Quantum Monte Carlo Simulations of the Holstein Model on a Strained Square Lattice

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Some of the most exciting physics in condensed matter systems is the result of interacting degrees of freedom giving rise to strongly correlated materials that, when the temperature is lowered, develop novel electronic phases. These emergent phases are characterized by intricate patterns of spin, charge and pairing. For instance, (anti-)ferromagnetic order is the result of interacting spin degrees of freedom, whereas electron pairing can lead to superconductivity in certain situations. In my oral exam I will discuss electron-phonon interactions, and their role in the emergence of Charge Density Wave order. This discussion will be within the context of a numerical study of the Holstein model, a model Hamiltonian describing electron-phonon interactions in solids, on a strained square lattice.

I. INTRODUCTION

As a member of Professor Richard Scalettar's research group, I study strongly correlated systems using quantum Monte Carlo techniques to simulate model Hamiltonians. Put simply, Monte Carlo simulations in physics are used to sample a system's equilibrium distribution of states at fixed temperature, where each sampled state describes a particular configuration of the degrees of freedom in the system. Measurements of physical quantities, like the specific heat, are extracted by averaging over the properties of the sampled states. Model Hamiltonians provide simplified descriptions of the most important interactions in strongly correlated materials, while remaining numerically tractable.

In my research I use determinant quantum Monte Carlo (DQMC) to investigate the Holstein model, a model Hamiltonian for describing electron-phonon interactions on a lattice. In my oral exam I will explain the Holstein model and the physics of Charge Density Wave (CDW) order, and how we simulate this system using DQMC. I will then describe the results of a research project studying CDW in a strained Holstein model, and finish by discussing avenues for future research and my path to writing my dissertation.

II. BACKGROUND

Electron-phonon interactions play an important role in explaining a variety of emergent phenomena in solids, including Charge Density Wave order, a phase characterized by a periodic modulation of electron density on a lattice. In the 1930's a physicist by the name of Rudolf Peierls first proposed the existence of CDW order for one-dimensional systems as the result of electron-phonon interactions. A uniform distribution of free electrons in a 1D chain is unstable, and introducing electron-phonon interactions results in a distortion of the underlying lattice such that the fermi momentum k_F becomes the boundary of a new Brillouin Zone. The electrons localize on a given sub-lattice, forming a CDW pattern that opens a gap at the Fermi Surface (FS), lowering the total energy of the system; this instability in the FS is called the Peierls instability. Since being first proposed, CDW order has been observed in a variety of systems. For instance, the quasi-1D material TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane) goes through a CDW transition at $T_{\text{cdw}} \approx 55\text{K}$ that is well described the Peierl's istability [1]. On the other hand, the quasi-2D material Niobium Diselenide ($2\text{H} - \text{NbSe}_2$) goes through a CDW transition that is not well explained by the Peierls instability, but is instead the result of a momentum dependent electron-phonon coupling.

Alteration of the band stucture via the application of strain provides specific insight into the nature of a native CDW phase, for instance into the role of Fermi surface nesting [2, 3]. Layered transition metal dichalcogenides (TMDs) are one of the most commonly investigated classes of CDW materials; their transitions have previously been tuned by varying the thickness or gate potential [4–9]. However, much of the existing theoretical work studying the effect of strain on a CDW phase has been within first-principles density functional theory (DFT). These studies find that for $1T\text{-TiSe}_2$ the CDW transition temperature can be enhanced or suppressed with the application of tensile or compressive strain, respectively [10]. In the latter case, the weakened CDW opens the door for superconductivity (SC). This difference in effect is linked to the distinct behavior of the band gap upon extension versus compression. Strain is therefore useful since it provides an alternate method for modulating CDW physics. Indeed, exploration of the potential use of strain to adjust optical, magnetic and conductive properties, especially in TMDs, has been referred to as 'strain engineering'.

III. THE HOLSTEIN MODEL

The role of electron-phonon interactions in CDW formation has been motivating theoretical studies of the Holstein model for years, and has been observed in a variety of lattice geometries, including the square lattice. The Holstein model on a strained square lattice that I will discuss in my oral exam is given by

$$\hat{\mathcal{H}} = \hat{K} + \hat{U} + \hat{V},$$

$$\hat{K} = -t_x \sum_{\mathbf{i},\sigma} \left(\hat{c}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{i}+\hat{x},\sigma} + \hat{c}^\dagger_{\mathbf{i}+\hat{x},\sigma} \hat{c}_{\mathbf{i},\sigma} \right) - t_y \sum_{\mathbf{i},\sigma} \left(\hat{c}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{i}+\hat{y},\sigma} + \hat{c}^\dagger_{\mathbf{i}+\hat{y},\sigma} \hat{c}_{\mathbf{i},\sigma} \right) - \mu \sum_{\mathbf{i},\sigma} \hat{n}_{\mathbf{i},\sigma},$$

$$\hat{U} = \frac{1}{2} \sum_{\mathbf{i}} \hat{P}^2_{\mathbf{i}} + \frac{\omega_0^2}{2} \sum_{\mathbf{i}} \hat{X}^2_{\mathbf{i}},$$

$$\hat{V} = \lambda \sum_{\mathbf{i},\sigma} \hat{n}_{\mathbf{i},\sigma} \hat{X}_{\mathbf{i}},$$

where $\hat{K}$ is the electron kinetic energy, $\hat{U}$ is the bare phonon term, and $\hat{V}$ is the electron-phonon interaction. $\hat{c}^\dagger_{\mathbf{i},\sigma}(\hat{c}_{\mathbf{i},\sigma})$ are creation (destruction) operators for a fermion of spin $\sigma =\uparrow,\downarrow$ at site $\mathbf{i}$ in the lattice. The two parameters t_x and t_y in $\hat{K}$ are hoppings in the x and y directions respectively, with a dispersion relation given by $\epsilon_{\mathbf{k}} = -2t_x \cos k_x - 2t_y \cos k_y$. At constant volume, compression along one axis is accompanied by an expansion in the orthogonal direction. Thus, in what follows, we set $t_x = t(1-\delta)$ and $t_y = t(1+\delta)$, a choice which keeps $t_x + t_y = 2t$, and hence the bandwidth $W = 4(t_x + t_y)$ constant. Introducing strain into the model this way also allows us to separate the effect of hopping anisotropy from changes which would accompany a simple isotropic reduction or enhancement of W. $\hat{P}_{\mathbf{i}}$ and $\hat{X}_{\mathbf{i}}$ describe a local phonon mode with frequency ω_0 on site $\mathbf{i}$, where the phonon mass has been normalized to $M = 1$. The electron-phonon coupling λ connects the electron density $\hat{n}_{\mathbf{i},\sigma} = \hat{c}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{i},\sigma}$ for spin σ at site $\mathbf{i}$ with the displacement $\hat{X}_{\mathbf{i}}$. Setting the chemical potential to $\mu = -\frac{\lambda^2}{\omega_0^2}$ fixes the system at half-filling $\langle n \rangle = 1$ regardless of temperature, where $\langle n \rangle = \langle n_\uparrow + n_\downarrow \rangle$ is the density. The electron-phonon interaction promotes local pairing of electrons, which is easily seen by considering the single site ($t = 0$) limit. Integrating out the phonon degrees of freedom leads to an effective attractive interaction between electrons with opposite spin given by $U_{\text{eff}} \hat{n}_\uparrow \hat{n}_\downarrow$, where $U_{\text{eff}} = -\lambda^2/\omega_0^2$. Associated with this attraction is an oscillator displacement $\langle X \rangle = -\lambda \langle n \rangle / \omega_0^2$.

IV. METHODOLOGY: DETERMINANT QUANTUM MONTE CARLO

The method I used in my project to investigate the strained Holstein model described above is determinant quantum Monte Carlo (DQMC). Here I will only briefly outline how DQMC works, and will discuss the technique in more detail in my oral exam. To understand how DQMC works, we start with the partition function:

$$Z = \operatorname{Tr} e^{-\beta \hat{\mathcal{H}}} = \operatorname{Tr} e^{-\beta(\hat{K}+\hat{U}+\hat{V})} \tag{1}$$

$$Z = \operatorname{Tr} \left[e^{-\Delta\tau(\hat{K}+\hat{U}+\hat{V})} \dots e^{-\Delta\tau(\hat{K}+\hat{U}+\hat{V})} \right], \tag{2}$$

where in the last line the argument of the trace is a product over $\tau = 1 \dots L_\tau$ exponents such that $\beta = L_\tau \, \Delta\tau$. The index τ is typically refereed to as the imaginary time, where $\Delta\tau$ is the chosen discretization of the imaginary time axis. Taking adavantage of the fact that $\Delta\tau$ is small, we apply the Suzuki-Trotter approximation $e^{\Delta\tau(\hat{A}+\hat{B})} = e^{\Delta\tau\hat{A}} \, e^{\Delta\tau\hat{B}} + \mathcal{O}\left(\Delta\tau^2[\hat{A},\hat{B}]\right)$ and write an approximate form for the partition function given by

$$Z \approx \operatorname{Tr} \left[e^{-\Delta\tau\hat{U}} e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} \dots e^{-\Delta\tau\hat{U}} e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} \right]. \tag{3}$$

Integrating out the phonon terms $e^{-\Delta\tau\hat{U}}$, and using the fact that

$$\operatorname{Tr} \left[e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}(1)} \dots e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}(L_\tau)} \right] = \det \left[\mathbb{1} + e^{-\Delta\tau K} e^{-\Delta\tau V(1)} \dots e^{-\Delta\tau K} e^{-\Delta\tau V(L_\tau)} \right],$$

where $V(\tau)$ and K are matrices filled with real (or in general complex) numbers, results in a final expression for the partition function given by

$$Z = \int_{-\infty}^{\infty} \prod_{i,\tau} dx_{i,\tau} W(\{x_{i\tau}\}) = \int_{-\infty}^{\infty} \prod_{i,\tau} dx_{i,\tau} \left\{ e^{-S_{\text{bose}}} \det[M]^2 \right\},$$

$$S_{\text{bose}}(\{x_{i\tau}\}) = \Delta\tau \left[\frac{\omega_0^2}{2} \sum_{i,\tau} x_\tau^2 + \frac{1}{2} \sum_{i,\tau} \left(\frac{x_{\tau+1} - x_\tau}{\Delta\tau} \right)^2 \right],$$

$$M = \mathbb{1} + e^{-\Delta\tau K} e^{-\Delta\tau V(1)} \ldots e^{-\Delta\tau K} e^{-\Delta\tau V(L_\tau)}.$$

$W(\{x_{i\tau}\})$ is the Monte Carlo weight used in DQMC to decide whether or not to update a given phonon field. Measurements are made using the Green's function, given by $G_{i,j} = \langle c_i c_j^\dagger \rangle = M_{i,j}^{-1}$.

V. RESULTS

Here I will present the results of my work studying a strained Holstein model; for additional information refer to a paper I recently posted on arXiv that is in the process of being submitted to PRB. All of the simulations that were done as part of this work used the parameter values $t = 1$, $\lambda = \sqrt{2}$, $\omega_0 = 1$ and $\lambda_D = 0.25$.

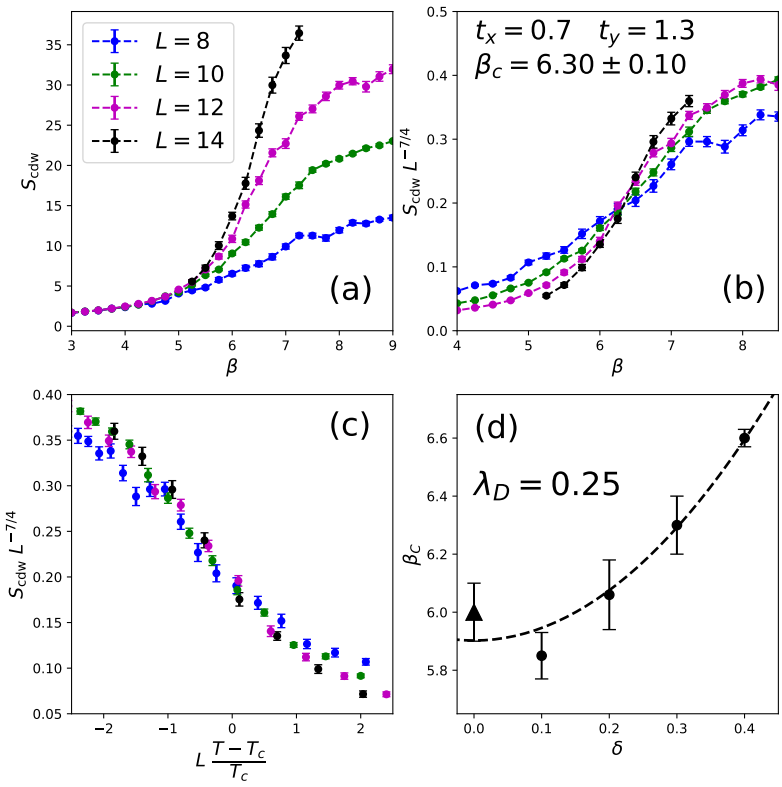

FIG. 1. Panel (a): S_{cdw} versus β for $\delta = 0.3$, $\lambda_D = 0.25$ and four different lattice size. Panel (b): A finite size scaling where the scaled structure factors $S_{\text{cdw}} L^{-\gamma/\nu}$ exhibit a crossing as a function of β for different lattice sizes L. We infer $\beta_c = 6.3 \pm 0.1$ is slightly increased from the isotropic $\beta_c = 6.0$. Panel (c): The full data collapse in which the temperature axis is also scaled by $L^{1/\nu} \left(\frac{T - T_{\text{cdw}}}{T_{\text{cdw}}} \right)$. Panel (d): β_c as a function of δ. The dashed line is a least squares fit to the data. The value of β_c at $\delta = 0$ (triangle) is from Ref. 11.

The quantity we measure in our DQMC simulations when looking for CDW order, and the corresponding critical

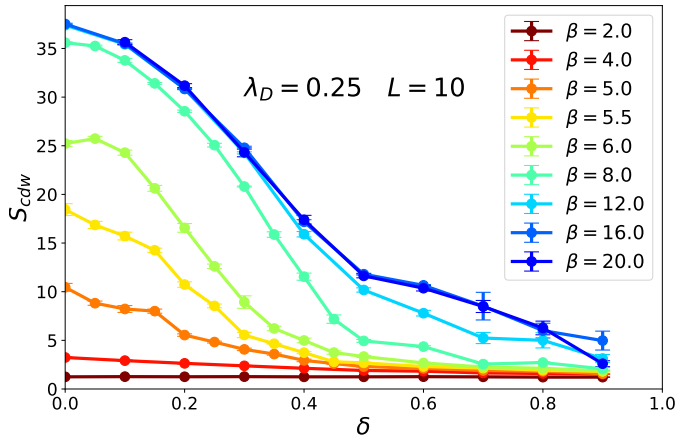

FIG. 2. CDW structure factor versus hopping anisotropy δ. The low temperature value of the CDW order parameter falls to approximately half of its isotropic value as $\delta \to 0.4$.

temperature $T_{\rm cdw}$, is the CDW Structure Factor given by

$$S_{\rm cdw} = S(\mathbf{q}_{\rm cdw}) = \frac{1}{N}\sum_{\mathbf{i},\mathbf{j}} e^{i\mathbf{q}_{\rm cdw}\cdot(\mathbf{i}-\mathbf{j})}\langle(n_{\uparrow,\mathbf{i}}+n_{\downarrow,\mathbf{i}})(n_{\uparrow,\mathbf{j}}+n_{\downarrow,\mathbf{j}})\rangle = \sum_{\mathbf{r}} e^{i\mathbf{q}_{\rm cdw}\cdot\mathbf{r}}c(\mathbf{r}) = \sum_{\mathbf{r}}(-1)^{\mathbf{r}}c(\mathbf{r}).$$

$S_{\rm cdw}$ is the Fourier transform of real space density-density correlation function

$$c(\mathbf{r}) = \langle(n_{\uparrow,\mathbf{i}}+n_{\downarrow,\mathbf{i}})(n_{\uparrow,\mathbf{i}+\mathbf{r}}+n_{\downarrow,\mathbf{i}+\mathbf{r}})\rangle$$

at $\mathbf{q}_{\rm cdw} = (\pi,\pi)$, the wavevector corresponding to checkerboard CDW order on a square lattice. At temperatures above the critical temperature, $T > T_{\rm cdw}$, the structure factor is independent of system size, $S_{\rm cdw} \perp N$, while at temperatures below the critical temperature, $T < T_{\rm cdw}$, the structure factor is proportional to the system size, $S_{\rm cdw} \sim N$. The Finite-Size scaling hypothesis says

$$S_{\rm cdw} = L^{2-2\beta/\nu} g(t\ L^{1/\nu}),$$

allowing us to perform a scaling analysis of the $S_{\rm cdw}$ in order to extract $T_{\rm cdw}$, the results of which are shown in Fig. 1. This analysis is simplified by the knowledge that the appropriate universality class is that of the 2D Ising model, as CDW order on the square lattice breaks a two-fold discrete symmetry.

Fig. 1(a) shows $S_{\rm cdw}$ increasing as the temperature is lowered for different lattice sizes and a strain of $\delta = 0.3$. Panels Fig. 1(b) and Fig. 1(c) shows the crossing and collapse of $S_{\rm cdw}$ respectively as a result of appropriately scaling the data, resulting in a critical temperature of $\beta = 6.30 \pm 0.10$. Finally, Fig. 1(d) shows the interesting result that $T_{\rm cdw}$ changes by less than 10% even out to a moderate strain of $\delta = 0.4$. This is in stark contrast to how $S_{\rm cdw}$ itself changes as δ is increased. Fig. 2 shows that as strain increases from $\delta = 0.0$ to $\delta = 0.4$, $S_{\rm cdw}$ fall off by approximately a half in the $\beta = 20$ low temperature limit, where the system is essentially in its ground state.

VI. FUTURE WORK

The results of my initial investigation into the effect of strain on charge ordering in the Holstein model can be easily extended. Performing analytic continuation in order to extract the momentum-resolved spectral function $A(\mathbf{k},\omega)$ would provide detailed information about the effect of strain on the quasiparticle dispersion, and in particular, the possibility that gaps might develop at distinct temperatures as the momentum $\mathbf{k}$ changes. Work to study that possibility is in progress. Also, moving away from half-filling in order to study the effect of strain on potential competition between checkerboard CDW, superconductivity and striped CDW would be a very interesting extension of the work presented here.

I am also currently working on another project studying CDW order in the Holstein model on a cubic lattice in three dimensions. In that project I am using a combination of Self-Learning Monte Carlo and Langevin techniques to simulate the system.

Finally, a recent paper showed that the half-filled Holstein model on a frustrated triangular lattice has a ground state characterized by superconductivity instead of charge order [12]. It would be an interesting project to study whether superconductivity also supplants charge order in a half-filled Holstein model on a frustrated Kagome lattice.

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