Pseudogap crossover in the electron-phonon system

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Thermodynamic properties of the square-lattice Holstein model of the electron-phonon problem with phonon frequencies small compared to the bare Fermi energy are obtained using Monte Carlo methods, a strong-coupling (bipolaronic) expansion, and a weak coupling Migdal-Eliashberg approach. Already at elevated temperatures where the charge-density wave (CDW) and superconducting (SC) correlations are very short-range, a crossover occurs as a function of increasing electron-phonon coupling, \( \lambda_0 \), from a normal metallic regime to a pseudogap regime. At sufficiently low \( T \), a SC phase is found for small \( \lambda_0 \) and a commensurate insulating CDW phase for large \( \lambda_0 \).

\[ H = H_c + H_p + H_{e-p}, \]
\[ H_c = - \sum_{ij \sigma} t_{ij} c_i^{\dagger \sigma} c_{j \sigma} - \mu \sum_{i \sigma} n_{i \sigma}, \]
\[ H_p = \sum_i \left( \frac{p_i^2}{2M} + \frac{1}{2} K x_i^2 \right), \]
\[ H_{e-p} = \alpha \sum_{i \sigma} x_i n_{i \sigma}, \]

and \( \omega_0 = \sqrt{K/M} \). The important dimensionless parameters are the coupling strength \( \lambda_0 \equiv \alpha^2 \rho(0)/K \) and the

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**Introduction** – Electron-phonon interactions determine many of the electronic properties of quantum materials; this includes the normal state electrical transport properties of most metals at all but the lowest temperatures, and of course the nature of the superconducting (SC) and/or charge-density-wave (CDW) ground-states of many “conventional” materials. In all but a few cases, the dimensionless electron-phonon coupling constant, \( \lambda_0 \), is of order one. Nonetheless, there is a genuine small parameter in the problem, the ratio of the phonon energy, \( \hbar \omega_0 \), to the bare Fermi energy, \( E_F^{(0)} \). While it has been argued that Migdal-Eliashberg (ME) theory provides an accurate solution to this problem provided \( \lambda_0 \ll E_F^{(0)}/\hbar \omega_0 \), we recently showed that ME theory breaks down when \( \lambda_0 \sim 1 \), even when the nominal condition for its validity is satisfied. As was already suggested in various earlier studies this breakdown is associated with the non-perturbative formation of bipolarons.

In the present paper, we explore the global phase diagram of the Holstein model – the paradigmatic model of the electron-phonon problem – over a broad range of temperatures, \( T \), and \( \lambda_0 \) in the physically important limit \( \hbar \omega_0/E_F^{(0)} \ll 1 \). We have carried out extensive Monte Carlo (MC) calculations, which we then compare with the results of ME theory and with a strong-coupling expansion (in powers of \( 1/\lambda_0 \)). As shown in the schematic phase diagram in Fig.1 there are two regions separated by a crossover line, \( T = T^*(\lambda_0) \); ME theory gives a good account of the physics only in the left region while a strong-coupling “polaronic” approach is accurate to the right. (Naturally, neither approach is entirely reliable close to the crossover line.)

The physics in the two regions is correspondingly distinct: In the weak coupling regime, the properties of the normal state are dominated by weakly scattered quasiparticle excitations near a well-defined Fermi surface with decay rates \( \hbar \gamma \sim \lambda_0 T \) and there is a low-\( T \) superconducting ground-state with a transition temperature \( T_c \) which is proportional to \( \hbar \omega_0 \) times a (possibly non-monotonic) function of \( \lambda_0 \). In the strong-coupling limit, there is a “pseudogap” to single-particle excitations, the normal state is a classical lattice gas of (effectively non-dynamical) bipolarons with binding energy \( \sim \lambda_0 E_F^{(0)} \) and at low temperatures the system has a tendency to commensurate CDW states, with ordering vectors unrelated to any Fermi-surface nesting vector. Depending on the electron density there may be a sequence of transitions to higher-order commensurate states or phase separation.

We will study the Holstein Hamiltonian

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**FIG. 1.** Schematic phase diagram of the electron-phonon problem with small \( \omega \equiv \hbar \omega_0/E_F^{(0)} \). Depending on details of the band-structure and the electron density, additional CDW phases can arise (including metallic ones at intermediate \( \lambda_0 \)).
retardation parameter \( w \equiv \hbar \omega_0/E_F^{(0)} \), where \( \rho^{(0)} \) is the bare (\( \alpha = 0 \)) density of states at the Fermi energy. While there are notable exceptions, the regime of the Holstein model relevant to most materials is \( w \ll 1 \).

We therefore study the phase diagram and thermodynamic correlation functions of the Holstein model in the limit \( w \ll 1 \). In previous work we carried out such a study via determinant quantum Monte Carlo (DQMC) for \( w = 0.1 \), but only for weak to moderate \( \lambda_0 : 0 \leq \lambda_0 \leq 0.6 \). The DQMC method is challenging to employ in the strong-coupling regime due to prohibitively long autocorrelation times for temperatures much lower than \( E_F^{(0)} \). Fortunately, in this strong-coupling regime especially, the results are not expected to depend strongly on \( M \) so long as \( w \ll 1 \), an expectation that we have confirmed where it can be tested. Thus, to analyze the full phase diagram, we will consider here the limit \( M \to \infty \), corresponding to \( w \to 0 \). In this limit the phonons become classical variables, and the MC calculations become substantially simpler. (See the Appendix for details of the MC algorithm employed.) We have chosen parameters to avoid any non-generic band features or special commensurate densities – specifically we take the matrix \( t_{ij} \) to contain both nearest-neighbor hopping \( t \) and next-nearest-neighbor hopping \( t' \), with the ratio \( t'/t = -0.3 \). We work at a fixed chemical potential, chosen such that the density is \( n = 0.8 \) at \( T = 0.25t \). We have studied systems of linear size \( L \leq 12 \) with periodic boundary conditions and temperatures \( T \geq t/40 \).

Results – The phase diagram derived from our MC studies in the \( M \to \infty \) limit is shown in Fig. 2. For \( \lambda_0 \ll 1 \) we find a translationally invariant Fermi liquid ground-state. At strong-coupling \( \lambda_0 \gg 1 \) the low-energy degrees of freedom are bipolarons, which have a binding energy \( V = \alpha^2/K \) and behave as a lattice gas of interacting hard-core classical charge 2e particles. (It is convenient to think of the bipolarons as hard-core bosons, but because they are non-dynamical in this limit, they in fact have no meaningful quantum statistics.) The change in the nature of the low-energy states manifests as a pseudogap in the single-particle electron spectrum, onsetting at a temperature \( T^* \sim V \). At lower \( T \) and for sufficiently large \( \lambda_0 \) we find a \((\pi, \pi)\) CDW state. While ME theory is extremely accurate for \( T > T^* \), we will see that it fails to describe the crossover at \( T \sim T^* \), and misses the strong-coupling physics when \( T < T^* \) entirely. By contrast, the strong-coupling expansion (also discussed below) gives a satisfactory account of the system in the strong-coupling regime; in particular, the CDW phase boundary labeled \( T_{c}^{\text{sing}} \) in the figure was computed to leading order in the strong-coupling expansion for the same parameters as in the DQMC study. Variations of the density with temperature and coupling strength are shown in Figure 3.

We have previously carried out DQMC results for this model with large but finite \( M \) such that \( w = 0.1 \). We expect the thermodynamic properties for \( w = 0 \) to be similar to those with \( w = 0.1 \) when \( T > \hbar \omega_0 \) or to the right of the \( T^*(\lambda_0) \) line. While we have not explicitly tested this in all cases (especially at large \( \lambda_0 \) and low \( T \), where the \( w \neq 0 \) DQMC is most difficult), we have verified the validity of this expectation wherever we have \( w \neq 0 \) results. Even to the left of the \( T^*(\lambda_0) \) line, the results with \( w = 0 \) and \( w = 0.1 \) differ little down to temperatures that are a small fraction of \( \hbar \omega_0 \). However, in this weak coupling regime, for finite \( w \) (but still \( w \ll 1 \)) we expect a SC transition at \( T_c \sim \hbar \omega_0 \exp(-1/\lambda) \). This accounts for the one qualitative difference between Fig.
where \( \omega/t _0 \) as a function of \( T \) is provided in the Appendix.

where \( \lambda _0 \) is the linear system size, assuming the transition to be in the Ising universality class. Details of this analysis are provided in the Appendix.

From a strong-coupling expansion in \( 1/\lambda _0 \) one finds the effective Hamiltonian for the system (which gives a valid description for temperatures \( T \ll V \)) is an antiferromagnetic Ising model in a uniform external field \( \delta_0 \).

\[
H_{\text{eff}} = \sum_{ij} J_{ij} \sigma_i \sigma_j - \hbar \sum_i \sigma_i ,
\]

where \( \sigma_i \) are classical Ising variables taking on the values \( \pm 1 \) and \( J_{ij} = 2 \lambda \sigma_i /U \). The relation to the electronic degrees of freedom is that \( \sigma_i = 1 \) if a site is occupied by a bipolaron and zero otherwise. The density \( n \) of the original electrons and the magnetization \( m \) of the Ising spins are related by \( n = 1 + m \). In the parameter regime where the nearest-neighbor \( J \) is much stronger than all further neighbor couplings and also near to half-filling \( (m = 0) \), this model has a transition from a paramagnetic phase to a \( (\pi, \pi) \) antiferromagnetic phase at a temperature \( T_{\text{Ising}} \sim J \). Depending on \( m \) and the nature of the further neighbor couplings there may be additional ordering transitions or phase separation at lower temperatures. \( \delta_0 \), we have computed \( T_{\text{Ising}} \) for the parameters relevant to the model under consideration – nearest-neighbor \( J = 2t^2 /U \), next-nearest-neighbor \( J' = 2t'^2 /U \), and external field \( h \) tuned such that \( m(T = 0.25t) = -0.2 \) and in Figure 2 we show that the transition temperature coincides very accurately with \( T_{\text{cdw}} \) of the full Holstein model for \( \lambda_0 \gtrsim 1 \).

\( \delta_0 \), \( \delta_0 \), \( \delta_0 \), \( \delta_0 \)

\[
\rho_X(\omega) = \frac{1}{L^2} \sum_{\lambda} \delta(\omega - E_\lambda[X]),
\]

where \( E_\lambda \) are the single-particle energies in the phonon configuration \( X \). The DOS is then obtained by averaging over phonon configurations (This procedure is explained in more detail in the Appendix). In practice the delta functions in \( \delta_0 \) are resolved with a Lorentzian broadening, with broadening parameter \( \eta \) chosen to be on the order of the finite size gaps in the single-particle spectrum for a given system size. The DOS for representative weak and strong-coupling values is shown in Figure 4.
FIG. 5. Temperature averaged DOS at the Fermi-energy $\rho_3$ at $T = 0.25t$, normalized by the zero-temperature, non-interacting DOS $\rho^{(0)}$. At this elevated temperature $\rho_3 < \rho^{(0)}$ even for $\lambda_0 = 0$. The breakdown of ME theory occurs for $\lambda_0 \approx 0.5$. Linear system size is $L = 12$.

The appearance of a pseudogap is also evident in thermodynamic observables. In the $w = 0$ limit of the current model, the charge and spin susceptibilities are degenerate and we therefore define a single static susceptibility

$$\chi = \frac{\beta}{L^2} \left( \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 \right) = \frac{\beta}{L^2} \left( \langle \hat{M}^2 \rangle - \langle \hat{M} \rangle^2 \right), \quad (8)$$

were $\hat{N} = \sum_i \hat{n}_i$ and $\hat{M} = \sum_i \hat{s}_i^z$. In Figure 4 we see there is indeed a depression of $\chi$ below $T^*$.  

**ME theory** – Migdal-Eliashberg (ME) theory purports to solve the electron-phonon problem for any coupling strength $\lambda_0$, provided the product $\lambda_0w \ll 1$ [11] for $w = 0$ the ME theory should therefore be valid for arbitrary $\lambda_0$. To assess the validity of this statement we compare the single-particle DOS computed within ME theory to that obtained with MC results. Our ME calculations are carried out in imaginary time and therefore comparison with dynamical quantities (e.g., single-particle DOS) requires analytic continuation. Rather than dealing with complications associated with analytic continuation we will work with a proxy for the low-energy DOS:

$$\rho_3 = \frac{\beta}{\pi} G(x = 0, \tau = \beta/2) = \frac{\beta}{2\pi} \int d\omega \frac{\rho(\omega)}{\cos(\beta\omega/2)}. \quad (9)$$

This quantity is essentially the single-particle DOS averaged over an energy window of order the temperature. At low-temperatures $\rho^{(0)} \approx \rho_3$. In Figure 5 we show $\rho_3$ computed with MC and within ME theory, at $T = 0.25t$ where the density in both calculations is $n = 0.8$. We find ME becomes qualitatively incorrect for $\lambda_0 \gtrsim 0.5$, where the MC shows a precipitous drop due to the onset of the pseudogap ($T^* \approx 0.25t$ for $\lambda_0 = 0.5$), while the ME shows a much weaker dependence. We emphasize that this temperature is well above $T_{cdw}$ ($T_{cdw} \approx 0.1t$ for $\lambda_0 = 0.5$) and therefore the breakdown of ME theory is unrelated with the onset of CDW order. Indeed, we find that $T_{cdw}$ drops rapidly as the density decreases from $n = 1$, while $T^*$ is essentially unchanged. Rather, the breakdown occurs because of a dramatic rearrangement in the low-energy spectrum upon entering the pseudogap regime. When $\lambda_0 > 1$, and even when $\lambda_0w = 0$, the ME perturbation theory breaks down because it is a perturbative expansion around the wrong state.

**Conclusion** – While ME theory works well for sufficiently weak coupling, it breaks down to the right of the $T^*(\lambda_0)$ line where the system is described by a classical lattice gas whose low-energy excitations are bipolarons. Because $T^*$ exceeds significantly the ordering temperature $T_{cdw}$ we do not associate the breakdown of ME theory with a competing order or fluctuations near $T_{cdw}$.

Interesting materials typically have multiple phonon branches, often multiple electronic bands crossing the Fermi energy, and generally more structured electron-phonon coupling, so quantitative comparison with the results for the Holstein model are of course not possible. However, we feel that aspects of the present results are of general relevance. Two aspects of the results, in particular, are relevant to phonon-mediated superconductivity. On the one hand, the breakdown of ME theory when $\lambda_0 \sim 1$ appears to be unavoidable; for example, seeking ways to prevent a lattice instability (e.g., CDW ordering) does not, by itself, extend the range of validity of ME theory. Moreover, while large $\lambda_0$ can indeed produce a large pairing scale, the resulting bipolaron formation is accompanied by a drop in the superconducting susceptibility. These results further corroborate our earlier inference that there is an optimal value of $\lambda_0 \sim 1$ at which $T_c$ is maximal, and that $T_c$ always drops quickly to zero for larger $\lambda_0$.

In exploring whether the optimal $\lambda_0$ obtained here is consistent with experimental data, it is important to distinguish the bare value of the electron-phonon coupling – our $\lambda_0$ – from the renormalized value, $\lambda$, which can be extracted, for example, from tunneling data. The induced phonon softening that is prominent at larger coupling strength results in values of $\lambda > \lambda_0$. For example, for the Holstein model with the same parameters studied here $\lambda_0 = 0.5$ corresponds to $\lambda \approx 2$. In this context, we note that in the famous Allen-Dynes compilation of experimental values of $\lambda$ and $T_c$ for a large number of conventional superconductors, all the entries are roughly in the range $\lambda \lesssim 2$. The presence of an apparent upper bound on $\lambda$ in SCs is something that is not expected on the basis of ME theory.

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Appendix A: Monte-Carlo algorithm

We study the Hamiltonian \[ H = H' + H_p, \] where

\[ H' = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \sum_{i\sigma} (\mu - \alpha x_i) n_{i\sigma}, \]

\[ H_p = K \sum_i x_i^2. \]

The partition function is

\[ Z = \text{Tr} e^{-\beta (H' + H_p)} = \int DX \ e^{-\beta H_p[X]} Z_e[X], \]

where \( \beta = 1/T \) is the inverse temperature, \( X \equiv \{ x_i \} \) denotes a configuration of the phonon fields, and \( Z_e = \text{Tr} \exp(-\beta H_p^e) \) is the electronic partition function in (classical) phonon configuration \( X \). The trace for \( Z_e \) can be computed explicitly and the result is

\[ Z = \int DX \ det \left( 1 + e^{-\beta K[X]} \right)^2 e^{-\beta H_p[X]} \]

\[ = \int DX \ e^{-\beta H_p^eff[X]}, \]

where \( K \) is the bilinear form

\[ K_{ij} = -t_{ij} - (\mu - \alpha x_i) \delta_{ij}, \]

which is a functional of the phonon configuration, and

\[ H_p^eff = H_p - 2 \log \{ \det[1 + \exp(\beta K)] \} / \beta \]

is the effective Boltzmann weight. The partition function is classical – i.e., the phonon configurations have no time dependence – and is amenable to classical MC simulation. Matrix \( K \) is Hermitian, implying that its eigenvalues are real and hence the determinant appearing in (A8) is non-negative. Therefore, there is no sign problem. Let \( N \) denote the number of lattice sites. To perform the MC, the \( N \times N \) matrix \( K \) must be diagonalized for each configuration \( X \). The diagonalization step is the mostly costly and makes the computational time scale as \( N^3 \).

Thermal expectation values \( \langle O \rangle \) are computed according to

\[ \langle O \rangle = \frac{1}{Z} \text{Tr} O e^{-\beta (H' + H_p)} = \frac{1}{Z} \int DX \ e^{-\beta H_p^eff[X]} O[X], \]

where

\[ O[X] = \frac{1}{Z_e} \text{Tr} O e^{-\beta H_p^eff}. \]

The functional \( O[X] \) is easily computed given the single-particle spectrum of \( H' \).

To accelerate convergence to the thermodynamic limit, the calculations presented in this paper have been carried out in the presence of weak, uniform magnetic field.

Appendix B: Zero temperature mean-field theory

At \( T = 0 \), where thermal fluctuations of the phonons are absent, mean-field theory is exact in the \( M \rightarrow \infty \) limit. The ground-state energy of the Hamiltonian \[ (A1) \]

\[ E_0[X] = \varepsilon_0[X] + \frac{K}{2} \sum_i x_i^2, \]

where \( \varepsilon_0 \) is the ground-state energy of \( H'_e \) in phonon configuration \( X \). The ground-state phonon configuration is obtained by minimizing \( E_0 \):

\[ \frac{\partial E_0}{\partial x_i} = \frac{\partial \varepsilon_0}{\partial x_i} + K x_i = 0. \]

By the Feynman-Hellmann theorem, \( \partial \varepsilon_0 / \partial x_i = \alpha \langle n_i \rangle_0 \), where \( \langle \ldots \rangle_0 \) is the ground-state expectation value. This yields the self-consistency condition

\[ x_i = -\frac{\alpha}{K} \langle n_i \rangle_0. \]

Solving the \( N \) equations in (B3) for \( X \) gives the ground-state phonon configuration.

From our finite \( T \) DQMC studies, we see that the ground-state for the range of parameters studied here is always either translationally invariant, or has \((\pi,\pi)\) CDW order. The \( T = 0 \) calculation is greatly simplified if we take this as justification to assume that in the ground-state \( x_i = \bar{x} + (-1)^{i_x+i_y} \delta x \). In this case the Hamiltonian \( (A1) \) takes the following form in momentum-space:

\[ H = \sum_k \epsilon_k - (\mu + \bar{\mu}) c_k^{\dagger} c_k + \Delta \sum_k c_k^{\dagger} Q \sigma c_k + Q \sigma + \frac{1}{2V} \Delta^2 N + \frac{1}{2V} \Delta^2 N. \]
where $\bar{\mu} = \alpha \bar{x}$, $\Delta = \alpha \delta x$, and $V = \alpha^2/K$. Rather than the full set of phonon coordinates there are now only two variational parameters $\bar{\mu}$ and $\Delta$. The self-consistency condition \[ \text{(B3)} \] can now be written as two coupled equations:

$$
\bar{\mu} = -V\langle n_0 \rangle, \quad \Delta = -V\langle n_\mathbf{Q} \rangle_{0}.
$$

To compute the $T = 0$ portion of the phase diagram in Fig. 2 we solve Equations \[ \text{(B5)} \] with $t'/t = -0.3$ and $\mu = \mu_0$ such that $n(T = 0.25t) = 0.8$. The function $\mu_0$ is obtained from the finite $T$ MC calculations. In Figure 6 we show the ground-state energy, $E_0$, order parameter $\Delta$, and density $n$ as a function of $\lambda_0$. The transition to the $(\pi, \pi)$ state is first-order, as can be seen from the discontinuous onset of $\Delta$ for $\lambda = \lambda_0 \approx 0.31$. A second critical point can be seen at $\lambda_0 \approx 0.39$, beyond which $n = 1$.

**Appendix C: Determination of $T_{\text{CDW}}$**

The CDW transition temperature $T_{\text{CDW}}$ is obtained from the finite size scaling behavior of the phonon correlation function

$$
D(\mathbf{Q}) = \frac{1}{L^2} \sum_{ij} \langle e^{i\mathbf{Q} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \rangle_{x_i x_j} \tag{C1}
$$

at wave-vector $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$. Near the transition $D(\mathbf{Q})$ has the scaling form

$$
\frac{1}{L^2} D(\mathbf{Q}) = L^{-2\beta/\nu} f[L^{1/\nu}(T - T_c)/T_c]. \tag{C2}
$$

FIG. 7. Finite-size scaling of phonon correlation function $D(\mathbf{Q})$, with $\mathbf{Q} = (\pi, \pi)$ for (a) $\lambda_0 = 0.54$ and $T_{\text{CDW}} \approx 0.12t$ and (b) $\lambda = 2.43$ and $T_{\text{CDW}} \approx 0.09t$. Ising exponents $\nu = 1$ and $\beta = 1/8$ are used.

FIG. 8. System size dependence of the Binder cumulant $U_L$ for (a) $\lambda_0 = 0.54$ and (b) $\lambda_0 = 2.43$. Vertical dashed lines indicate $T_{\text{CDW}}$ obtained from finite-size scaling of $D(\mathbf{Q})$.

FIG. 9. (a) Specific heat $C_V$ as a function of temperature $T$ for various coupling strengths. The dashed line indicates the contribution from non-interacting phonons. Arrows show the $T_{\text{CDW}}$ inferred from finite-size scaling. Linear system size is $L = 12$. Finite size scaling of $C_V$ for (b) $\lambda_0 = 0.54$ and (c) $\lambda_0 = 2.43$.

The $(\pi, \pi)$ transition spontaneously breaks $Z_2$ symmetry and we therefore use exponents for the 2D Ising universality class: $\nu = 1$ and $\beta = 1/8$. The transition temperature $T_{\text{CDW}}$ is obtained by looking for the best data collapse. This procedure is shown in Figure 7 for representative weak and strong-coupling values, $\lambda_0 = 0.54$ and $\lambda_0 = 2.43$.

The value of $T_{\text{CDW}}$ obtained from finite-size scaling is consistent with the expected behavior of the Binder cumulant of the order parameter and the specific heat near a continuous phase transition. We take the order parameter to be the staggered phonon displacement

$$
\phi = \frac{1}{L^2} \sum_i (-1)^{i_x + i_y} x_i \tag{C3}
$$
and define the Binder cumulant $U_L^{(23)}$ in the usual way

$$U_L = 1 - \frac{\langle \phi^4 \rangle}{3 \langle \phi^2 \rangle^2}. \quad \text{(C4)}$$

The Binder cumulant has the property that, in the thermodynamic limit, $U_L \to 0$ for $T > T_{cdw}$ and $U_L \to 2/3$ for $T < T_{cdw}$. The intersection point of $U_L$ for different system sizes gives an estimate of $T_{cdw}$. In Figure 8 we show $U_L$ in the weak and strong-coupling regimes. The values of $U_L$ for different system sizes indeed intersect at temperatures near $T_{cdw}$ obtained from finite-size scaling.

In Figure 9 we show the specific heat $C_V$ as a function of $T$ for several values of $\lambda_0$. The $(\pi, \pi)$ CDW transition is in the 2D Ising universality class, for which the specific heat exponent is known to be $\alpha = 0$, implying a logarithmic divergence of the specific heat at $T_{cdw}$ upon approaching the thermodynamic limit $C_V \sim C_0 \ln L$. While we do not access sufficiently large systems to see scaling behavior in the specific heat, Fig. 9 shows the position of the specific heat maxima is consistent with our estimates of $T_{cdw}$. Furthermore, the evolution of the peak positions with system size tends toward the estimated $T_{cdw}$, as can be seen in Fig. 9.