Temperature-Doping Phase Diagram of the 2D Holstein Model

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Model and Methods

$$\hat{H} = -\sum_{\langle i,j\rangle,\sigma} t_{i,j}\,\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} - \mu\sum_{i,\sigma}\hat{n}_{i,\sigma} + \sum_{i}\left[\frac{\hat{P}_i^2}{2M} + \frac{1}{2}M\Omega^2\hat{X}_i^2\right] - \sum_{i,\sigma} g\left(\hat{n}_{i,\sigma} - \frac{1}{2}\right)\hat{X}_i$$

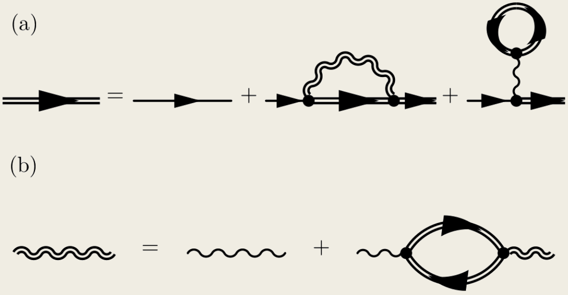


Figure: P. Dee, *et. al.* (To be published)

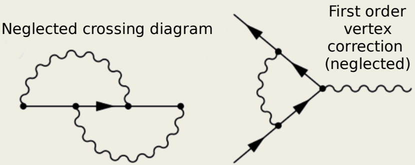
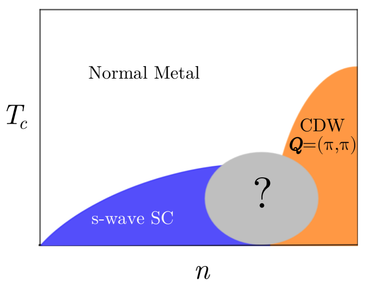


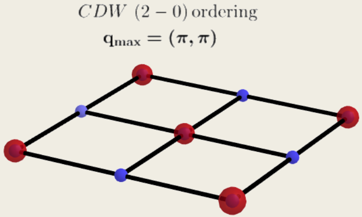
Figure: Y. Wang, *et. al.* (2016) Superconductor Science and Technology. 29

- Migdal's Approx: $\Gamma \sim \lambda\Omega/E_F \sim \sqrt{m/M} \sim 0.01$ where $\lambda = g^2/(W\Omega^2) = 0.3$

What we know and what we don't.

- Holstein exhibits metal-insulator transition as function of doping[1].
- Peierls-CDW at half-filling and s-wave SC at lower doping[1].
- NNN hopping enhances pairing correlations[2]
- What is the nature of phase boundary (T_c vs. $\langle n \rangle$)?
- Is there a SC dome?





[1] R. Noack. *et al.*, Phys. Rev. Lett. **66**,778-781 (1991)

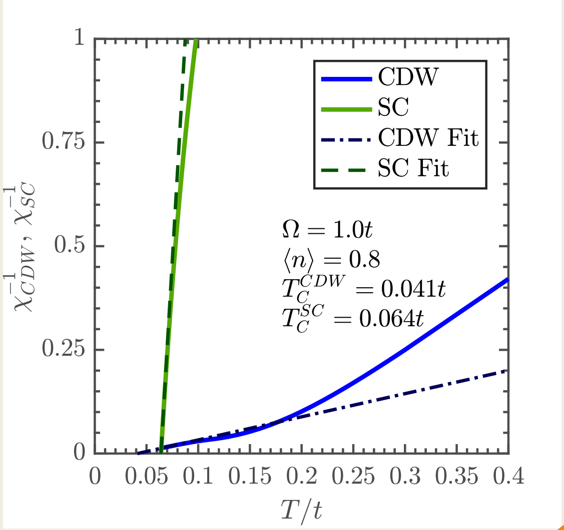
[2] Hirsch, J. E. *et al.* (1986) Phys. Rev. Lett., **56**, 2732-2735.

How do we obtain T_c?

- Extrapolate inverse susceptibilities.
- Works well for χ^{SC}.
- χ^{CDW} is expected to obey Ising universality class

$$\chi^{\text{CDW}} \propto \left|\frac{T - T_c}{T_c}\right|^{-7/4}$$

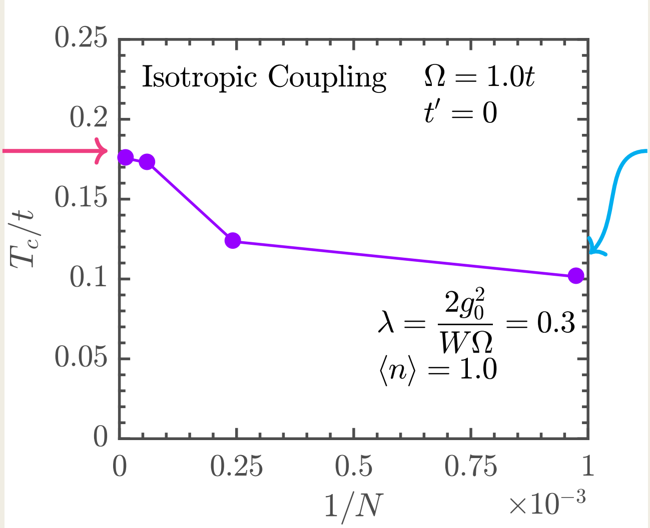
- We notice significant finite size effects in χ^{CDW}.



Finite-size effects on T_c: $L = \sqrt{N} = 256, 128, 64,$ and 32

$T_c^{\text{CDW}}(L \geq 128)$

$\approx \lim_{L\to\infty} T_c^{\text{CDW}}(L)$

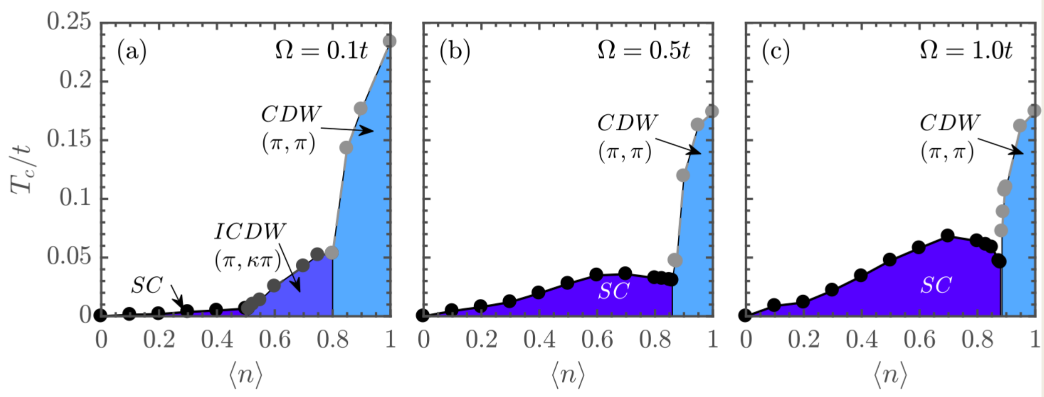


Most finite size calculations are even smaller

$L < 32$ poorly represented by Ising-like susceptibility fit.

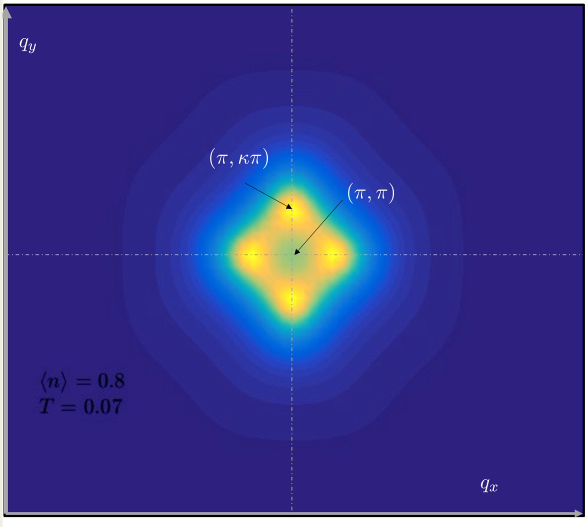
ME Theory Phase Diagram

Isotropic e-ph coupling and NN hopping only. All points obtained from lattice sizes $\geq 128 \times 128$.

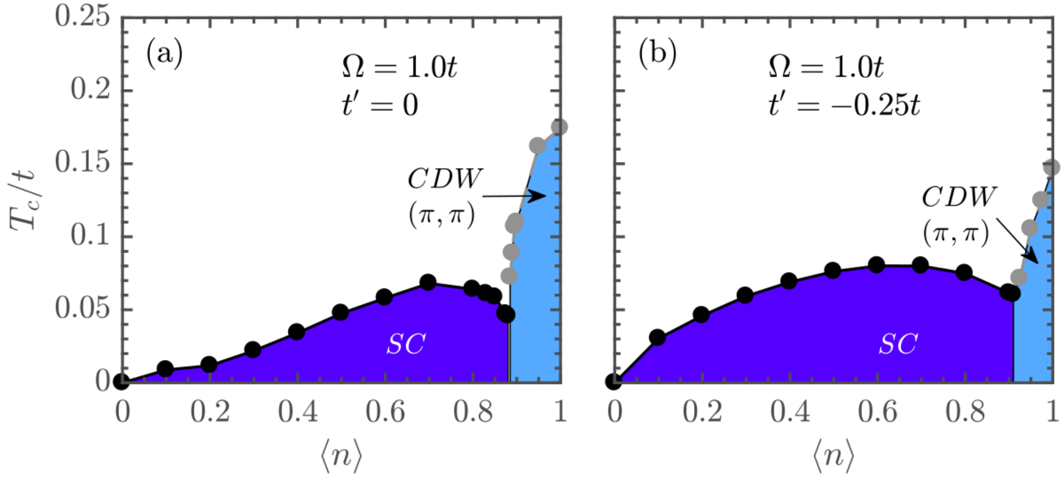


The SC region is not simply monotonic as expected for conventional SC, rather we get a dome-like structure.

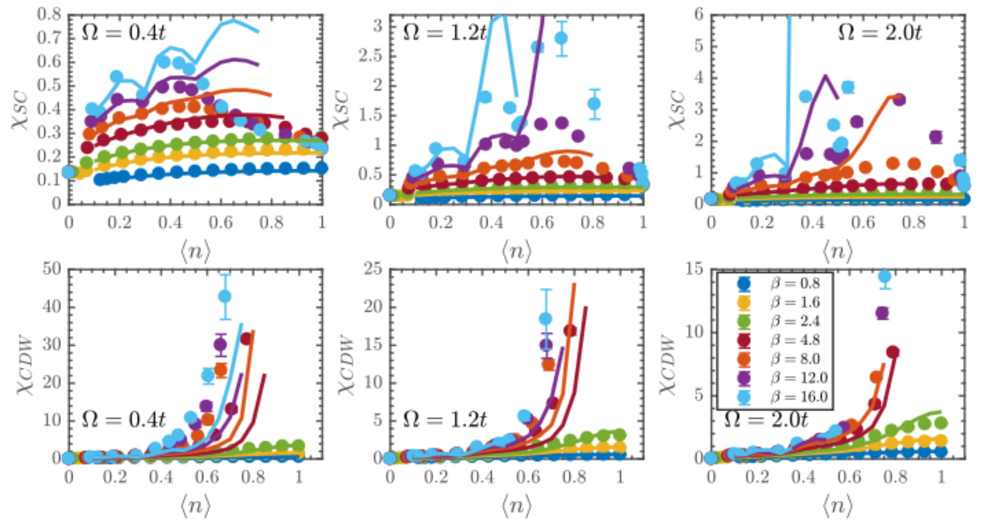
Incommensurate Peaks in $\chi^{\text{CDW}}(\mathbf{q})$



Addition of NNN Hopping



Results: DQMC vs. ME Theory $\lambda = 0.30$ (12×12)



Conclusion and Further Questions

...on the phase diagram

- Distinct CDW phase near half-filling and s-wave SC phase away from half-filling.
- SC enhanced by increasing phonon frequency and NNN hopping. CDW is suppressed by both.
- Non-monotonic behavior seen in SC phase. **Will it remain even with vertex corrections?**

...on our method

- Access to large finite clusters $\sim 256 \times 256 \rightarrow$ largest value tested.
- Qualitatively agrees with DQMC on most doping, but overestimates T_c on the average.

Thank you for your attention!

The finite-temperature Green's function

Imaginary time-ordering operator

Fermion operators: $\hat{c}_{\mathbf{k},\sigma}(\tau) = \mathrm{e}^{\hat{\mathsf{H}}\tau}\hat{c}_{\mathbf{k},\sigma}\mathrm{e}^{-\hat{\mathsf{H}}\tau}$

$$\mathcal{G}_{\sigma,\sigma'}(\mathbf{k},\tau;\mathbf{k}',\tau') = -\left\langle \hat{T}_\tau \hat{c}_{\mathbf{k},\sigma}(\tau)\hat{c}^\dagger_{\mathbf{k}',\sigma'}(\tau') \right\rangle$$

$$= -\mathrm{Tr}\left[\hat{\rho}\,\hat{T}_\tau\left\{\hat{c}_{\mathbf{k},\sigma}(\tau)\hat{c}^\dagger_{\mathbf{k}',\sigma'}(\tau')\right\}\right]$$

Statistical operator: $\hat{\rho} = \mathrm{e}^{-\beta(\hat{\mathsf{H}}-\hat{\Omega})}$

$$\mathcal{G}_{\lambda,\lambda'}(\mathrm{i}\omega_n) = \frac{1}{\beta}\int_0^\beta \mathcal{G}_{\lambda,\lambda'}(\tau)\mathrm{e}^{\mathrm{i}\omega_n\tau}, \quad \text{where} \quad \omega_n = \frac{(2n+1)\pi}{\beta} \quad \text{(fermions)}$$

Working in Momentum space

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \Omega \sum_{\mathbf{k}} \left(\hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} + \frac{1}{2} \right)$$
$$- \frac{g}{\sqrt{2N_s M \Omega}} \sum_{\mathbf{k},\mathbf{k}',\sigma} \left(\hat{a}_{\mathbf{k}'-\mathbf{k}} + \hat{a}^\dagger_{-(\mathbf{k}'-\mathbf{k})} \right) \hat{c}^\dagger_{\mathbf{k}',\sigma} \hat{c}_{\mathbf{k},\sigma}$$

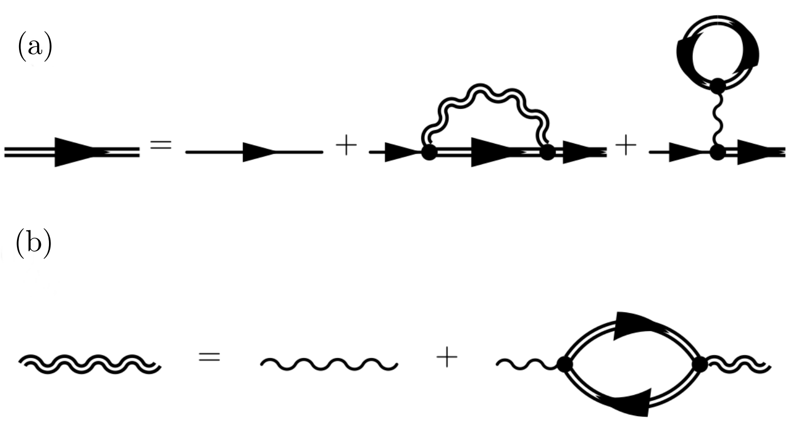
- Electron dispersion:

$$\epsilon_{\mathbf{k}} = -2t \left(\cos(k_x d) + \cos(k_y d) \right) - \left(\mu - \frac{\alpha^2}{K} \right).$$

- We will use finite temperature many-body Green's functions to make equilibrium calculations.

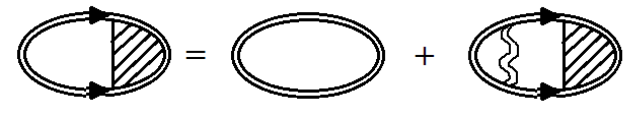
$$\mathcal{G}_\sigma(\mathbf{k}, i\omega_n) = [i\omega_n - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\mathbf{k}, i\omega_n)]^{-1}$$
$$\mathcal{D}(\mathbf{q}, i\nu_n) = \left[-M(\Omega^2 + \nu_n^2) - \Pi(\mathbf{q}, i\nu_n) \right]^{-1}$$

Propagators in Migdal Theory



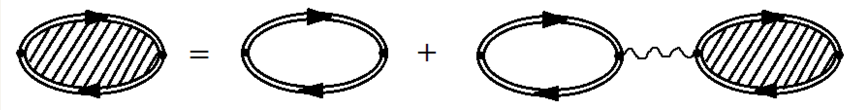
Susceptibilities

- Singlet Pairing (SC) Susceptibility



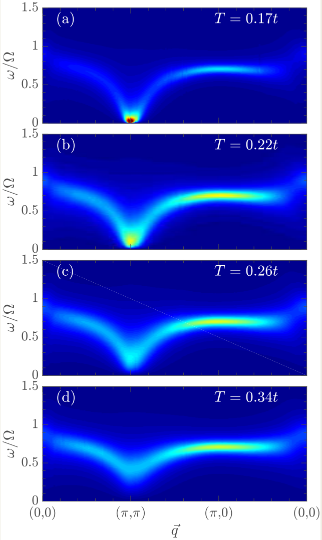
$$\chi^{\mathrm{SP}}(\mathbf{q}=0) = \frac{1}{N}\sum_{i,j}\int_0^\beta \mathrm{d}\tau \,\langle\, \hat{c}_{i\uparrow}(\tau)\hat{c}_{i\downarrow}(\tau)\hat{c}^\dagger_{j\downarrow}(0)\hat{c}^\dagger_{j\uparrow}(0)\,\rangle$$

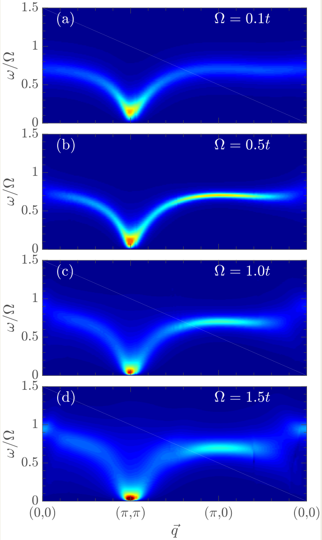
- CDW Susceptibility



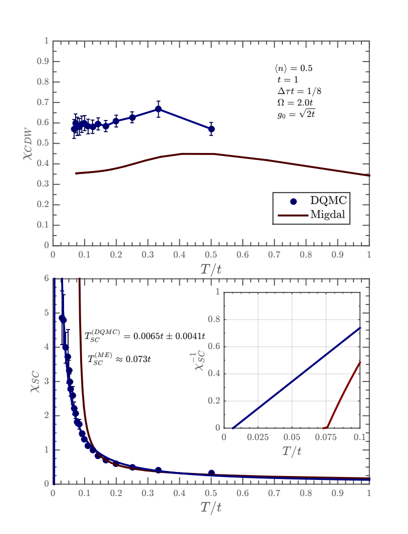
$$\chi^{\mathrm{CDW}}(\mathbf{q}) = \frac{1}{N}\sum_{i,j,\sigma,\sigma'} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot(\mathbf{R_i}-\mathbf{R_j})}\int_0^\beta \mathrm{d}\tau\,\langle \hat{n}_{i,\sigma}(\tau)\hat{n}_{j,\sigma'}(0)\rangle_{\mathrm{c}}$$

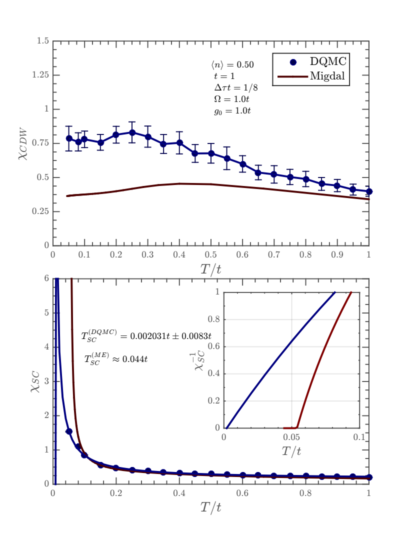
Phonon Dispersion: $\lambda = 0.3$



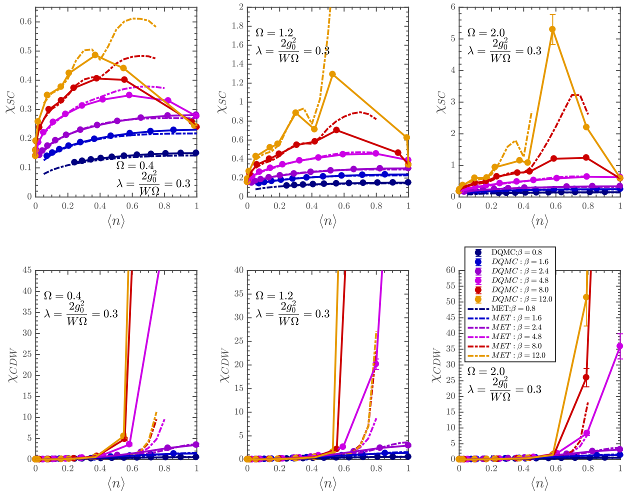


Results: One-Quarter Filling $\langle n \rangle = 0.50$ (4×4)





Results: DQMC vs. ME Theory $\lambda = 0.30$ (10×10)



Results: DQMC vs. ME Theory $\lambda = 0.50$ (10×10)

- Large enough λ reveals breakdown of ME theory.
- DQMC shows rapid enhancement of CDW and weak pairing correlations.
- I. Esterlis *et al.*(2017) claim ME theory agrees for $\lambda \lesssim 0.4$ around half-filling.