Quantum Monte Carlo Study of the Doped Holstein Model

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1 Introduction

One of the central themes of condensed matter physics over the past few decades has been that of *emergence*, i.e. the onset of new kinds of phenomena which can arise from the collective behavior of large numbers of particles. In principle, one could determine the behavior of a large number of interacting particles by solving the many-body Schrödinger equation, which governs their time evolution. However, this becomes completely infeasible for systems of more than a couple of particles, and computationally, the amount of storage one would require to solve the many-body Schrödinger equation grows exponentially with the number of particles. This is the essence of the 'many-body problem' in quantum mechanics.

The approach taken by my group to resolve this problem can be separated into two main pieces: (i) the choice of a 'model Hamiltonian' which, although a simplification of the system, captures the essential physics we wish to study, and (ii) using a stochastic Monte Carlo method to simulate the system on a computer. The model Hamiltonian which I am currently studying is the *Holstein model*, which is a simplified description of electron-phonon interactions on a lattice, providing insight into the interplay between charge density wave order and the superconducting phase. The method I employ in my research is Determinant Quantum Monte Carlo (*DQMC*). I will now explain both the Holstein model and the DQMC method in more detail below, along with some of my results to date.

2 The Holstein Model

In 1950, the discovery of the isotope effect, i.e. the dependence of the superconducting transition temperature in a material on the ionic mass ($T_c \sim M^{-1/2}$) was the first indication that interactions between electrons and the underlying lattice could be related to superconductivity. Since then, the study of electron-phonon interactions as a mechanism for superconductivity has attracted a great deal of interest. One of the most prominent effective models for the electron-phonon interaction is the Holstein model [1], which is described by the following Hamiltonian:

$$\hat{H} = \underbrace{-t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}) - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma}}_{\equiv \hat{K}} + \underbrace{\frac{1}{2}\sum_i \hat{P}_i^2 + \frac{\omega_0^2}{2}\sum_i \hat{X}_i^2}_{\equiv \hat{U}} + \underbrace{\lambda \sum_{i,\sigma} \hat{n}_{i,\sigma}\hat{X}_i}_{\equiv \hat{V}} \tag{1}$$

Here, $\hat{c}^\dagger_{i\sigma}$ and $\hat{c}_{i\sigma}$ are creation and annihilation operators for an electron of spin $\sigma = \{\uparrow, \downarrow\}$ at site i of the lattice. The notation $\langle i, j\rangle$ means that the sum in the first term is over all nearest-neighbor pairs of sites. The first term therefore represents itinerant electrons hopping between neighboring sites. The parameter t is the nearest-neighbor hopping integral, which sets the energy scale — we typically set $t = 1$ in our simulations.

In the second term, μ is the chemical potential, which controls the overall filling (i.e. the total number of electrons) of the system. $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$ is the number operator, which gives the number of electrons occupying a site. Due to the exclusion principle, the possible occupation states for a single site are $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$ and $|\uparrow\downarrow\rangle$ only. For convenience, this term is grouped with the hopping term to define $\hat{K}$ — the electron kinetic energy. In the Holstein model, on each site of the lattice there is a local harmonic oscillator with fixed frequency ω_0. That is, we consider there to be a dispersionless optical phonon mode associated with each site of the lattice, with $\hat{X}_i$ and $\hat{P}_i$ the corresponding displacement and momentum variables. The third and fourth terms in Eq. 1 are thus the phonon kinetic energy and potential energy,

which we group together to define $\hat{U}$. Electrons are coupled to the local phonon modes through an on-site electron-phonon interaction $\hat{V}$, with a fixed coupling strength λ. The electron-phonon coupling can also be written in terms of a variable $g \equiv \lambda/\sqrt{2\omega_0}$.

Although the Holstein model is quite a simplified description of the electon-phonon interaction, the electron-phonon coupling term crucially gives rise to an effective electron-electron interaction. As a result, some interesting phases can emerge as the temperature is lowered. At half-filling (one electron on average per site), one finds a periodic modulation of charge on bipartite lattices. For the square lattice, this is a checkerboard pattern of alternating doubly occupied and empty sites — this is called charge density wave (CDW) order. Previous studies of the Holstein model have mostly focused on systems at half-filling [2, 3, 4]. However, when the system is doped away from half-filling, the CDW order is weakened, and a superconducting (SC) phase can emerge. The main goal of my project is to study the *doped* Holstein model, focusing on the competition between CDW and SC order on the square lattice. Although there have been attempts to estimate SC transition temperatures in the doped case [5, 6, 7], computational limitations have rendered this mostly unfeasible in the past. I will provide some estimates of T_C found using a finite-size scaling method, obtained by accessing lower temperatures and simulating larger lattice sizes than attempted in previous studies.

3 Determinant Quantum Monte Carlo

In the classical Monte Carlo approach (for example, in simulations of the Ising model) a stochastic procedure is used to generate configurations of a system according to a desired probability distribution, e.g. the Boltzmann distribution. Measurements of physical quantities (e.g. magnetization) can then be made on these samples. The key idea is that after enough iterations, the average value of an observable O should approximate the ensemble average $\langle O \rangle = Z^{-1} \sum_i O_i e^{-\beta E_i}$, where Z is the partition function of the system, $\beta = 1/T$ is the inverse temperature, and the sum is over all possible configurations. The same general idea is used in quantum Monte Carlo, however there is some additional effort required in transforming the quantum problem into a form suitable for Monte Carlo simulation.

The initial step is to rewrite the partition function of the Holstein Hamiltonian $Z = Tr\left(e^{-\beta \hat{H}}\right)$ by expressing the inverse temperature as $\beta = \Delta\tau L$:

$$Z = Tr\left[e^{-\Delta\tau\hat{H}} e^{-\Delta\tau\hat{H}} \dots e^{-\Delta\tau\hat{H}}\right] \tag{2}$$

$$= Tr\left[e^{-\Delta\tau(\hat{K}+\hat{V}+\hat{U})} e^{-\Delta\tau(\hat{K}+\hat{V}+\hat{U})} \dots e^{-\Delta\tau(\hat{K}+\hat{V}+\hat{U})}\right] \tag{3}$$

$$\approx Tr\left[\left(e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{U}}\right)\left(e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{U}}\right) \dots \left(e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{U}}\right)\right] \tag{4}$$

The previous step uses the Suzuki-Trotter approximation, which states that for non-commuting operators ($[\hat{A}, \hat{B}] \neq 0$) we have that $e^{-\Delta\tau(\hat{A}+\hat{B})} = e^{-\Delta\tau\hat{A}} e^{-\Delta\tau\hat{B}} + O(\Delta\tau)^2$. If $\Delta\tau$ is kept small then the error (which scales as $(\Delta\tau)^2$) becomes negligible and we can perform the decomposition shown in Eq. 4. The trace is now over the product of L terms, which we can index by $\tau = 1, \dots, L$, where τ is known as the 'imaginary time'. Let us now perform the trace over both the electron and phonon degrees of freedom:

$$Z = \underset{\{n_{i\sigma}\}}{Tr} \underset{\{x_{i\tau}\}}{Tr}\left[\left(e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{U}}\right)\left(e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{U}}\right) \dots \left(e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} e^{-\Delta\tau\hat{U}}\right)\right] \tag{5}$$

$$Z = \int_{-\infty}^{\infty} \prod_{i,\tau} dx_{i\tau} \underset{\{n_{i\sigma}\}}{Tr}\Big[\langle x_{i,1}| e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{U}} e^{-\Delta\tau\hat{V}} |x_{i,2}\rangle \langle x_{i,2}| e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{U}} e^{-\Delta\tau\hat{V}} |x_{i,3}\rangle \dots \tag{6}$$

$$\dots \langle x_{i,L}| e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{U}} e^{-\Delta\tau\hat{V}} |x_{i,1}\rangle\Big] \tag{7}$$

where we note that the phonon field $\{x_{i\tau}\}$ has two indices: i denotes the spatial site, and τ denotes the 'time slice' along the imaginary time axis. In the last step, the identity operator for the phonon position has been inserted at each imaginary time slice. $|x_{i,\tau}\rangle$ represents the phonon field (i.e. the phonon displacements) for a particular imaginary time τ.

We want to eventually show that the partition function can be written in terms of the phonon variables $x_{i\tau}$ only. To do this, we let the $\hat{K}$ and $\hat{V}$ terms act on the states $\langle x_{i,\tau}|$ and evaluate the resultant $\langle x_{i,\tau}|e^{-\Delta\tau\hat{U}}|x_{i,\tau+1}\rangle$ terms, which give:

$$\langle x_{i,\tau}|e^{-\Delta\tau\hat{U}}|x_{i,\tau+1}\rangle = \exp\left(-\Delta\tau\left[\frac{\omega_0}{2}\sum_i x_{i,\tau}^2 - \frac{1}{2}\sum_i\left(\frac{x_{i,\tau+1}-x_{i,\tau}}{\Delta\tau}\right)^2\right]\right) \tag{8}$$

The partition function can now be written as

$$Z = \int_{-\infty}^{\infty}\prod_{i,\tau}dx_{i,\tau}e^{-S}\prod_{\sigma}\underset{\{n_i\}}{Tr}\left[e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,1})}e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,2})}\dots e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,L})}\right] \tag{9}$$

where

$$S = \Delta\tau\left[\frac{\omega_0^2}{2}\sum_{i,\tau}x_{i,\tau}^2 - \frac{1}{2}\sum_{i,\tau}\left(\frac{x_{i,\tau+1}-x_{i,\tau}}{\Delta\tau}\right)^2\right] \tag{10}$$

is referred to as the 'phonon action'. Since $\hat{K}$ and $\hat{V}$ are quadratic in fermion creation and annihilation operators, they can be expressed as $\hat{K} = \underline{\hat{c}}^\dagger\bar{K}\underline{\hat{c}}$ and $\hat{V}(x_{i,\tau}) = \underline{\hat{c}}^\dagger\bar{V}(x_{i,\tau})\underline{\hat{c}}$, where $[\underline{\hat{c}}^\dagger]^T = (\hat{c}_1^\dagger, \hat{c}_2^\dagger \dots \hat{c}_N^\dagger)$ is a row vector containing fermion creation operators for each site in the lattice. $\bar{K}$ and $\bar{V}$ are both $N\times N$ matrices. Now, since $\hat{K}$ and $\hat{V}$ are quadratic in fermion operators they obey the following identity:

$$Tr\left[e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,1})}\dots e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{V}(x_{i,L})}\right] = \det\left[\mathbb{1} + e^{-\Delta\tau\bar{K}}e^{-\Delta\tau\bar{V}(x_{i,1})}\dots e^{-\Delta\tau\bar{K}}e^{-\Delta\tau\bar{V}(x_{i,L})}\right] \tag{11}$$

On the right-hand side, the expression in square brackets is another $N\times N$ matrix which we denote by $\bar{M}$. The partition function now becomes:

$$Z = \int_{-\infty}^{\infty}\prod_{i,\tau}dx_{i,\tau}e^{-S}\left[\det(\bar{M})\right]^2 \tag{12}$$

$$= \int_{-\infty}^{\infty}\prod_{i,\tau}dx_{i,\tau}W(\{x_{i\tau}\}) \tag{13}$$

where $W(\{x_{i\tau}\}) = e^{-S}\left[\det(\bar{M})\right]^2$ is a function of the phonon field only. We can now perform random sampling over the phonon field (using the Metropolis-Hastings algorithm), where $W(\{x_{i\tau}\})$ plays the role of a Monte Carlo 'weight' for a given configuration. As in classical Monte Carlo simulations, we can calculate various physical quantities for each sampled configuration, with the resulting measurements becoming precise after a sufficient number of Monte Carlo steps.

4 Results

Using DQMC, we can obtain measurements of various physical quantities which can indicate different phases. I will mainly discuss measurements of the CDW structure factor $S(\mathbf{q})$, which measures charge ordering on the square lattice, and the s-wave superconducting pair susceptibility P_s, which analyzes pairing features. These quantities are given by:

$$S(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{i},\mathbf{j}}e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\langle n_\mathbf{i}n_\mathbf{j}\rangle \tag{14}$$

$$P_s = \frac{1}{N}\int_0^\beta\langle\Delta(\tau)\Delta^\dagger(0)\rangle d\tau \tag{15}$$

where we define $\Delta(\tau) = \sum_\mathbf{i}c_{\mathbf{i}\downarrow}(\tau)c_{\mathbf{i}\uparrow}(\tau)$. Our simulations allow us to study a range of lattice sizes (up to 12×12 here), for temperatures as low as $\beta = 28$. The density is varied by changing the chemical potential, in order to study how the CDW and SC correlations change as the system is doped away from half-filling. We can also define a dimensionless electron-phonon coupling $\lambda_D = \frac{\lambda^2}{\omega_0^2 W} \equiv \frac{2g^2}{\omega_0 W}$ where $W = 8t$ is the electronic bandwidth for the square lattice. In this work we fix $\lambda_D = 0.25$ and focus on two parameter sets: $g = 1$, $\omega_0 = 1$ and $g = 2$, $\omega_0 = 4$. In both cases, measurements of $S(\pi,\pi)$ indicate strong CDW order at half-filling, which is greatly reduced as the system is doped away from

half-filling. Simultaneously, SC correlations become stronger away from half-filling, with measurements of P_s appearing to peak within the density range $0.6 \leq \rho \leq 0.85$, as shown in Fig. 1. By tuning the chemical potential, we can fix the electron density at a desired target value and study P_s as a function of temperature. We fix the density at $\rho = 0.6$ and $\rho = 0.7$ for $g = 1$, $\omega_0 = 1$ and $\rho = 0.6$ and $\rho = 0.85$ for $g = 2$, $\omega_0 = 4$, and plot P_s vs β in each case. At high temperatures (low β), P_s is relatively small and independent of lattice size L, however as the temperature is lowered, P_s grows and becomes dependent on lattice size, e.g. as shown in Fig. 2 for one particular parameter set. This indicates the superconducting phase transition, since when correlations become long range, they will be sensitive to the lattice size in a finite system. We can therefore apply a finite-size scaling analysis described below to obtain the transition temperature T_c.

Generally, near a phase transition, physical quantities (such as the pair susceptibility P_s) should scale with the reduced temperature $t = (T - T_c)/T_c$ raised to the power of some *critical exponent*. The correlation length for the system ξ in turn scales with t to the power of some critical exponent. However, for a finite-size system, the more relevant length scale becomes the linear dimension L of the lattice. In this case, P_s should scale as some power of L multiplied by a function of the ratio L/ξ. This is known as the 'scaling hypothesis', and forms the basis for the finite size scaling approach. For the 2D superconducting transition, which is known to belong to the Kosterlitz-Thouless universality class, one has $P_s \sim L^{7/4} f(L/\xi)$ with $\xi \sim \exp\left(At^{-1/2}\right)$, where A and T_c are unknown variables. Plotting $P_s L^{-7/4}$ as a function of $L \exp[-A(T - T_c)^{-1/2}]$ for different lattice sizes L should result in all the data collapsing onto a single curve, which allows us to estimate T_c.

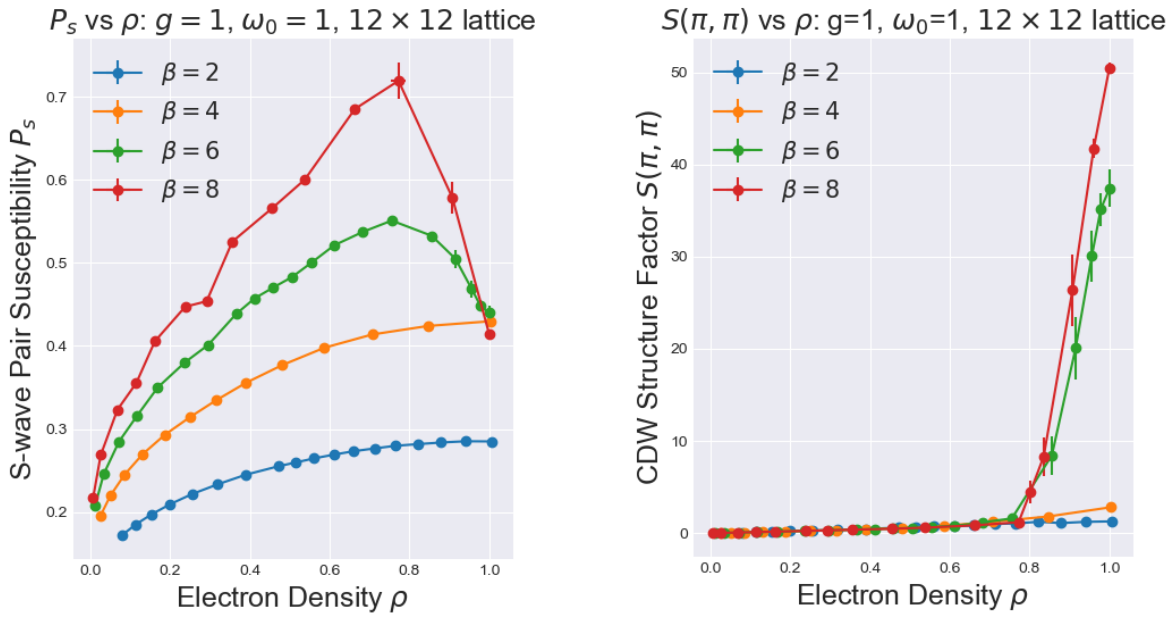

Figure 1: Left: Pair susceptibility data is shown as a function of electron density for $\beta = 2, 4, 6, 8$ for a 12×12 lattice (for $g = 1$, $\omega_0 = 1$). At low temperature, the superconducting correlations are enhanced when the system is doped away from $\rho = 1$. Right: The CDW structure factor $S(\pi, \pi)$ which measures charge ordering is shown as a function of electron density. CDW order dominates at half-filling, but this is greatly suppressed as electron density is reduced. These plots illustrate the competition between CDW and SC in the Holstein model.

For the two densities studied at $g = 1$, $\omega_0 = 1$ the data collapses onto a single curve at around $\beta_c \approx 28.5$. When the phonon frequency is increased to $\omega_0 = 4$, the SC transition temperature is raised: for $g = 2$, $\omega_0 = 4$ we find approximately $\beta_c \approx 22.5 - 23.5$. When phonon frequency is increased, CDW order in the Holstein model is weakened, which favors superconducting order. Measurements of density-density correlations on the square lattice also illustrate a weakening of the checkerboard charge ordering when ω_0 is increased. It should be noted these values of $T_c = 1/\beta_c$ are only approximate, as we are quite

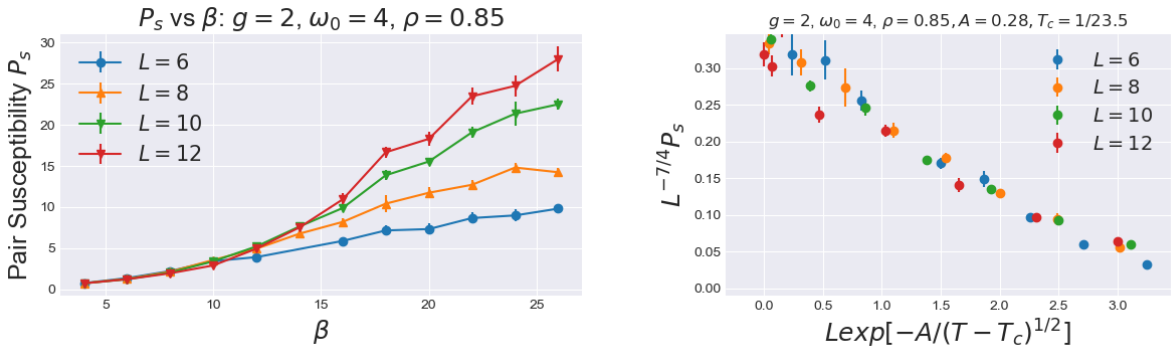

Figure 2: Left Pair susceptibility as a function of the inverse temperature β is shown for the $g = 2$, $\omega_0 = 4$, $\rho = 0.85$ parameter set, for lattice sizes of linear dimension $L = 6, 8, 10, 12$. Right: Finite-size scaling of the pair susceptibility data for $g = 2$, $\omega_0 = 4$, $\rho = 0.85$, which gives an estimated $\beta_c \approx 23.5$.

limited by the range of lattice sizes we can study with DQMC. However, previous attempts to estimate T_c in the Holstein model have been unable to perform any such scaling analysis, due to computational limitations in the past. Indeed, previous works such as [5] study temperatures down to $\beta = 12$ only, for lattices no larger than 8×8, and provide only a broad estimate of $\beta_c \approx 30$–40 for $g = 1$, $\omega_0 = 1$. Since we previously set the energy scale by taking $t = 1$, our estimates of β can be converted to Kelvin given an electronic bandwidth $W = 8t$ in eV. For example, if $W = 8t = 1eV \approx 12000K$, then $\beta_c = 28.5$ corresponds to $T_c = (1/28.5)t = (1/28.5)(12000/8) \approx 50K$.

5 Future work

This study is ongoing and work is currently in progress to estimate T_c for lower phonon frequencies for the doped Holstein model on the square lattice. Newly developed algorithms have also made studies of the Holstein model in three-dimensional systems feasible [8, 9], although it remains to be seen whether one can determine estimates of T_c for the superconducting transition. Future work will involve studying the Holstein model on the cubic lattice, where we hope to be able to find a superconducting transition away from half-filling.

Although not the topic of my oral presentation, I have also done some work on the thermodynamics of spin systems along with my co-advisor Prof. Rajiv Singh, resulting in a recent Physical Review B publication on the triangular Ising antiferromagnet [10], and another work (recently submitted to Physical Review B) on a variant of a spin model defined on the honeycomb lattice [11].

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