Quantum Monte Carlo Study of the Effect of Dirac Spectrum Gap Opening on Charge Ordering

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September 06, 2019

Outline

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  - The Holstein Model
  - A Decorated Honeycomb Lattice
  - Charge Density Wave (CDW)
- **Methodology**
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  - Quantum Monte Carlo
  - Determinant Quantum Monte Carlo (DQMC)
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  - Phase Diagram
- **Future Work**

The Holstein Model

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$

Electron:

$$\hat{H}_{el} = -t \sum_{<i,j>,\sigma} \left(\hat{c}^{+}_{i,\sigma} \hat{c}_{j,\sigma} + h.c. \right) - \mu \sum_{i,\sigma} \hat{c}^{+}_{i,\sigma} \hat{c}_{i,\sigma}$$

Phonon:

$$\hat{H}_{ph} = \frac{{\omega_0}^2}{2} \sum_i {\hat{x}_i}^2 + \frac{1}{2} \sum_i {\hat{p}_i}^2$$

Electron-Phonon Interaction:

$$\hat{H}_{el-ph} = \lambda \sum_{i,\sigma} \hat{x}_i \hat{c}^{+}_{i,\sigma} \hat{c}_{i,\sigma}$$

Half filling:

$$\mu = -\frac{\lambda^2}{{\omega_0}^2}$$

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$t = 0$ limit: The Single Site Holstein Model at Half Filling

Half Filling: $\mu = -\frac{\lambda^2}{{\omega_0}^2}$

The Single Site Holstein Model:

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

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$$= \frac{1}{2}\hat{p}^2 + \frac{1}{2}{\omega_0}^2\left[\hat{x} + \frac{\lambda}{{\omega_0}^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)\right]^2 - \frac{\lambda^2}{{\omega_0}^2}\hat{n}_\uparrow\hat{n}_\downarrow + \frac{\lambda^2}{2{\omega_0}^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)$$

$t = 0$ limit: The Single Site Holstein Model at Half Filling

Half Filling: $\mu = -\frac{\lambda^2}{{\omega_0}^2}$

$U_{eff} = -\frac{\lambda^2}{{\omega_0}^2}$

Attractive electron-electron interaction

The Single Site Holstein Model:

$$
\begin{aligned}
H &= \frac{1}{2}\hat{p}^2 + \frac{1}{2}{\omega_0}^2\hat{x}^2 + \lambda\hat{x}(\hat{n}_\uparrow + \hat{n}_\downarrow) - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow) \\
&= \frac{1}{2}\hat{p}^2 + \frac{1}{2}{\omega_0}^2\left[\hat{x} + \frac{\lambda}{{\omega_0}^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)\right]^2 - \frac{\lambda^2}{{\omega_0}^2}\hat{n}_\uparrow\hat{n}_\downarrow + \frac{\lambda^2}{2{\omega_0}^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)
\end{aligned}
$$

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$$\begin{cases} |0\rangle \\ |\uparrow\cdot\rangle, |\cdot\downarrow\rangle \\ |\uparrow\downarrow\rangle \end{cases} \rightarrow \begin{matrix} 0 \\ \frac{\lambda^2}{2{\omega_0}^2} \\ 0 \end{matrix}$$

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$$= \frac{1}{2}\hat{p}^2 + \frac{1}{2}{\omega_0}^2\left[\hat{x} + \frac{\lambda}{{\omega_0}^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)\right]^2 - \frac{\lambda^2}{{\omega_0}^2}\hat{n}_\uparrow\hat{n}_\downarrow + \frac{\lambda^2}{2{\omega_0}^2}(\hat{n}_\uparrow + \hat{n}_\downarrow)$$

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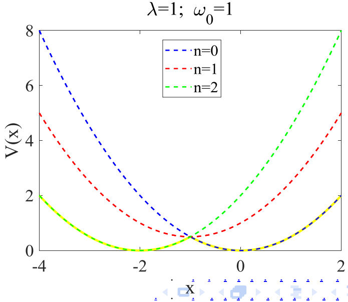
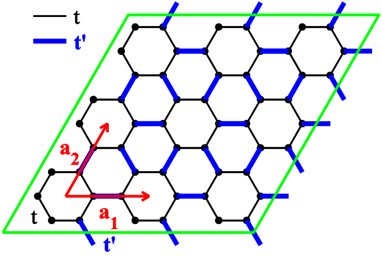


Holstein Model on a Decorated Honeycomb Lattice



- A $3 \times 3 \times 6$ decorated honeycomb lattice
- $\begin{cases} \overrightarrow{a_1} = (1,0) \\ \overrightarrow{a_2} = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \end{cases}$
- 6 sites per unit cell
- Periodic boundary condition

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$

$$= -t \sum_{<i,j>,\sigma} \left(\hat{c}_{i,\sigma}^{+} \hat{c}_{j,\sigma} + h.c.\right) - t' \sum_{<i',j'>,\sigma} \left(\hat{c}_{i',\sigma}^{+} \hat{c}_{j',\sigma} + h.c.\right) - \mu \sum_{i,\sigma} \hat{c}_{i,\sigma}^{+} \hat{c}_{i,\sigma}$$

$$+ \frac{{\omega_0}^2}{2} \sum_i {\hat{x}_i}^2 + \frac{1}{2} \sum_i {\hat{p}_i}^2 + \lambda \sum_{i,\sigma} \hat{x}_i \hat{c}_{i,\sigma}^{+} \hat{c}_{i,\sigma}$$

$\lambda = 0$ limit:

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$

$$= -t \sum_{<i,j>,\sigma} \left(\hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + h.c.\right) - t' \sum_{<i',j'>,\sigma} \left(\hat{c}^{+}_{i',\sigma}\hat{c}_{j',\sigma} + h.c.\right) - \mu \sum_{i,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

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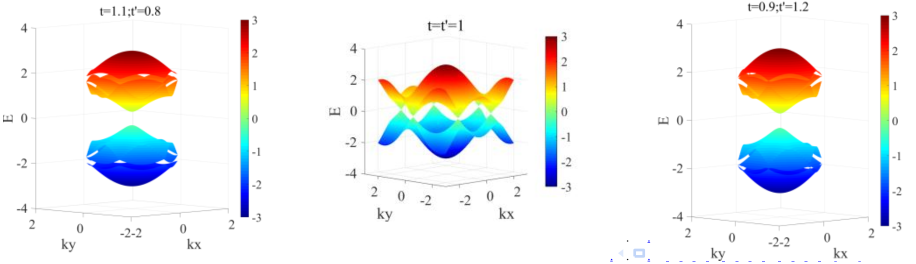
$t = t' = 1$: Dirac Spectrum; $t \neq t'$: Gap Opening   Effect on Charge Ordering?



$\lambda = 0$ limit:

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$
$$= -t \sum_{<i,j>,\sigma} \left(\hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + h.c.\right) - t' \sum_{<i',j'>,\sigma} \left(\hat{c}^{+}_{i',\sigma}\hat{c}_{j',\sigma} + h.c.\right) - \mu \sum_{i,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$
$$+ \frac{{\omega_0}^2}{2}\sum_i {\hat{x}_i}^2 + \frac{1}{2}\sum_i {\hat{p}_i}^2 + \lambda \sum_{i,\sigma} \hat{x}_i \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

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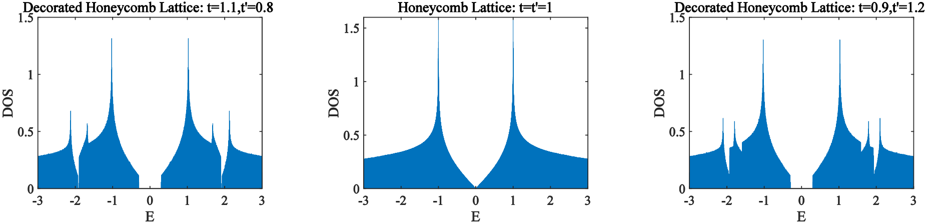
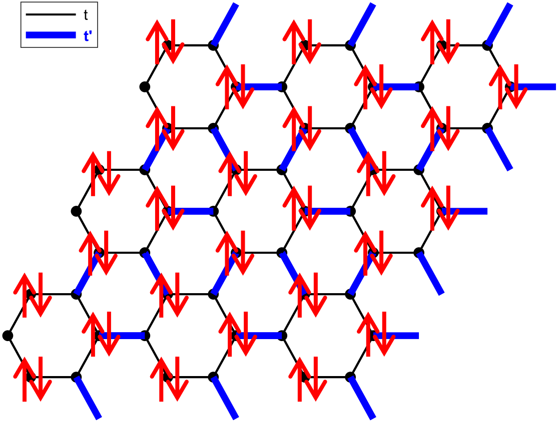


Charge Density Wave (CDW)

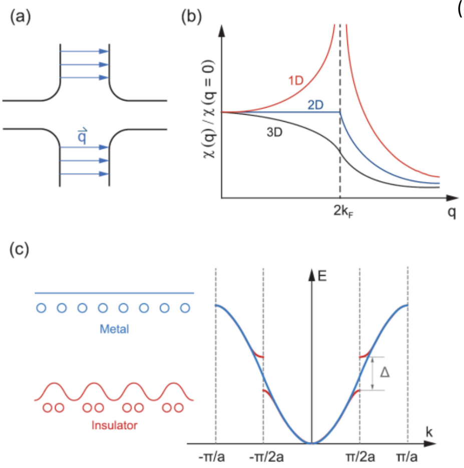


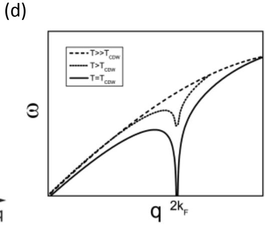
The Origin of Charge Density Wave (CDW)

1D: Peierls's picture

Key features:

$$\chi(q) = \sum_{\boldsymbol{k}} \frac{f(\varepsilon_{\boldsymbol{k}}) - f(\varepsilon_{\boldsymbol{k+q}})}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k+q}}}$$





Zhu, X., Guo, J., Zhang, J., & Plummer, E. W. (2017). *Advances in Physics: X*, *2*(3), 622-640.

(a) Fermi Surface Nesting (FSN)

(b) A sharp peak in Lindhard function

(c) A structural transition in lattice
A metal-insulator transition

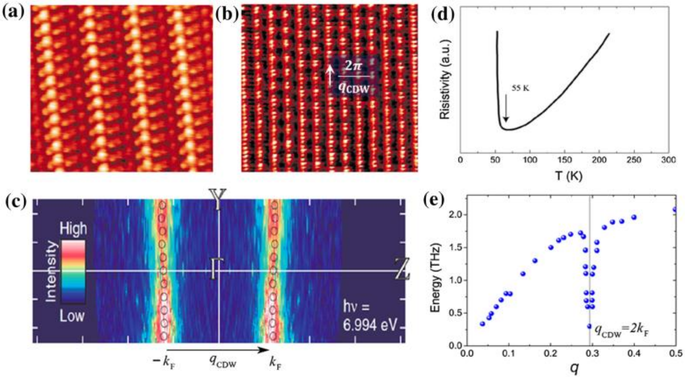
(d) Kohn anomaly in phonon spectra

Chen, C. W., Choe, J., & Morosan, E. (2016). *Reports on Progress in Physics*, *79*(8), 084505.

The Origin of Charge Density Wave (CDW)

1D: Peierls's picture

Example: the CDW state of TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane)



(a) STM image at 63 K showing the normal state. (b) STM image at 36 K showing the CDW state.
(c) ARPES intensity mapping at EF of TTF-TCNQ at 60 K, showing a clear 1D FSN.
(d) Resistivity vs. temperature measurements showing a clear metal–insulator transition at 55 K.
(e) Inelastic neutron scattering results of the acoustic phonon dispersion showing a strong Kohn anomaly.

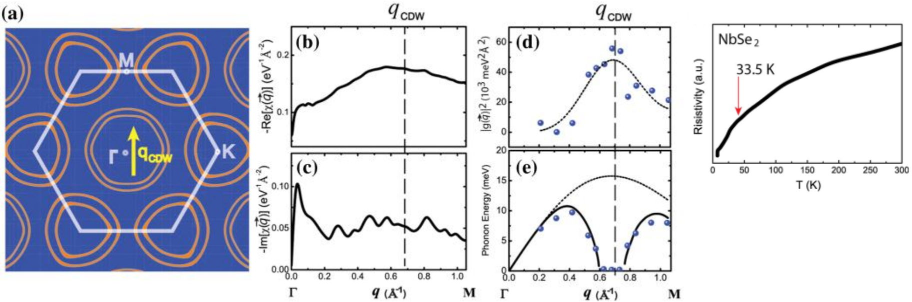
Zhu, X., Guo, J., Zhang, J., & Plummer, E. W. (2017). *Advances in Physics: X*, *2*(3), 622-640.

The Origin of Charge Density Wave (CDW)

2D: Electron Phonon Coupling?

Example: $NbSe_2$

- × Fermi Surface Nesting (FSN)
- × Sharp peak in Lindhard function
- × Metal-insulator transition
- √ Kohn Anomaly
- √ Structural Transition



3D: Highly material-dependent

Zhu, X., Guo, J., Zhang, J., & Plummer, E. W. (2017). *Advances in Physics: X*, *2*(3), 622-640.

Classical Monte Carlo

The probability of being in state $|n\rangle$ with energy E_n is given by the Boltzmann distribution,

$$P(n) = \frac{1}{Z} e^{-E_n/k_B T}$$

,in which

$$Z = \sum_n e^{-E_n/k_B T}$$

The Master Equation:

$$\frac{dP_\upsilon(t)}{dt} = \sum_{\sigma \neq \upsilon} P_\sigma(t) W(\sigma \to \upsilon) - P_\upsilon(t) W(\upsilon \to \sigma)$$

$P_\upsilon(t)$: the probability of having configuration υ at time t

$W(\sigma \to \upsilon)$: the probability per unit time for the system to go from configuration σ to υ.

Classical Monte Carlo

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$W(\sigma \to \upsilon)$： the probability per unit time for the system to go from configuration σ to υ

$$\lim_{t \to \infty} P_\upsilon(t) = P_\upsilon$$

Impose the sufficient but not necessary condition: ***Detailed Balance***

$$P_\sigma W(\sigma \to \upsilon) = P_\upsilon W(\upsilon \to \sigma)$$

Metropolis Algorithm: $W(\upsilon \to \sigma) = \begin{cases} 1 & for\ P_\sigma \geq P_\upsilon \\ \frac{P_\sigma}{P_\upsilon} & for\ P_\sigma < P_\upsilon \end{cases}$

Quantum Monte Carlo

Example: Quantum Harmonic Oscillator $\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{{\omega_0}^2}{2}\hat{x}^2$

$Z = Tr\left(e^{-\beta\hat{H}}\right) = Tr\left(e^{-\Delta\tau\hat{H}} \dots \dots e^{-\Delta\tau\hat{H}}\right)$

Quantum Monte Carlo

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Suzuki-Trotter Approximation: $e^{-\Delta\tau(\hat{A}+\hat{B})} = e^{-\Delta\tau\hat{A}}e^{-\Delta\tau\hat{B}} + \mathcal{O}(\Delta\tau^2)$

$$Z = Tr\left(e^{-\beta\widehat{H}}\right) = Tr\left(e^{-\Delta\tau\widehat{H}} \dots\dots e^{-\Delta\tau\widehat{H}}\right) \approx Tr\left(e^{-\Delta\tau\frac{1}{2}\hat{p}^2}e^{-\Delta\tau\frac{{\omega_0}^2}{2}\hat{x}^2} \dots\dots e^{-\Delta\tau\frac{1}{2}\hat{p}^2}e^{-\Delta\tau\frac{{\omega_0}^2}{2}\hat{x}^2}\right)$$

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$$= \int_{-\infty}^{+\infty} dx_1 \cdots dx_L \left\langle x_1 \middle| e^{-\Delta\tau\frac{1}{2}\hat{p}^2} e^{-\Delta\tau\frac{{\omega_0}^2}{2}\hat{x}^2} \middle| x_2 \right\rangle \left\langle x_2 \middle| e^{-\Delta\tau\frac{1}{2}\hat{p}^2} e^{-\Delta\tau\frac{{\omega_0}^2}{2}\hat{x}^2} \middle| x_3 \right\rangle \ldots \left\langle x_L \middle| e^{-\Delta\tau\frac{1}{2}\hat{p}^2} e^{-\Delta\tau\frac{{\omega_0}^2}{2}\hat{x}^2} \middle| x_1 \right\rangle$$

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$$\sim \int_{-\infty}^{+\infty} e^{-\Delta\tau\frac{{\omega_0}^2}{2}{x_1}^2} \left\langle x_1 \middle| e^{-\Delta\tau\frac{1}{2}\hat{p}^2} \middle| p \right\rangle \langle p | x_2 \rangle dp$$

$$= e^{-\Delta\tau\frac{{\omega_0}^2}{2}{x_1}^2} \int_{-\infty}^{+\infty} e^{-\Delta\tau\frac{1}{2}p^2} e^{ip(x_1-x_2)/\hbar} dp \sim e^{-\Delta\tau\frac{{\omega_0}^2}{2}{x_1}^2} e^{-\frac{(x_1-x_2)^2/\hbar^2}{2\Delta\tau}}$$

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$$= \int dx_1 \cdots dx_L \exp[-\Delta\tau(\frac{{\omega_0}^2}{2}\sum_l {x_l}^2 + \frac{1}{2}\sum_l \left(\frac{x_{l+1} - x_l}{\Delta\tau}\right)^2) \equiv \int e^{-S_{bose}(\{x_l\})} \prod_{l=1}^{L} dx_l$$

Determinant Quantum Monte Carlo (DQMC)

$$\hat{H} = -t \sum_{<i,j>,\sigma} \left(\hat{c}_{i,\sigma}^{+}\hat{c}_{j,\sigma} + h.c.\right) - t' \sum_{<i',j'>,\sigma} \left(\hat{c}_{i',\sigma}^{+}\hat{c}_{j',\sigma} + h.c.\right) - \mu \sum_{i,\sigma} \hat{c}_{i,\sigma}^{+}\hat{c}_{i,\sigma}$$
$$+\lambda \sum_{i,\sigma} \hat{x}_i \hat{c}_{i,\sigma}^{+}\hat{c}_{i,\sigma} + \frac{{\omega_0}^2}{2} \sum_i {\hat{x}_i}^2 + \frac{1}{2} \sum_i {\hat{p}_i}^2 = \hat{H}_{el} + \hat{V} + \hat{H}_{ph}$$

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$$Z = Tr\left(e^{-\beta \hat{H}}\right) = Tr\left(e^{-\Delta\tau \hat{H}} \dots \dots e^{-\Delta\tau \hat{H}}\right) \approx Tr\left(e^{-\Delta\tau \hat{H}_{el}} e^{-\Delta\tau \hat{V}} e^{-\Delta\tau \hat{H}_{ph}} \dots \dots e^{-\Delta\tau \hat{H}_{el}} e^{-\Delta\tau \hat{V}} e^{-\Delta\tau \hat{H}_{ph}}\right)$$

Determinant Quantum Monte Carlo (DQMC)

$$\hat{H} = -t \sum_{<i,j>,\sigma} \left(\hat{c}_{i,\sigma}^{+}\hat{c}_{j,\sigma} + h.c.\right) - t' \sum_{<i',j'>,\sigma} \left(\hat{c}_{i',\sigma}^{+}\hat{c}_{j',\sigma} + h.c.\right) - \mu \sum_{i,\sigma} \hat{c}_{i,\sigma}^{+}\hat{c}_{i,\sigma}$$

$$+\lambda \sum_{i,\sigma} \hat{x}_i \hat{c}_{i,\sigma}^{+}\hat{c}_{i,\sigma} + \frac{{\omega_0}^2}{2}\sum_i {\hat{x}_i}^2 + \frac{1}{2}\sum_i {\hat{p}_i}^2 = \hat{H}_{el} + \hat{V} + \hat{H}_{ph}$$

$$Z = Tr\left(e^{-\beta\hat{H}}\right) = Tr\left(e^{-\Delta\tau\hat{H}} \ldots\ldots e^{-\Delta\tau\hat{H}}\right) \approx Tr\left(e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}} \ldots\ldots e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}}\right)$$

$$= \int \prod_l d\vec{\boldsymbol{x}}_l\, Tr_{el} \langle\vec{\boldsymbol{x}}_1|e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}}|\vec{\boldsymbol{x}}_2\rangle\langle\vec{\boldsymbol{x}}_2|e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}}|\vec{\boldsymbol{x}}_3\rangle\cdots\langle\vec{\boldsymbol{x}}_L|e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}}|\vec{\boldsymbol{x}}_1\rangle$$

$$= \sum_l \langle\vec{\boldsymbol{x}}_1|e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}|\vec{\boldsymbol{x}}_l\rangle\langle\vec{\boldsymbol{x}}_l|e^{-\Delta\tau\hat{H}_{ph}}|\vec{\boldsymbol{x}}_2\rangle = e^{-\Delta\tau H_{el}}e^{-\Delta\tau V(\vec{\boldsymbol{x}}_1)}\langle\vec{\boldsymbol{x}}_1|e^{-\Delta\tau\hat{H}_{ph}}|\vec{\boldsymbol{x}}_2\rangle$$

Determinant Quantum Monte Carlo (DQMC)

$$\hat{H} = -t \sum_{<i,j>,\sigma} (\hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + h.c.) - t' \sum_{<i',j'>,\sigma} (\hat{c}^{+}_{i',\sigma}\hat{c}_{j',\sigma} + h.c.) - \mu \sum_{i,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

$$+\lambda \sum_{i,\sigma} \hat{x}_i \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma} + \frac{{\omega_0}^2}{2}\sum_i {\hat{x}_i}^2 + \frac{1}{2}\sum_i {\hat{p}_i}^2 = \hat{H}_{el} + \hat{V} + \hat{H}_{ph}$$

$$Z = Tr(e^{-\beta\hat{H}}) = Tr(e^{-\Delta\tau\hat{H}} \ldots\ldots e^{-\Delta\tau\hat{H}}) \approx Tr(e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} \ldots\ldots e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}})$$

$$= \int \prod_l d\vec{x}_l \, Tr_{el} \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle \langle \vec{x}_2 | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_3 \rangle \cdots \langle \vec{x}_L | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_1 \rangle$$

$$= \sum_l \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} | \vec{x}_l \rangle \langle \vec{x}_l | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle = e^{-\Delta\tau H_{el}} e^{-\Delta\tau V(\vec{x}_1)} \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle$$

$$= \int \prod_l d\vec{x}_l \, \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle \langle \vec{x}_2 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_3 \rangle \cdots \langle \vec{x}_L | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_1 \rangle \, Tr_{el}(e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}(\vec{x}_1)} \ldots e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}(\vec{x}_L)})$$

Determinant Quantum Monte Carlo (DQMC)

$$\hat{H} = -t \sum_{<i,j>,\sigma} (\hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + h.c.) - t' \sum_{<i',j'>,\sigma} (\hat{c}^{+}_{i',\sigma}\hat{c}_{j',\sigma} + h.c.) - \mu \sum_{i,\sigma} \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma}$$

$$+\lambda \sum_{i,\sigma} \hat{x}_i \hat{c}^{+}_{i,\sigma}\hat{c}_{i,\sigma} + \frac{{\omega_0}^2}{2}\sum_i {\hat{x}_i}^2 + \frac{1}{2}\sum_i {\hat{p}_i}^2 = \hat{H}_{el} + \hat{V} + \hat{H}_{ph}$$

$$Z = Tr\left(e^{-\beta\hat{H}}\right) = Tr\left(e^{-\Delta\tau\hat{H}} \dots\dots e^{-\Delta\tau\hat{H}}\right) \approx Tr\left(e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} \dots\dots e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}}\right)$$

$$= \int \prod_l d\vec{x}_l\, Tr_{el} \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle \langle \vec{x}_2 | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_3 \rangle \cdots \langle \vec{x}_L | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_1 \rangle$$

$$= \sum_l \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}} | \vec{x}_l \rangle \langle \vec{x}_l | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle = e^{-\Delta\tau H_{el}} e^{-\Delta\tau V(\vec{x}_1)} \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle$$

$$= \int \prod_l d\vec{x}_l \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle \langle \vec{x}_2 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_3 \rangle \cdots \langle \vec{x}_L | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_1 \rangle\, Tr_{el}\left(e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}(\vec{x}_1)} \dots e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}(\vec{x}_L)}\right)$$

$$= \int \prod_l d\vec{x}_l \prod_l exp\left\{-\Delta\tau \left[\frac{1}{2}{\omega_0}^2 {\vec{x}_l}^2 + \frac{1}{2}\left(\frac{\vec{x}_{l+1} - \vec{x}_l}{\Delta\tau}\right)^2\right]\right\} Tr_{el}\left(e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}(\vec{x}_1)} \dots e^{-\Delta\tau\hat{H}_{el}} e^{-\Delta\tau\hat{V}(\vec{x}_L)}\right)$$

Determinant Quantum Monte Carlo (DQMC)

$$\hat{H} = -t \sum_{<i,j>,\sigma} (\hat{c}_{i,\sigma}^{+}\hat{c}_{j,\sigma} + h.c.) - t' \sum_{<i',j'>,\sigma} (\hat{c}_{i',\sigma}^{+}\hat{c}_{j',\sigma} + h.c.) - \mu \sum_{i,\sigma} \hat{c}_{i,\sigma}^{+}\hat{c}_{i,\sigma}$$

$$+\lambda \sum_{i,\sigma} \hat{x}_i \hat{c}_{i,\sigma}^{+}\hat{c}_{i,\sigma} + \frac{{\omega_0}^2}{2}\sum_i {\hat{x}_i}^2 + \frac{1}{2}\sum_i {\hat{p}_i}^2 = \hat{H}_{el} + \hat{V} + \hat{H}_{ph}$$

$$Z = Tr(e^{-\beta\hat{H}}) = Tr(e^{-\Delta\tau\hat{H}} \dots\dots e^{-\Delta\tau\hat{H}}) \approx Tr(e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}} \dots\dots e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}})$$

$$= \int \prod_l d\vec{x}_l \, Tr_{el} \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle \langle \vec{x}_2 | e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_3 \rangle \cdots \langle \vec{x}_L | e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_1 \rangle$$

$$= \sum_l \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}} | \vec{x}_l \rangle \langle \vec{x}_l | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle = e^{-\Delta\tau H_{el}}e^{-\Delta\tau V(\vec{x}_1)} \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle$$

$$= \int \prod_l d\vec{x}_l \langle \vec{x}_1 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_2 \rangle \langle \vec{x}_2 | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_3 \rangle \cdots \langle \vec{x}_L | e^{-\Delta\tau\hat{H}_{ph}} | \vec{x}_1 \rangle \, Tr_{el}(e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}(\vec{x}_1)} \dots e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}(\vec{x}_L)})$$

$$= \int \prod_l d\vec{x}_l \prod_l exp\left\{-\Delta\tau\left[\frac{1}{2}{\omega_0}^2{\vec{x}_l}^2 + \frac{1}{2}(\frac{\vec{x}_{l+1}-\vec{x}_l}{\Delta\tau})^2\right]\right\} Tr_{el}(e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}(\vec{x}_1)} \dots e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}(\vec{x}_L)})$$

$$\equiv \int \prod_l d\vec{x}_l e^{-S_{bose}(\{\vec{x}_l\})} Tr_{el}(e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}(\vec{x}_1)} \dots e^{-\Delta\tau\hat{H}_{el}}e^{-\Delta\tau\hat{V}(\vec{x}_L)})$$

Determinant Quantum Monte Carlo (DQMC)

$$Z = \int \prod_l d\vec{\boldsymbol{x}}_l e^{-S_{bose}(\{\vec{x}_l\})}\, Tr_{el}\left(e^{-\Delta\tau \hat{H}_{el}} e^{-\Delta\tau \hat{V}(\vec{x}_1)} \dots e^{-\Delta\tau \hat{H}_{el}} e^{-\Delta\tau \hat{V}(\vec{x}_L)}\right)$$

,where

$$\hat{H}_{el} = \hat{\boldsymbol{C}}_\uparrow{}^\dagger \boldsymbol{H}_{el} \hat{\boldsymbol{C}}_\uparrow + \hat{\boldsymbol{C}}_\downarrow{}^\dagger \boldsymbol{H}_{el} \hat{\boldsymbol{C}}_\downarrow$$

$$= \begin{pmatrix} c_{1\uparrow}^\dagger & c_{2\uparrow}^\dagger & \cdots & c_{N\uparrow}^\dagger \end{pmatrix} \begin{pmatrix} -\mu & -t & \cdots & -t \\ -t & -\mu & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -t & 0 & \cdots & -\mu \end{pmatrix} \begin{pmatrix} c_{1\uparrow} \\ c_{2\uparrow} \\ \vdots \\ c_{N\uparrow} \end{pmatrix} + \begin{pmatrix} c_{1\downarrow}^\dagger & c_{2\downarrow}^\dagger & \cdots & c_{N\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} -\mu & -t & \cdots & -t \\ -t & -\mu & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -t & 0 & \cdots & -\mu \end{pmatrix} \begin{pmatrix} c_{1\downarrow} \\ c_{2\downarrow} \\ \vdots \\ c_{N\downarrow} \end{pmatrix}$$

$$\hat{V}(\vec{\boldsymbol{x}}_l) = \hat{\boldsymbol{C}}_\uparrow{}^\dagger \boldsymbol{V}(\vec{\boldsymbol{x}}_l) \hat{\boldsymbol{C}}_\uparrow + \hat{\boldsymbol{C}}_\downarrow{}^\dagger \boldsymbol{V}(\vec{\boldsymbol{x}}_l) \hat{\boldsymbol{C}}_\downarrow$$

$$= \begin{pmatrix} c_{1\uparrow}^\dagger & c_{2\uparrow}^\dagger & \cdots & c_{N\uparrow}^\dagger \end{pmatrix} \begin{pmatrix} \lambda x_{1,l} & 0 & \cdots & 0 \\ 0 & \lambda x_{2,l} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda x_{N,l} \end{pmatrix} \begin{pmatrix} c_{1\uparrow} \\ c_{2\uparrow} \\ \vdots \\ c_{N\uparrow} \end{pmatrix} + \begin{pmatrix} c_{1\downarrow}^\dagger & c_{2\downarrow}^\dagger & \cdots & c_{N\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} \lambda x_{1,l} & 0 & \cdots & 0 \\ 0 & \lambda x_{2,l} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda x_{N,l} \end{pmatrix} \begin{pmatrix} c_{1\downarrow} \\ c_{2\downarrow} \\ \vdots \\ c_{N\downarrow} \end{pmatrix}$$

$$Z = \int \prod_l d\vec{\boldsymbol{x}}_l e^{-S_{bose}(\{\vec{x}_l\})} \prod_\sigma \det\left(\boldsymbol{I} + e^{-\Delta\tau \boldsymbol{H}_{el}} e^{-\Delta\tau \boldsymbol{V}(\vec{\boldsymbol{x}}_1)} \dots e^{-\Delta\tau \boldsymbol{H}_{el}} e^{-\Delta\tau \boldsymbol{V}(\vec{\boldsymbol{x}}_L)}\right)$$

$$\equiv \int \prod_l d\vec{\boldsymbol{x}}_l e^{-S_{bose}(\{\vec{x}_l\})} \det[\boldsymbol{M}(\{\vec{\boldsymbol{x}}_{l\uparrow}\})] \det[\boldsymbol{M}(\{\vec{\boldsymbol{x}}_{l\downarrow}\})] = \int \prod_l d\vec{\boldsymbol{x}}_l P(\{\vec{\boldsymbol{x}}_l\})$$

DQMC Measurements: CDW Structure Factor

Density-Density Correlation:

$$c(\boldsymbol{r}) = \langle n_{\boldsymbol{i}} n_{\boldsymbol{i+r}} \rangle$$

CDW Structure Factor:

$$S_{cdw} = \sum_{n=1}^{N} (-1)^n c(\boldsymbol{r}_n)$$

Disordered Phase: $c(\boldsymbol{r}) \sim r^{-\frac{1}{2}(d-1)} \exp\left(-\frac{r}{\xi}\right)$, when $r \gg \xi$

$\Rightarrow \quad S_{cdw}$ is independent of N

Ordered Phase: $c(\boldsymbol{r}) \sim const.$ $\quad \Rightarrow \; S_{cdw} \propto N$

DQMC Measurements: CDW Structure Factor

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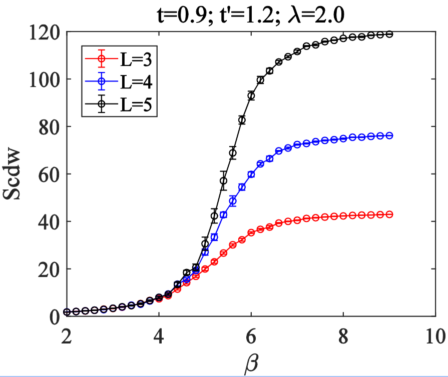


$$\beta = \frac{1}{T}$$

Finite Size Scaling → T_c

Correlation length: $\xi \sim |t|^{-\nu} \rightarrow t \sim \xi^{-1/\nu}$, where $t = \frac{T-T_c}{T_c}$

Order parameter: $\langle n \rangle \sim t^{\beta}$

Density-density correlation: $c(\boldsymbol{r}) = \langle n_{\boldsymbol{i}} n_{\boldsymbol{i}+\boldsymbol{r}} \rangle \sim t^{2\beta} \sim \xi^{-2\beta/\nu}$

Finite Size Scaling Hypothesis: $c(\boldsymbol{r}) = L^{\sigma} f\left(\frac{\xi}{L}\right) = L^{-2\beta/\nu} g\left(|t| L^{1/\upsilon}\right)$

Structure Factor:

$$S_{cdw} = \sum_{n=}^{N} (-1)^n c(\boldsymbol{r}_n) \sim L^2 L^{-2\beta/\nu} g\left(|t| L^{1/\upsilon}\right) \rightarrow L^{2-2\beta/\nu} g\left(|t| L^{1/\upsilon}\right)$$

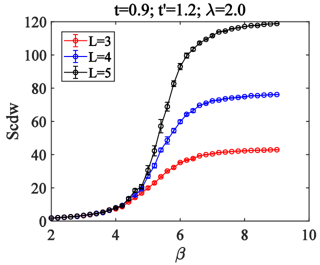
Finite Size Scaling → T_c

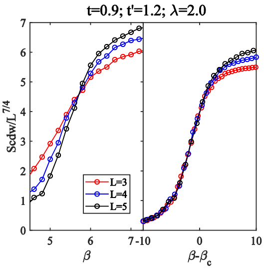
Structure Factor:

$$S_{cdw} = \sum_{n=}^{N} (-1)^n c(\boldsymbol{r}_n) \sim L^2 L^{-2\beta/\nu} g\left(|t| L^{1/\upsilon}\right) \to L^{2-2\beta/\nu} g\left(|t| L^{1/\upsilon}\right)$$

Ising Universality Class: $\beta = \frac{1}{8}, \upsilon = 1$

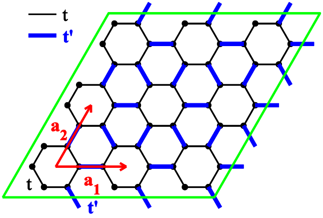
$$S_{cdw} \sim L^{7/4} g(|t| L)$$

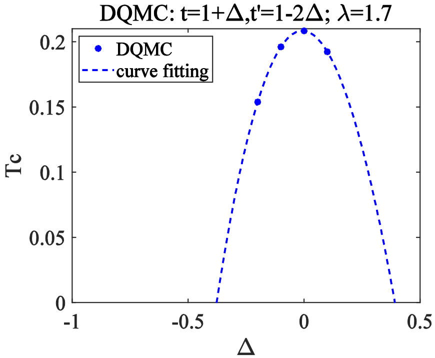


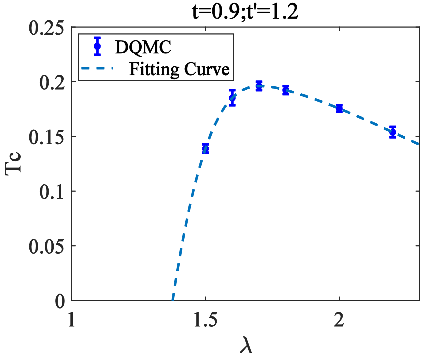


$$\beta = \frac{1}{T}, \quad \beta_c = \frac{1}{T_c}$$

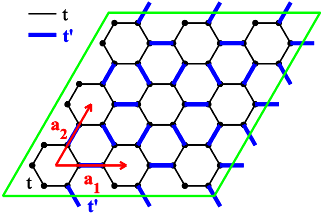
Results: Phase Diagram

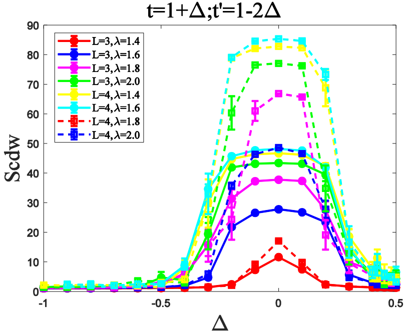






More Results





Future Work

- Holstein Model on Lieb Lattice
- Move away from half-filling: CDW and/or SC?
- ......

Thank You!