Langevin simulations of the Half-Filled Cubic Holstein Model

- Holstein Hamiltonian- Polarons and Pairing
- Holstein Hamiltonian- Charge Density Wave Order
- Langevin-based Quantum Monte Carlo Algorithm
- Honeycomb Lattice
- Cubic Lattice
- Conclusions

Funding:
Holstein Hamiltonian- Polarons and Pairing

Holstein: wave function $a_i$ probability amplitude for (*single*) electron on site $i$.

Modern (many body) notation. Noninteracting electron kinetic energy:

$$\hat{H}_{\text{el-ke}} = -t \sum_{\langle ij \rangle \sigma} \left( \hat{c}_{i \sigma}^\dagger \hat{c}_{j \sigma} + \hat{c}_{j \sigma}^\dagger \hat{c}_{i \sigma} \right)$$

Spin $\uparrow, \downarrow$ electrons interact with boson displacement on site $i$

$$\hat{H}_{\text{el-ph}} = \lambda \sum_i \hat{X}_i (\hat{n}_{i \uparrow} + \hat{n}_{i \downarrow})$$

$$\hat{H}_{\text{boson}} = \frac{1}{2} \omega_0^2 \sum_i \hat{X}_i^2 + \frac{1}{2} \sum_i \hat{P}_i^2$$

Bosons local $\Rightarrow$ energy independent of momentum (*dispersionless*) $\omega(q) = \omega_0$.

Similarly, electron-boson coupling is local $\Rightarrow$ independent of momentum.

Dimensionless coupling: $\lambda_D = \lambda^2 / (\omega_0^2 W)$ where $W =$ electronic bandwidth.
Initial insight from $t = 0$ \(\text{ (Independent sites)}\)

Complete the square

$$\frac{1}{2} \omega_0^2 X^2 + \lambda X (n_\uparrow + n_\downarrow) = \frac{1}{2} \omega_0^2 (X + \frac{\lambda}{\omega^2} (n_\uparrow + n_\downarrow))^2 - \frac{\lambda^2}{2 \omega_0^2} (n_\uparrow + n_\downarrow)^2$$

Integrate out the phonon coordinate $X$.

**Effective attraction**

$$-\frac{\lambda^2}{\omega_0^2} n_\uparrow n_\downarrow = U_{\text{eff}} n_\uparrow n_\downarrow \quad U_{\text{eff}} = -\frac{\lambda^2}{\omega_0^2}$$

Imagine you are at half-filling. Then turn on $t$ perturbatively.

**Attractive interaction** ($-U$ Hubbard; Holstein):

- Local pairs form.
- Double occupied/empty alternation favored:
  - Charge Density Wave.

**Repulsive interaction** ($+U$ Hubbard):

- Local moments form.
- up/down spin alternation favored by $J$:
  - Antiferromagnetism.
Holstein Hamiltonian- Charge Density Wave Order

Local order can become long ranged if thermal/quantum fluctuations reduced.

\begin{align*}
\text{Repulsive (AF)} & \quad \text{Attractive (CDW)} \\
\downarrow & \quad \uparrow \\
\downarrow & \quad \uparrow \\
\downarrow & \quad \uparrow \\
\uparrow & \quad \downarrow \\
\downarrow & \quad \uparrow \\
\downarrow & \quad \uparrow \\
\uparrow & \quad \downarrow \\
\uparrow & \quad \downarrow \\
\end{align*}

Holstein Model:
- Charge order at half-filling (bipartite lattice).
- Superconducting order when doped.

CDW transition at finite $T$ in 2D (Ising universality class).
Contrast to Hubbard: AF order only at $T = 0$ in 2D (Heisenberg universality).
Quantitative values for $T_c$ obtained for square lattice only relatively recently!

Weber and Hohenadler, Phys. Rev. B 98, 085405 (2018).
Langevin-Based QMC Algorithm

Many QMC approaches propose local moves.
Inexpensive to evaluate change in action.
In the case of DQMC: $o(N^2)$ to update boson coordinate.
$N\beta$ boson degrees of freedom: Complete scaling is $o(N^3\beta)$.

Alternate approach in Lattice Gauge Theory QMC:
Update all bosonic field variables at same time via Langevin equation.
In principle complete scaling is $o(N\beta)$.
Assumes number of (conjugate gradient) iterations to compute $\mathcal{M}^{-1}\vec{v}$
is independent of system size $N$ and inverse temperature $\beta$.

Does not work for Hubbard Model!
Matrix $\mathcal{M}$ is much more ill-conditioned than LGT.
Number of conjugate gradient iterations grows catastrophically with $\beta$.

Key observation: $\hat{P}_i^2 \Rightarrow \left[ \frac{X_i(\tau+\Delta\tau)-X_i(\tau)}{\Delta\tau} \right]^2$ moderates eigenspectrum of $\mathcal{M}$.
(No such term for auxiliary bosonic field in Hubbard model.)
Left: Langevin CPU time is indeed nearly linear in $N$.

Below:
Increase in accessible system size improves scaling collapse.
DQMC (left) vs. Langevin (right).
Honeycomb Lattice

Dirac spectrum for fermions.

Quantum critical point for Hubbard Model:
Minimal $U_c/t \gtrsim 3.87$ to induce antiferromagnetic order.

Effect of electron-boson interactions on Dirac fermions and charge order?

(a)

(b) Long range real space charge correlations develop as $\beta$ increases.
CDW structure $o(N)$ when charge correlations long range ($\beta > \beta_c$).

Data collapse/crossing yield critical temperature.
Quantum critical point from \( T = 0 \)
Invariant correlation length crossing

\[
R_c \equiv 1 - \frac{S(Q + \delta q)}{S(Q)}
\]

“Charge Order in the Holstein Model on a Honeycomb Lattice,” Y.-X. Zhang, W.-T. Chiu, N.C. Costa, G.G. Batrouni, and RTS, Phys. Rev. Lett. 122, 077602 (2019).

“Charge-Density-Wave Transitions of Dirac Fermions Coupled to Phonons,” C. Chen, X.Y. Xu, Z.Y. Meng, and M. Hohenadler, Phys. Rev. Lett. 122, 077601 (2019).
Cubic Lattice

Thermodynamics

Structure in Energies → peak in specific heat
Real space density correlations and structure factor.

\[
\lambda_D = 0.33 \quad L = 12 \quad T_{cdw} = 0.392 \pm 0.007
\]
Conclusions

- At half-filling, Holstein model in $d > 1$ undergoes a finite temperature phase transition to state with long range charge order $K_* = (\pi, \pi)$.
- Critical temperature has a maximum at intermediate el-ph coupling $\lambda_D$.

“Langevin Simulations of the Half-Filled Cubic Holstein Model”, B. Cohen-Stead, K. Barros, Z.Y. Meng, Chuang Chen, and R. Scalettar, Phys. Rev. B102, 161108R (2020).
Autocorrelations in Langevin Simulations:

(a) $\omega_0 = 0.7 \; \lambda = 1.0 \; \lambda_D = 0.17 \; \beta = 4.7 \; L = 8$

$\beta = 4.7 \; \Delta \tau = 0.10 \; L = 8 \; dt = 0.001$

(b) $m = 15.0$

$m = 10.0$

$m = 5.0$

$m = 2.0$

$m = 1.5$

$m = 0.5$
Momentum Dependence of Structure Factor

\[ \lambda_D = 0.33 \]
\[ \omega_0 = 0.5 \]
\[ L = 12 \]
\[ T_{cdw} = 0.392 \pm 0.008 \]
CDW Transition in Mean Field Theory

Overestimates transition temperature: \( T_c = \beta_c^{-1} \sim (2 - 5)t \)
Spectral Function

Gap opens below $T_c$

$\omega_0 = 0.7$, $\lambda_D = 0.17$

$T_{cdw} = 0.215 \pm 0.002$

$L = 10$
Correlation Length:

\[ T_{cdw} = 0.315 \pm 0.005 \]

- \( L = 8 \)
- \( L = 10 \)
- \( L = 12 \)

\[ \omega_0 = 0.60, \lambda = 1.00 \]
\[ \lambda_D = 0.23 \]
Momentum Dependence of Structure Factor

\[ \lambda_D = 0.33 \]
\[ \omega_0 = 0.5 \]
\[ L = 12 \]
\[ T_{\text{cdw}} = 0.392 \pm 0.008 \]