Temperature and Doping Phase Diagrams For the Holstein Model in the Migdal Approximation.

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ABSTRACT: Within this manuscript and the associated seminar presentation, I present results from a soon-to-be-released open-source code that simulates the two-dimensional Holstein model within the Migdal approximation. This algorithm implements fast Fourier transforms to evaluate the momentum and Matsubara frequency sums pertinent to the expressions defining the fully renormalized electron and phonon propagators and evaluates them self-consistently. This routine has given us access to finite-size lattice simulations previously unseen in similar calculations. Most importantly, we were able to study pairing and charge density correlations over a wide range of electron doping and frequency and have observed the emergence of a superconducting dome with increasing phonon frequency.

INTRODUCTION: The electron-phonon (e-ph) interaction (EPI) is pervasive in solids and supports the transport and other properties of many poor metals and semiconductors. The EPI is now commonly associated with conventional superconductivity (SC) where the pairing between electrons is understood to be mediated by virtual phonon exchange[1]. In addition to SC, the EPI is also responsible for charge-density-wave (CDW) insulators [2]. Landau was the first to propose the existence of the lattice polaron[3], which is a quasiparticle known to form if the EPI is sufficiently large. Effective models dealing with polaron physics have been an active field of study since the development of the Fröhlich[4] and Holstein[5] Hamiltonians, and even the more recent *ab initio* treatments of the EPI have made remarkable progress[6].

Despite the long and arduous effort to study these systems, many issues remain to be addressed, even for the simplest models. Among these models, the Holstein-model (and its extension: the Hubbard-Holstein model) has served as the most straightforward way to describe systems of electrons interacting with the crystal lattice. Approximating the ionic motion using a system of independent oscillators with a non-dispersive phonon energy scale given by Ω, the electrons and phonons have a purely local on-site coupling $g = \alpha / (2M\Omega)$ where M is the ion mass and α is the EPI strength. This isotropic e-ph coupling is assumed momentum independent in the Holstein model, but this is not necessarily true in general; i.e. we should expect some anisotropic form $g_{\mathbf{k},\mathbf{q}}$. The second quantized single-band Holstein Hamiltonian in 2D is expressed in real space as

$$\hat{H} = -\sum_{i,j,\sigma} t_{i,j}(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{h.c.}) - \mu\sum_{i,\sigma}\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma} + \sum_{i}\left[\frac{\hat{P}_i^2}{2M} + \frac{1}{2}M\Omega^2\hat{X}_i^2\right] + \sum_{i,\sigma}\alpha\left(\hat{n}_{i,\sigma} - 1\right)\hat{X}_i \qquad (1.1)$$

where the hopping $t_{i,j} \to t$ is to nearest neighbor (NN) sites, μ is the chemical potential, $\hat{c}^{\dagger}_{i,\sigma}$ ($\hat{c}_{i,\sigma}$) creates (annihilates) an electron on site i with spin σ, $\hat{n}_{i,\sigma} = \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma}$ is the electronic number operator, and $\hat{P}_i$ ($\hat{X}_i$) represents the momentum (position) operator for the i^{th} ion in the lattice.

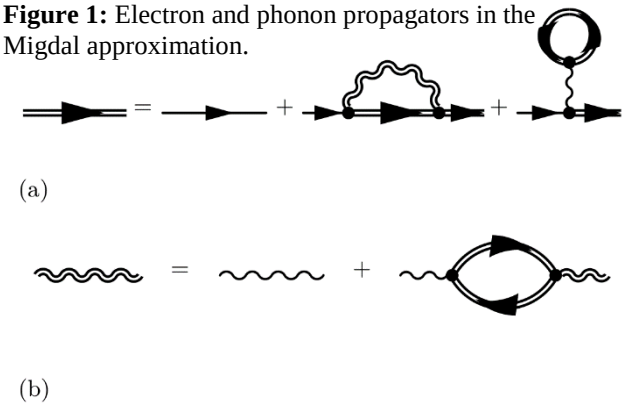
The Holstein model as defined in Eqn.(1.1) has been studied extensively via analytical and numerical techniques including diagrammatic expansions [7], variational approaches[8], dynamical mean-field theory[9,10], and quantum Monte Carlo methods[7,8,11–15]. Collectively,

these studies confirm that the Holstein model exhibits CDW and superconducting instabilities, the latter in the s-wave channel. The associated transition temperatures for these phases vary as a function of doping, phonon frequency, and Fermi surface topology. However, there does not seem to be any comprehensive study of the temperature-doping phase diagram for this model.

The Holstein model is often studied diagrammatically within the Migdal approximation[16]. Migdal's original theory made the argument that corrections to the e-ph vertex function were of $\mathcal{O}(\lambda(\Omega / E_F))$ where λ is the dimensionless e-ph coupling and E_F is the Fermi-energy. If the e-ph coupling is not too large and the renormalization of both the electron and phonon properties are accounted for self-consistently, the Migdal approximation compares well with QMC near half-filling[7,10,15]. It should be stated that these studies do not comprehensively prove this to be true, rather they show this to be the case for select parameters. In what follows, we will show that the diagrammatic approach can be used to obtain temperature vs. doping phase diagrams.

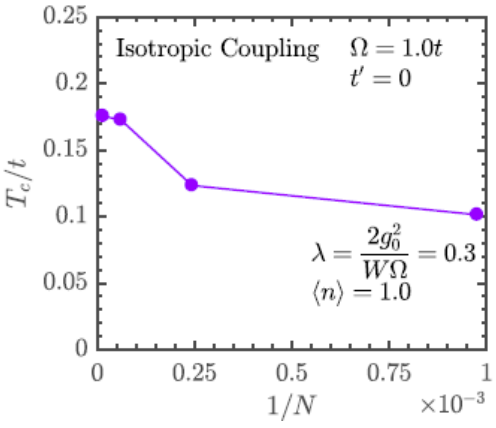
PROCEDURE: In the Migdal theory, we calculate the electron and phonon propagators and self-energies in a self-consistency loop. We can do this because we have analytical expressions from the diagrammatic expansion. The figure on the right depicts the (a) fully-dressed single-particle propagator and (b) the fully dressed phonon propagator. The electron self-energy is composed of two pieces, the (non-crossing) rainbow diagrams, and the Hartree term. Finding the values of these propagators numerically allows us to calculate higher particle number correlations such as two particle susceptibilities. Since we are interested in pairing and CDW correlations, we have calculated the temperature dependence of the singlet-pairing (superconducting) susceptibility χ^{SC} and the CDW susceptibility $\chi^{CDW}(\mathbf{q})$ where $\mathbf{q}$ is a momentum transfer (a.k.a. scattering) vector.

Figure 1: Electron and phonon propagators in the Migdal approximation.



In the thermodynamic limit, each of these two susceptibilities can diverge as the calculation approaches their respective quantum critical temperatures T_c^{SC} and T_c^{CDW}. Usually, the system has an instability that favors one phase over the other, with the other correlations being suppressed. Our calculations are performed on a finite-size lattice, hence they only approximate the thermodynamic limit and thus also the asymptotic behavior for χ. Careful extrapolation of the inverse susceptibilities to the temperature axis is one way to find estimates for the critical temperatures, but we find that this is only reliable for the SC-transition because χ^{SC} approaches its thermodynamic limit behavior even for modestly sized lattices (e.g. N=64[2]). For $\chi^{CDW}(\mathbf{q})$ it is well known[12] that this function should obey the Ising universality class in two dimensions so that we can fit χ^{CDW} (for a single $\mathbf{q}$ vector) with $\chi(\mathbf{q}_{max}) = A|T/T_c - 1|^{-7/4}$, and with this fit we obtain T_c^{CDW}. We find that the finite size dependence is rather significant as seen in the figure to the right. For

Figure 2: Finite-size dependence. Hopping beyond NN sites is 0, i.e. t'=0.



lattice sizes smaller than N=32^2 , the Ising class is a very poor descriptor of the functional behavior of χ^{CDW} and thus we omit those fit results smaller than this value.

RESULTS: After collecting the critical temperatures across a wide range of electron doping $\langle n \rangle$ from 0 to 1.0 (where $\langle n \rangle$ =1.0 =half-filling), we plotted the phase diagrams in the three-panel plot (Fig. 3). We performed all these calculations for a constant dimensionless coupling $\lambda = 2g^2 / W\Omega = 0.3$ but examined three phonon frequencies $\Omega / t =$ 0.1, 0.5, and 1.0. In all cases there exists a commensurate CDW phase peaked at half-filling with at scattering vector $\mathbf{q}_{\max} = (\pi, \pi)$ which is suppressed with increasing Ω. For panel (a), we observe an incommensurate CDW where $\mathbf{q}_{\max} = (\pi, \kappa\pi)$ with $\kappa < 1$. Most notably, we see that increasing Ω reveals a larger non-monotonic SC region which can effectively be called a dome. This behavior is only thought to be associated with unconventional SC, however, we see it here under the Migdal approximation which is associated with BCS-like superconductivity.

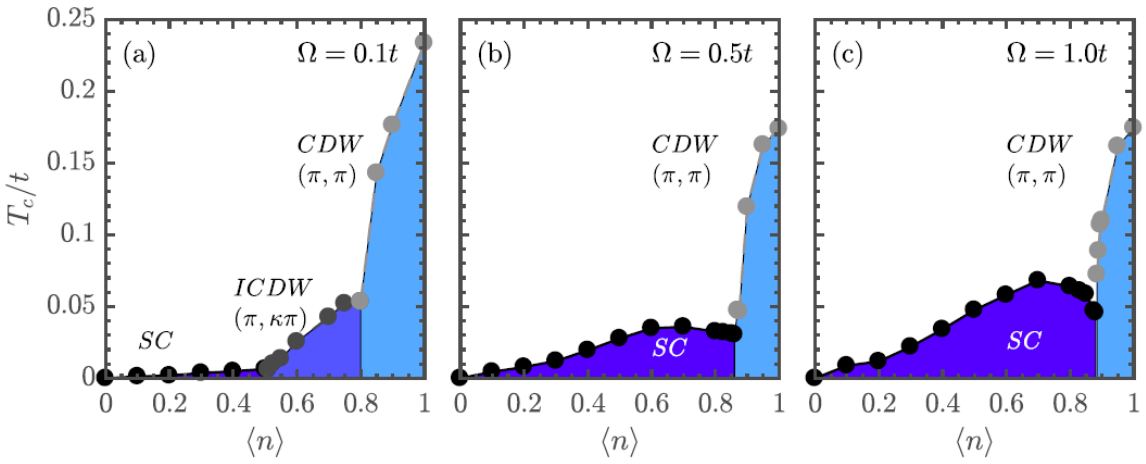


Figure 3. The temperature-doping phase diagram for (a) $\Omega / t = 0.1$(b) $\Omega / t = 0.5$, and (c) $\Omega / t = 1.0$. Results were obtained for $N = 128^2$ site lattice and dimensionless coupling $\lambda = 0.3$.

CONCLUSION: Here we have shown the emergence of an SC-dome within the framework of a theory associated with conventional superconductivity. Moreover, we have also shown that using finite-size calculations to approximate the thermodynamic limit needs to be carefully investigated as our relatively large calculations up to $N = 128^2$ were especially important for capturing the proper universality class behavior of the CDW correlations. Both findings should be of importance to those who work with effective models aimed at studying emergent phenomena. Namely, a SC dome may emerge in a conventional superconductor and more justification may be required when studies claim to study the thermodynamic limit with finite-size calculations.

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