The Effect of Strain on Charge Density Wave Order in the Holstein Model

Benjamin Cohen-Stead

May 13, 2019

Outline for Talk

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Model Hamiltonians:

- Simple $\Longrightarrow$ small number of parameters
- Describes most important interactions
- Reproduces underlying physics of emergent phases
- Does not incorporate details of real materials

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- **Dimensionless Coupling Constant:** $\lambda_D = \frac{\lambda^2}{\omega_0^2 W}$ where $W \sim t$ is bandwidth

The Holstein Electron-Phonon Interaction Term

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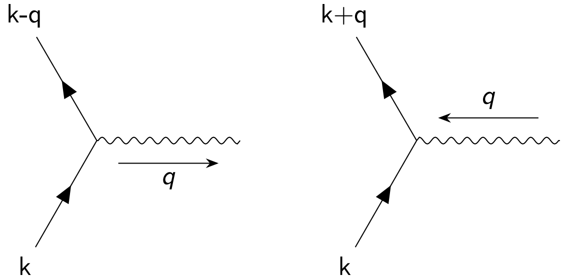
$$\hat{V} = \frac{g}{\sqrt{N}} \sum_{k,q,\sigma} \left[\hat{b}_q^\dagger \ \hat{c}_{k-q,\sigma}^\dagger \hat{c}_{k,\sigma} + \hat{b}_q \ \hat{c}_{k+q,\sigma}^\dagger \hat{c}_{k,\sigma} \right], \ g \ = \frac{\lambda}{\sqrt{2\omega_0}}$$



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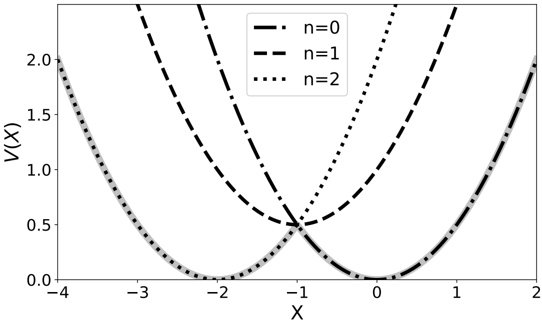
$\lambda = 1.0 \quad \omega = 1.0 \quad U_{eff} = -\frac{\lambda^2}{\omega^2} = -1 \quad -\frac{\lambda}{\omega^2} = -1.0$

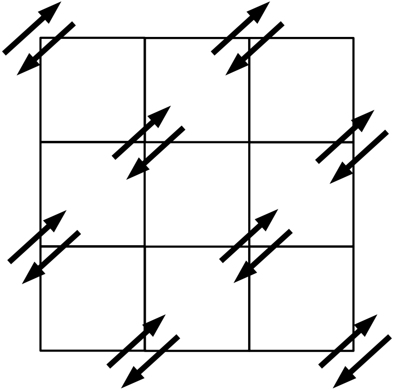


Charge-Density Wave Order

Effective Electron-Electron Attraction Mediated by Phonons

$\Longrightarrow$ Charge-Density Wave Order:

Periodic Spatial Modulation of the Electron Density



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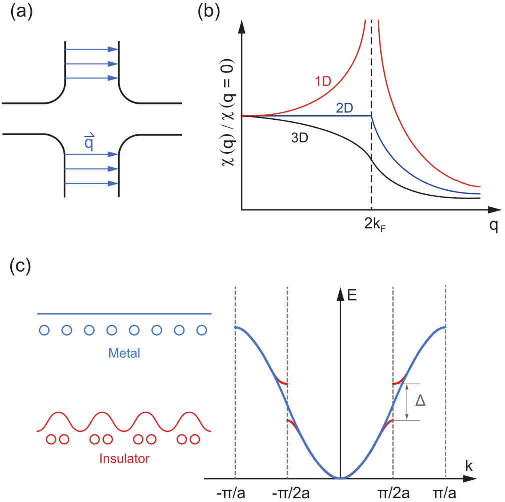

Peierls Instability

In a 1D chain, a uniform distribution of non-interacting electrons is unstable.

$$\chi_0(\mathbf{q}) = \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k}+\mathbf{q}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}}$$

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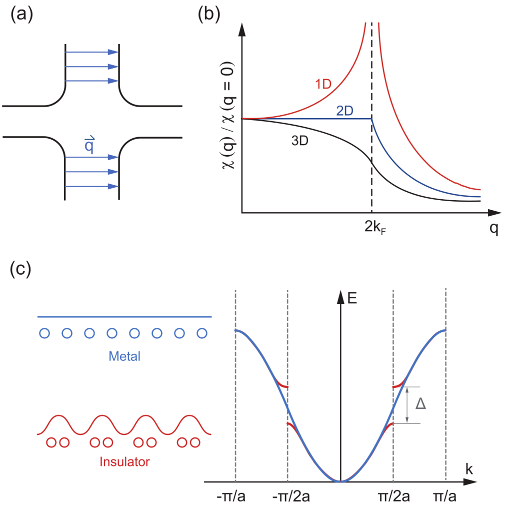

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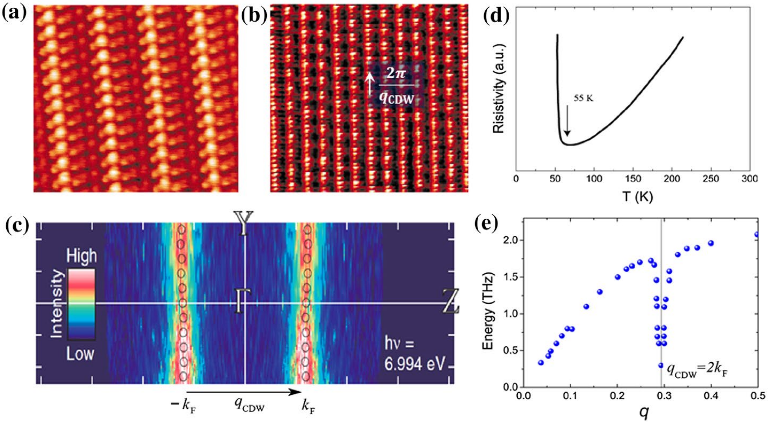
Fermi Surface Nesting allows Peierl's explanation of CDW to be applied in $D > 1$ dimensions.

An example of a Peierls CDW in the quasi-1D material TTF-TCNQ

(tetrathiafulvalene-tetracyanoquinodimethane)



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

Charge-Density Wave Order

The Peierl's Instability does not explain all CDW order in $D > 1$ dimensions.

- No FSN
- No Phonon Softening
- No Peak in χ_0
- No Metal-Insulator Transition

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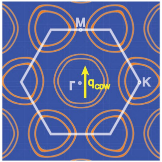
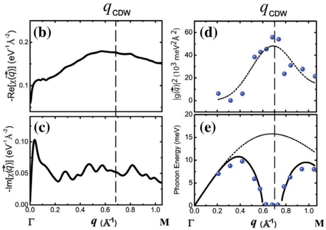
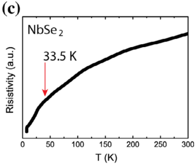
Ex: $\mathrm{2H-NbSe_2}$

(Niobium diselenide)

- Quasi-2D System
- $g(\mathbf{q}) \Rightarrow$ CDW at $T_{\mathrm{cdw}} \approx 33.5\mathrm{K}$
- $q_{\mathrm{cdw}} = 0.7\,\text{Å}^{-1} \quad (a = 3.443\,\text{Å})$







Effect of Strain on Charge Density Wave Order in the Holstein Model

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[2] *International School for Advanced Studies (SISSA), Via Bonomea 265, 34136, Trieste, Italy*
[3] *Instituto de Física, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil*
[4] *Department of Physics and Astronomy, San José State University, San José, CA 95192*

(Dated: May 7, 2019)

We investigate charge ordering in the Holstein model in the presence of anisotropic hopping, $t_x, t_y = 1-\delta, 1+\delta$, as a model of the effect of strain on charge density wave (CDW) materials. Using Quantum Monte Carlo simulations, we show that the CDW transition temperature is relatively insensitive to moderate anisotropy $\delta \lesssim 0.3$, but begins to decrease more rapidly at $\delta \gtrsim 0.4$. However, the density correlations, as well as the kinetic energies parallel and perpendicular to the compressional axis, change significantly for moderate δ. Accompanying mean-field theory calculations show a similar qualitative structure, with the transition temperature relatively constant at small δ and a more rapid decrease for larger strains. We also obtain the density of states $N(\omega)$, which provides clear signal of the charge ordering transition at large strain, where finite size scaling of the charge structure factor is extremely difficult because of the small value of the order parameter.

PACS numbers: 71.10.Fd, 71.30.+h, 71.45.Lr, 74.20.-z, 02.70.Uu

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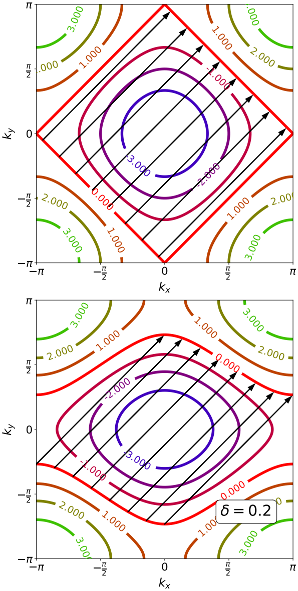
- $\mathbf{q}_{\mathrm{cdw}} = (\pi, \pi) \implies$ Checkerboard



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$$F = \frac{N}{2}\omega_0^2(x_0^2+x_1^2) - \frac{2}{\beta}\sum_{\mathbf{k}} \ln\left(1+e^{-\beta E_{\mathbf{k}}(x_1)}\right)$$

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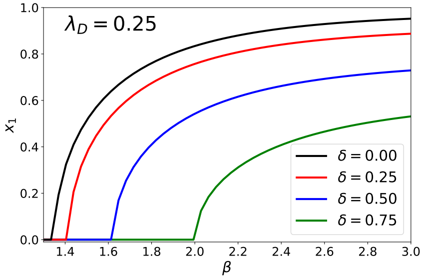

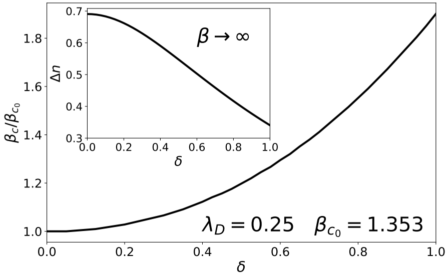

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- **Ergodicity:** sampling protocol can access all microstates
- Irreducibility, Aperiodicity
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$$\frac{\pi(A)}{\pi(B)} = \frac{e^{-\beta E_A}/Z}{e^{-\beta E_B}/Z} = e^{-\beta(E_A - E_B)} = e^{-\beta \Delta E}$$

Quantum Monte Carlo: Quantum Harmonic Oscillator

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] \quad \text{where} \quad \hat{H} = \tfrac{1}{2}\hat{P}^2 + \tfrac{\omega_0^2}{2}\hat{X}^2$$

$$Z = \mathrm{Tr}\left[e^{-\Delta\tau \hat{H}} \dots e^{-\Delta\tau \hat{H}}\right] \quad \text{where} \quad \tau = 1 \dots L_\tau \quad \text{and} \quad \beta = L_\tau \Delta\tau$$

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

$$Z \approx \mathrm{Tr}\left[e^{-\Delta\tau\left(\frac{1}{2}\hat{P}^2\right)} e^{-\Delta\tau\left(\frac{1}{2}\omega_0^2\hat{X}^2\right)} \dots e^{-\Delta\tau\left(\frac{1}{2}\hat{P}^2\right)} e^{-\Delta\tau\left(\frac{1}{2}\omega_0^2\hat{X}^2\right)}\right]$$

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$$\langle x_{L_\tau} | e^{-\Delta\tau\left(\frac{1}{2}\hat{P}^2\right)} e^{-\Delta\tau\left(\frac{1}{2}\omega_0^2\hat{X}^2\right)} | x_1 \rangle$$

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$$Z = \int_{-\infty}^{\infty} dx_1 \dots dx_{L_\tau} e^{-\Delta\tau\left(\frac{\omega_0^2}{2}\sum_\tau x_\tau^2\right)} \dots \int_{-\infty}^{\infty} e^{-\frac{\Delta\tau}{2}p^2 + ip(x_{\tau+1}-x_\tau)} \dots$$

$$Z = \int_{-\infty}^{\infty} dx_1 \dots dx_{L_\tau} \exp\left\{-\Delta\tau\left[\frac{\omega_0^2}{2}\sum_\tau x_\tau^2 + \frac{1}{2}\sum_\tau\left(\frac{x_{\tau+1}-x_\tau}{\Delta\tau}\right)^2\right]\right\} = \int e^{-S_{\mathrm{bose}}(\{x_\tau\})}$$

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$$Z \approx \mathrm{Tr}\left[e^{-\Delta\tau\left(\frac{1}{2}\hat{P}^2\right)} e^{-\Delta\tau\left(\frac{1}{2}\omega_0^2\hat{X}^2\right)} \dots e^{-\Delta\tau\left(\frac{1}{2}\hat{P}^2\right)} e^{-\Delta\tau\left(\frac{1}{2}\omega_0^2\hat{X}^2\right)}\right]$$

$$Z = \int_{-\infty}^{\infty} dx_1 \dots dx_{L_\tau} \langle x_1| e^{-\Delta\tau\left(\frac{1}{2}\hat{P}^2\right)} e^{-\Delta\tau\left(\frac{1}{2}\omega_0^2\hat{X}^2\right)} |x_2\rangle \langle x_2| \dots |x_{L_\tau}\rangle$$

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Quantum Monte Carlo: Quantum Harmonic Oscillator

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Determinant Quantum Monte Carlo

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

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

$$Z = \int_{-\infty}^{\infty}\prod_{\tau,i} dx_{\tau,i}\; e^{-S_{\mathrm{bose}}(\{x_{\tau,i}\})}\prod_{\sigma} Tr\left[e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(1)}\dots e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(L_\tau)}\right]$$

Note: $\hat{V}(\tau) = \hat{\mathbf{c}}^\dagger\bar{V}(\tau)\hat{\mathbf{c}}$ and $\hat{K} = \hat{\mathbf{c}}^\dagger\bar{K}\hat{\mathbf{c}}$

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Determinant Quantum Monte Carlo

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

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

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Detecting CDW Order:

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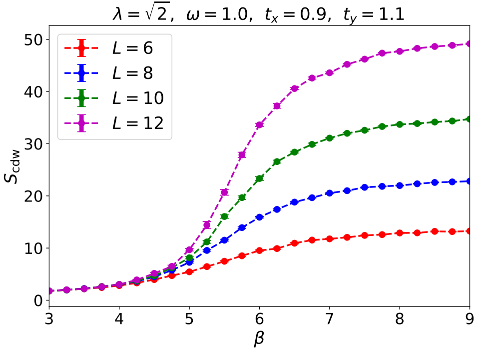

- $T > T_{\mathrm{cdw}} \Longrightarrow S_{\mathrm{cdw}} \perp N$
- $T < T_{\mathrm{cdw}} \Longrightarrow S_{\mathrm{cdw}} \sim N$
- Perfect CDW $\Longrightarrow S_{\mathrm{cdw}} = N$

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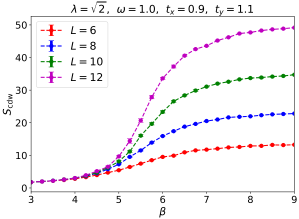
Getting T_{cdw} from S_{cdw}: Finite Size Scaling

Ising Universality Class: $\boxed{\beta = 1/8, \quad \nu = 1/4,} \quad \alpha = 0, \quad \gamma = 7/4, \quad \eta = 1/4$



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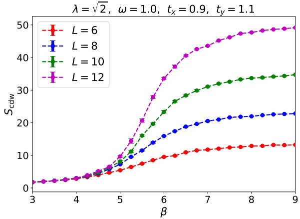

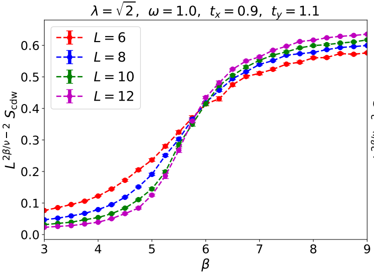

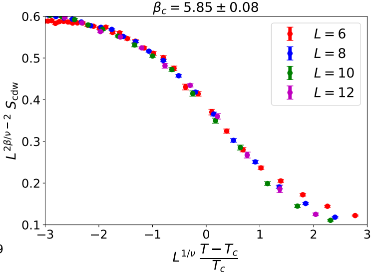

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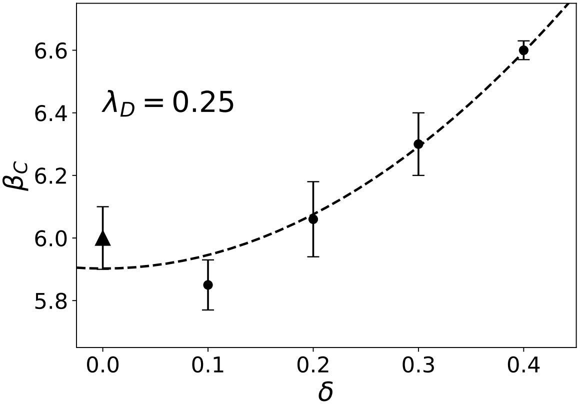
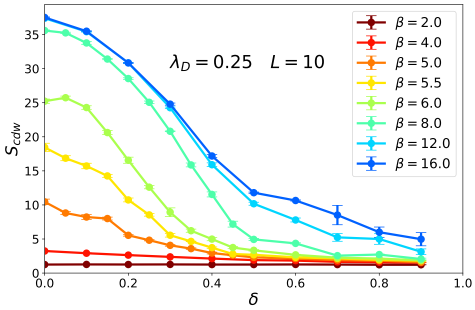
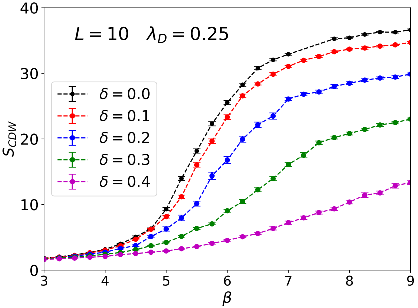


S_{cdw} Sensitive to δ





More Results: CDW as $\delta \to 1$

$$T_{\mathrm{cdw}} > 0 \quad \forall \quad \delta \in [0, 1)$$

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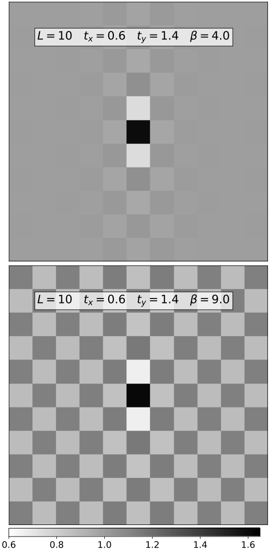

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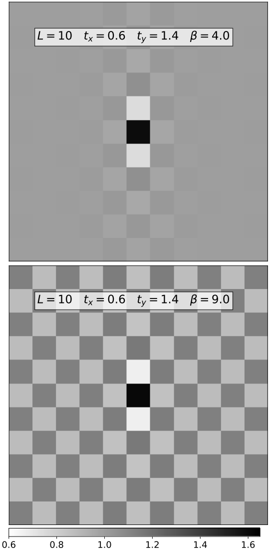
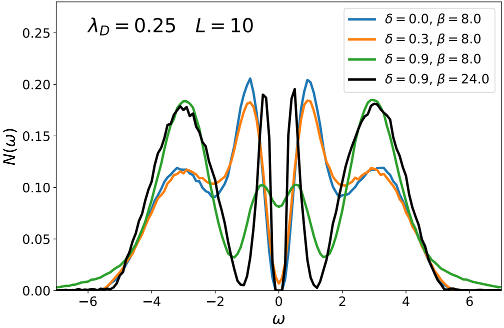


$$G(\mathbf{k}, \tau) = \int d\omega \frac{A(\mathbf{k}, \omega)\ e^{-\omega\tau}}{e^{-\beta\omega} + 1}$$

$$N(\omega) = \sum_{\mathbf{k}} A(\mathbf{k}, \omega)$$



Summary

- $\delta \lesssim 0.4 \implies T_{\mathrm{cdw}}$ Insensitive to δ

- δ Supresses S_{cdw}

- $T_{\mathrm{cdw}} > 0 \quad \forall \quad \delta \in [0, 1)$

Future Work

- Holstein Model on Cubic Lattice using SLMC + Langevin (ongoing)
- Move away from half-filling: striped CDW and/or SC?
- Kagome Lattice at Half-filling
- etc.

Thank You!