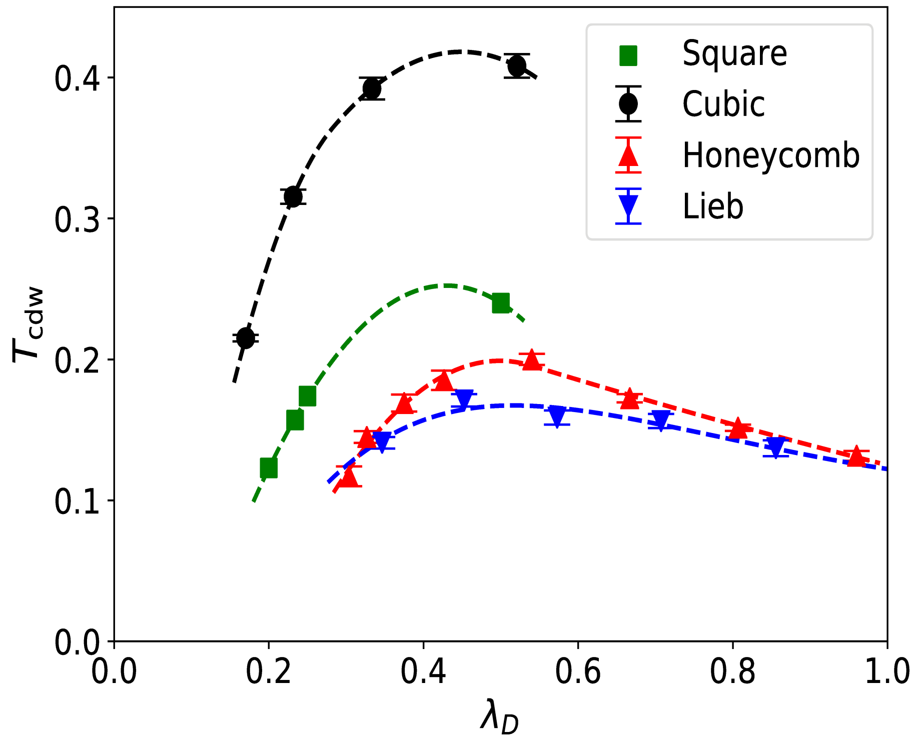


Real space density correlations and structure factor.





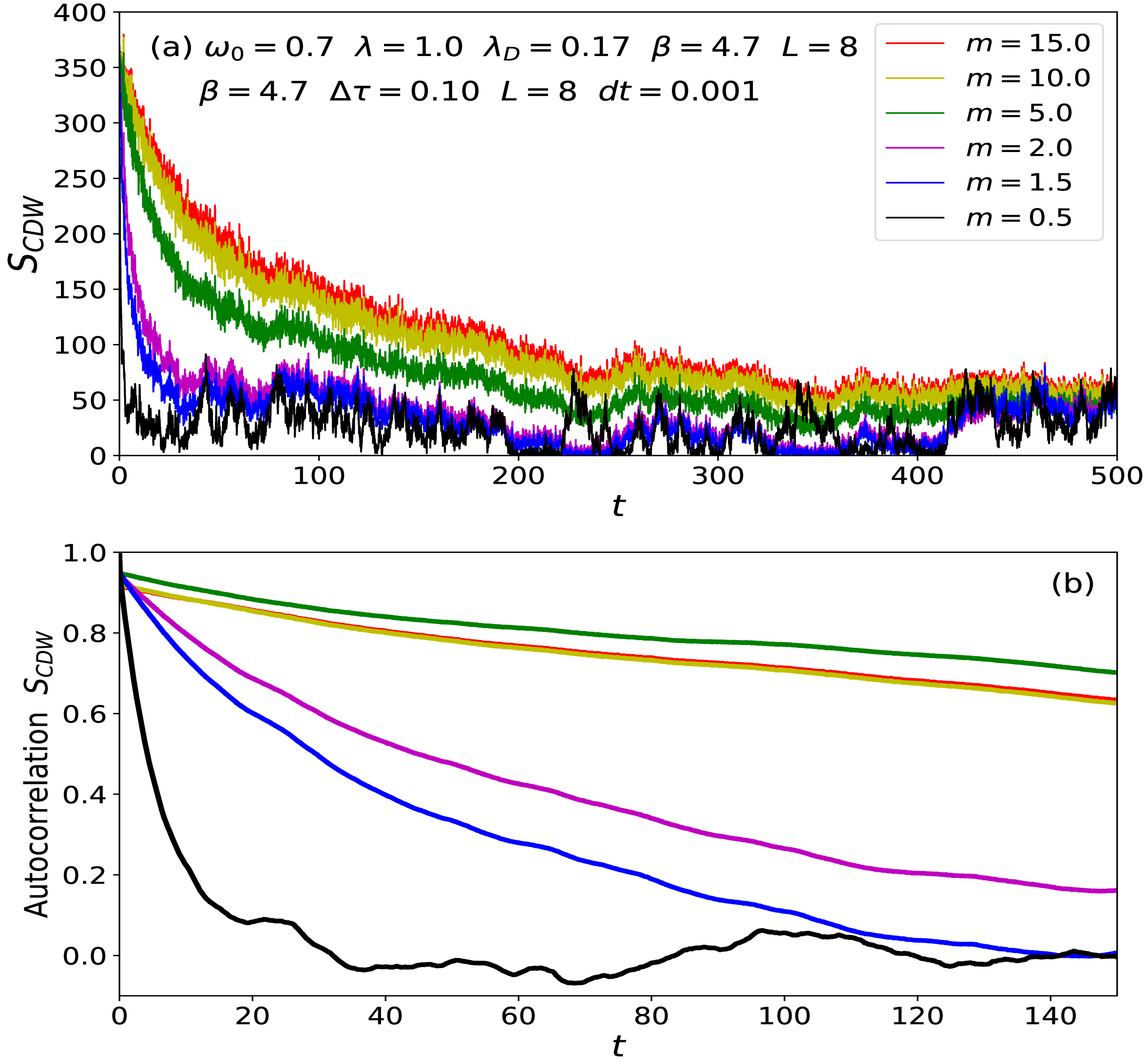
Conclusions



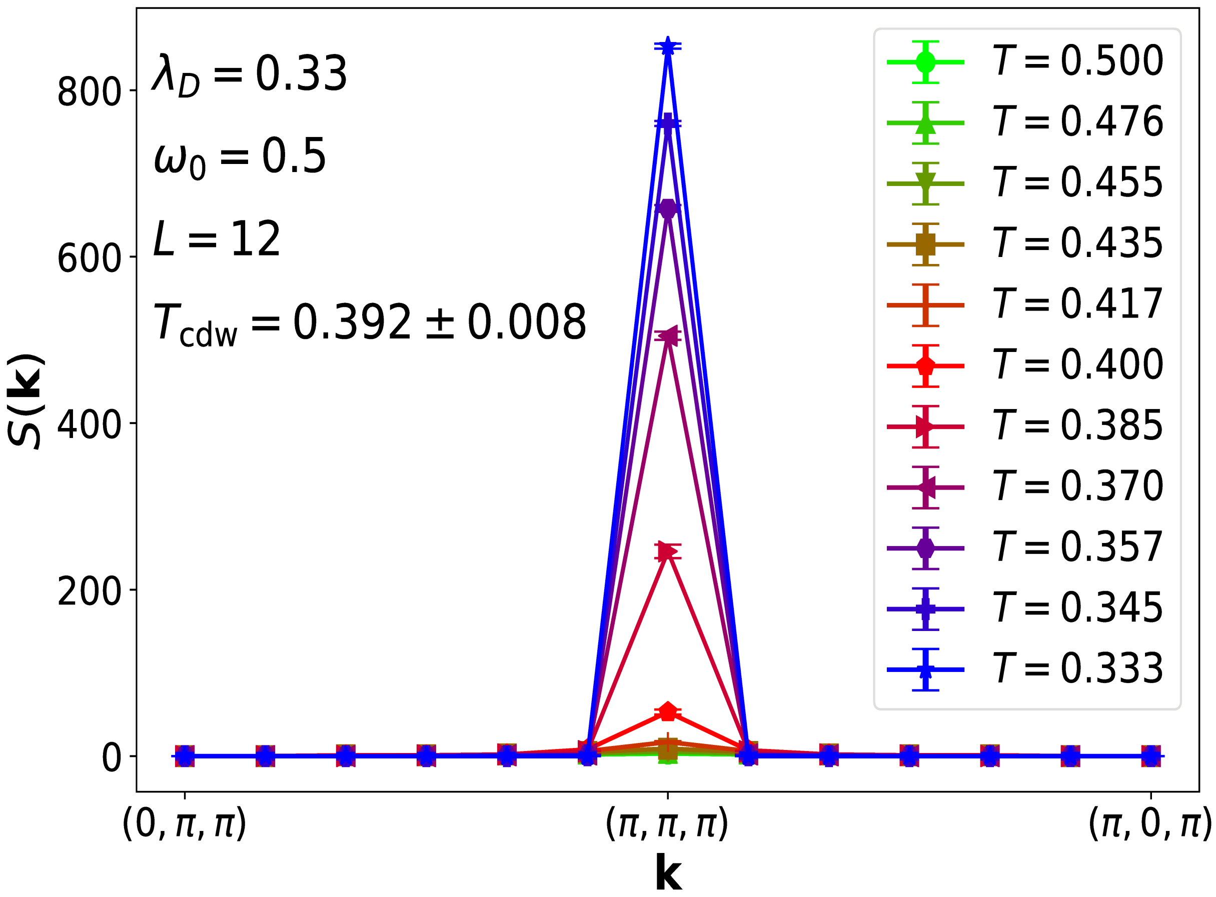
- At half-filling, Holstein model in $d > 1$ undergoes a finite temperature phase transition to state with long range charge order $K_* = (\pi, \pi)$.
- Critical temperature has a maximum at intermediate el-ph coupling λ_D.

"Langevin Simulations of the Half-Filled Cubic Holstein Model", B. Cohen-Stead, K. Barros, Z.Y. Meng, Chuang Chen, and R. Scalettar, Phys. Rev. B102, 161108R (2020).

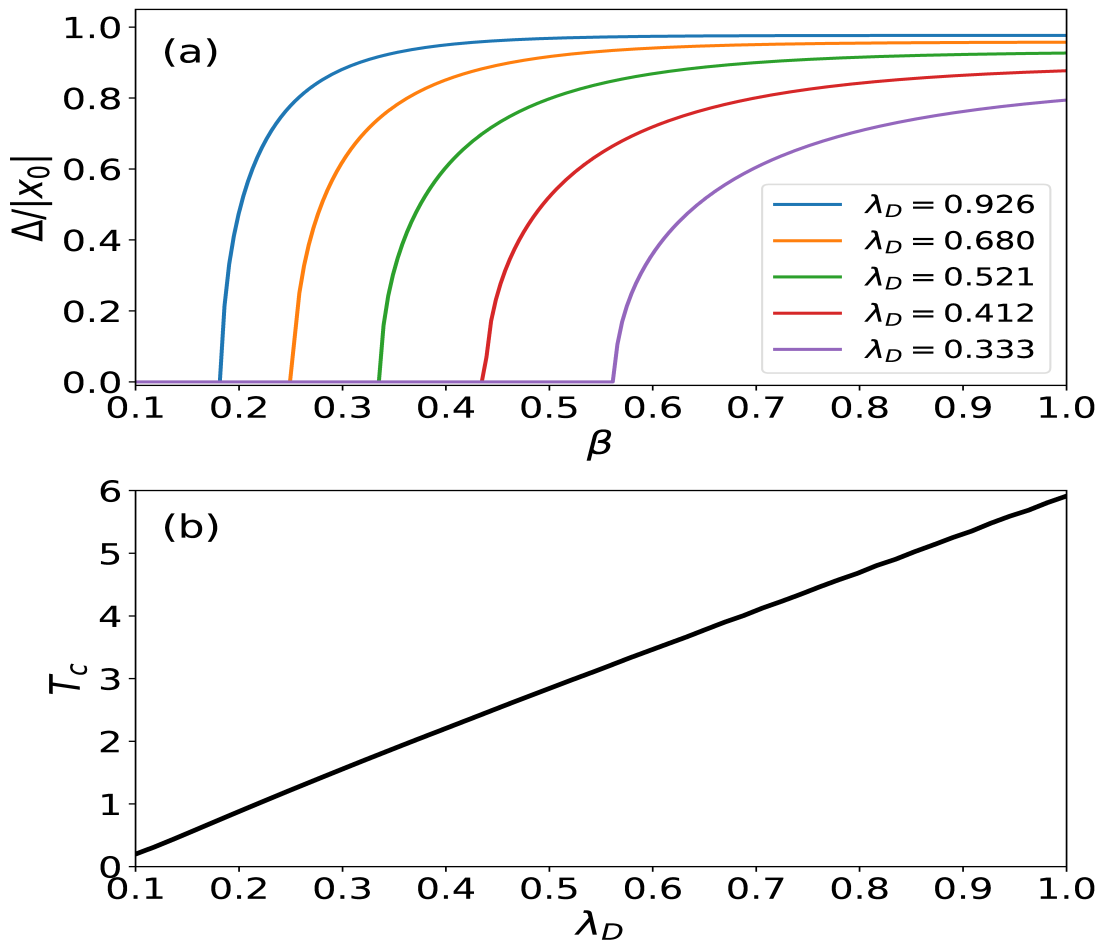
Autocorrelations in Langevin Simulations:



Momentum Dependence of Structure Factor

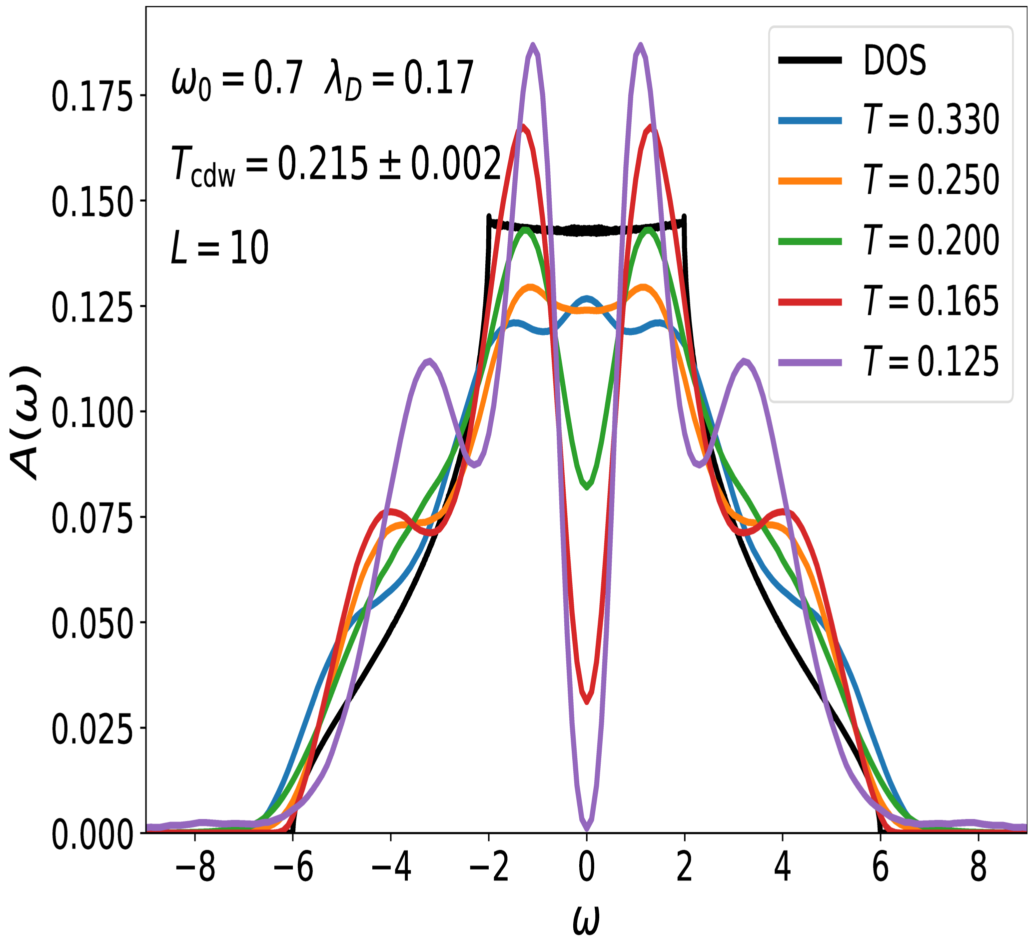


CDW Transition in Mean Field Theory



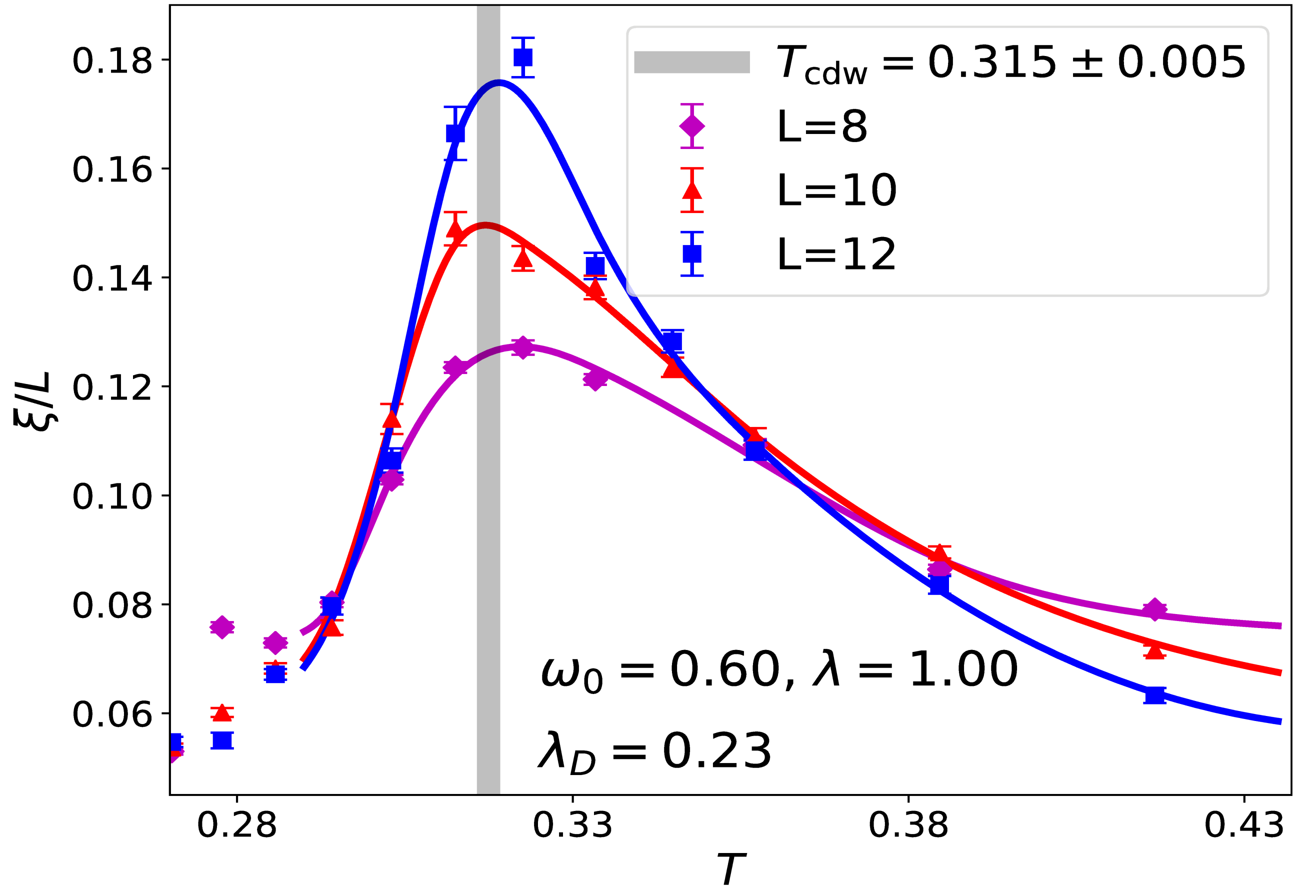
Overestimates transition temperature: $T_c = \beta_c^{-1} \sim (2-5)t$

Spectral Function



Gap opens below T_c

Correlation Length:



Momentum Dependence of Structure Factor