Temperature-Doping Phase Diagram of the 2D Holstein Model

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Model and Methods

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

(a)

\[ \overset{\sim}{\sim} = \overset{\sim}{\sim} + \text{Neglected crossing diagram} \]

(b)

\[ \text{First order vertex correction (neglected)} \]

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

Figure: Y. Wang, et. al. (2016)
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- 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?

How do we obtain $T_c$?

- Extrapolate inverse susceptibilities.
- Works well for $\chi^{\text{SC}}$.
- $\chi^{\text{CDW}}$ 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 $\chi^{\text{CDW}}$.  

\[ \Omega = 1.0t \]
\[ \langle n \rangle = 0.8 \]
\[ T_{C^{\text{CDW}}} = 0.041t \]
\[ T_{C^{\text{SC}}} = 0.064t \]
Finite-size effects on $T_c$: $L = \sqrt{N} = 256, 128, 64, \text{ and } 32$

\[ T_{c,\text{CDW}}(L \geq 128) \approx \lim_{L \to \infty} T_{c,\text{CDW}}(L) \]

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 $\chi_{\text{CDW}}(q)$

Figure: Incommensurate peaks in $\chi_{\text{CDW}}(q)$ for $\langle n \rangle \sim 0.8$ and $\Omega = 1.0$ near the phase transition temperature on a smaller $64 \times 64$ lattice.
Addition of NNN Hopping

\[ \Omega = 1.0t \]

\[ t' = 0 \]

\[ \frac{T_c}{t} \]

(a) $CDW$ $(\pi, \pi)$

(b) $CDW$ $(\pi, \pi)$

SC

Temperature-Doping Phase Diagram of the 2D Holstein Model
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: \( \hat{c}_{k,\sigma}(\tau) = e^{\hat{H}_\tau} \hat{c}_{k,\sigma} e^{-\hat{H}_\tau} \)

\[
G_{\sigma,\sigma'}(k, \tau; k', \tau') = -\left\langle \hat{T}_\tau \hat{c}_{k,\sigma}(\tau) \hat{c}_{k',\sigma'}^\dagger(\tau') \right\rangle \\
= -\text{Tr} \left[ \hat{\rho} \hat{T}_\tau \left\{ \hat{c}_{k,\sigma}(\tau) \hat{c}_{k',\sigma'}^\dagger(\tau') \right\} \right]
\]

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

\[
G_{\lambda,\lambda'}(i\omega_n) = \frac{1}{\beta} \int_0^\beta G_{\lambda,\lambda'}(\tau) e^{i\omega_n \tau}, \quad \text{where} \quad \omega_n = \frac{(2n + 1)\pi}{\beta} \quad \text{(fermions)}
\]
Working in Momentum space

\[ \hat{H} = \sum_{k,\sigma} \epsilon_k \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} + \Omega \sum_{k} \left( \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) - \frac{g}{\sqrt{2N_s M\Omega}} \sum_{k,k',\sigma} \left( \hat{a}_{k'-k} + \hat{a}_{-(k'-k)}^\dagger \right) \hat{c}_{k',\sigma}^\dagger \hat{c}_{k,\sigma} \]

- Electron dispersion:

\[ \epsilon_k = -2t \left( \cos(k_x d) + \cos(k_y d) \right) - \left( \mu - \frac{\alpha^2}{k} \right). \]

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

\[ G_{\sigma}(k, i\omega_n) = \left[ i\omega_n - \epsilon_k - \Sigma_{\sigma}(k, i\omega_n) \right]^{-1} \]

\[ D(q, i\nu_n) = \left[ -M(\Omega^2 + \nu_n^2) - \Pi(q, i\nu_n) \right]^{-1} \]
Propagators in Migdal Theory

(a) \[ \begin{align*}
\text{Propagators} &= \text{Propagators} + \text{Interaction} + \text{Propagators} \\
\end{align*} \]

(b) \[ \begin{align*}
\text{Propagators} &= \text{Propagators} + \text{Interaction} \\
\end{align*} \]
Susceptibilities

• Singlet Pairing (SC) Susceptibility

\[
\chi_{SP}(q = 0) = \frac{1}{N} \sum_{i,j} \int_0^\beta d\tau \langle \hat{c}_{i\uparrow}(\tau) \hat{c}_{i\downarrow}(\tau) \hat{c}_{j\downarrow}^\dagger(0) \hat{c}_{j\uparrow}^\dagger(0) \rangle
\]

• CDW Susceptibility

\[
\chi_{CDW}(q) = \frac{1}{N} \sum_{i,j,\sigma,\sigma'} e^{i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \int_0^\beta d\tau \langle \hat{n}_{i,\sigma}(\tau) \hat{n}_{j,\sigma'}(0) \rangle_c
\]
Phonon Dispersion: $\lambda = 0.3$

- (a) $\text{Im}[D(q, \omega)]$ for $\Omega = 1.0t$
- (b) $\text{Im}[D(q, \omega)]$ for $T = 0.17t$
- (c) $\text{Im}[D(q, \omega)]$ for $T = 0.22t$
- (d) $\text{Im}[D(q, \omega)]$ for $T = 0.26t$
- (e) $\text{Im}[D(q, \omega)]$ for $T = 0.34t$

- (a) $\text{Im}[D(q, \omega)]$ for $T = 0.17t$
- (b) $\text{Im}[D(q, \omega)]$ for $\Omega = 0.1t$
- (c) $\text{Im}[D(q, \omega)]$ for $\Omega = 0.5t$
- (d) $\text{Im}[D(q, \omega)]$ for $\Omega = 1.0t$
- (e) $\text{Im}[D(q, \omega)]$ for $\Omega = 1.5t$
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 $\lambda = 0.50$ ($10 \times 10$)

- Large enough $\lambda$ 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.