Numerical Study of Holstein Polarons

Part I. Self-Trapping Crossover
Part II. Disorder, Correlation, and Finite-Density Effects
Part III. Collective Phenomena – Quantum Phase Transitions

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Greifswald
KPM, CPT, statDMFT

Erlangen
ED, DMRG

Sydney
BO, KPM

Graz
QMC, CPT

Hannover
(D)DMRG

Prag
WC-SC A

Augsburg
PMT

Los Alamos
ILMs
Lecture III: Collective Phenomena – Quantum Phase Transitions

- **Introduction**
  - Peierls instability
  - Peierls-Mott competition

- **Metal insulator transition**
  - Luttinger liquid characterisation
  - CDW characterisation
  - Phase diagram of the spinless fermion Holstein model
  - Phonon softening

- **Peierls-insulator Mott-insulator transition**
  - Ground-state properties
    - Charge & spin structure factors
    - Phonon distribution function
    - Symmetry considerations
  - Excitations
    - Photoemission
    - Optical response
    - Spin & charge excitation gaps
  - Intrinsic localised modes

related publications ～ http://theorie2.physik.uni-greifswald.de
Effect of electron-phonon coupling in low-D systems?

\[ \sim \text{structural distortions at commensurate band fillings } \bar{n}, \]

famous example, Peierls instability:

\[ \chi(q) = \frac{\chi(q)}{\chi(0)} \]

EP driven metal insulator transition!

related:

Kohn anomaly

phonon softening

Lattice dynamics? Especially important in 1D!
Effect of Coulomb interaction?

Ground state:

Electron-hole pairs ↔ QP behaviour!

Quasi-1D materials: wide variety of broken-symmetry ground states & (partially) exotic excitations!
Part I: Metal-Insulator Transition

(Luttinger liquid vs charge-density-wave behaviour)

simplest model: 1D spinless fermion Holstein model at half-filling

\[ H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j - g \omega_0 \sum_i (b_i^\dagger + b_i) n_i + \omega_0 \sum_i b_i^\dagger b_i \]

N sites, \( N_e \) electrons with \( n = N_e/N = 0.5 \), dispersionless phonons, \( T = 0 \)

parameters: \( g^2 = \varepsilon_p/\omega_0; \ \lambda = \varepsilon_p/2t \), and \( \alpha = \omega_0/t \)

"known" results:

- \( \lambda \uparrow\): quantum phase transition from a metallic (LL) to an insulating (Peierls distorted) phase; RG, QMC, GFMC, ED, DMRG, . . . \( \sim \) phase boundary, \textit{but} significant discrepancies in the adiabatic intermediate coupling regime!
- \( \omega_0 \rightarrow 0: \lambda_c \rightarrow 0 \)
- strong-coupling anti-adiabatic regime \( \sim \) exactly solvable XXZ model: Kosterlitz - Thouless phase transition
Luttinger liquid parameters

- Characterisation of Luttinger liquids?
  - Holstein model - gapless for small couplings $\sim$ Tomonaga-Luttinger universality class [Haldane LL conjecture (PRL 45, 1358 (1980))]:
    - $n(k), \rho(\omega), G(x), \chi^{-1}, \kappa^{-1}, \ldots \Rightarrow K_\rho, u_\rho$
  - Interaction (stiffness) constant and charge velocity
  - Scaling relations!
    - (conformal field theory - Affleck, Cardy, Nomura, Okamoto, Voit, ...)

$$\varepsilon_0(\infty) - \frac{E_0(N)}{N} = \frac{\pi u_\rho}{3} \frac{1}{2} \frac{1}{N^2}$$ \quad \propto \text{ground-state energy}$$

$$E_0^{(\pm 1)}(N) - E_0(N) = \frac{\pi u_\rho}{2} \frac{1}{K_\rho} \frac{1}{N}$$ \quad \propto \text{charge excitation gap}$$

- Density Matrix Renormalisation Group:
  - Systems with $N=128 \ldots 512$ accessible
  - Determination of (non-universal) $K_\rho$ & $u_\rho$!
Effects of EP coupling?

Scaling relations are still fulfilled almost perfectly – ∀α!

(but, of course, they break down at large $g^2$)
Finite-size scaling

Extraction of LL parameters:

\[ g^2, \omega_0/t = 0.1, \omega_0/t = 10.0 \]

<table>
<thead>
<tr>
<th>( g^2 )</th>
<th>( \omega_0/t = 0.1 )</th>
<th>( \omega_0/t = 10.0 )</th>
</tr>
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<tbody>
<tr>
<td>( K_\rho )</td>
<td>( u_\rho/2 )</td>
<td>( K_\rho )</td>
</tr>
<tr>
<td>0.6</td>
<td>1.031</td>
<td>( \sim 1 )</td>
</tr>
<tr>
<td>2.0</td>
<td>1.055</td>
<td>0.995</td>
</tr>
<tr>
<td>4.0</td>
<td>1.091</td>
<td>0.963</td>
</tr>
</tbody>
</table>

\[ > 1 \quad < 1 \]

\( \rightarrow \) adiabatic regime: attractive interaction & weak \( u_\rho \)-renormalisation

\( \rightarrow \) anti-adiabatic regime: repulsive interaction & strong \( u_\rho \)-renormalisation!
**Charge density wave formation**

- **Charge structure factor at** $\pi$: 
  \[ S_c(\pi) = \frac{1}{N^2} \sum_{i,j} (-1)^j \langle (n_i - \frac{1}{2})(n_{i+j} - \frac{1}{2}) \rangle \]

existence of a Peierls-CDW phase above $g_c(\alpha)$!
Ground-state phase diagram

attractive LL

repulsive LL

metallic behaviour

\[ u_\rho, K_\rho \]

activated transport

\[ \sigma^{reg}(\omega) \]

Peierls distorted state
Photoemission spectra I

- Injection/emission of electrons? \( (c_{K\sigma}^+ = c_{K\sigma}^\dagger - \text{IPE}; c_{K\sigma}^- = c_{K\sigma} - \text{PE}; \sigma \equiv \uparrow) \)

\[
A_{K\sigma}^\pm(\omega) = \sum_m |\langle \psi_m^{(N_{el} \pm 1)} | c_{K\sigma}^\pm | \psi_0^{(N_{el})} \rangle|^2 \delta[\omega \mp (E_m^{(N_{el} \pm 1)} - E_0^{(N_{el})})]
\]

- weak coupling:

- metal
- QP peak
- phonon satellites
• critical coupling:

- gap feature emerges
- redistribution of QP weight
- phonon absorption bands

weak coupling:

- N=8 M=28
- \(\epsilon_p/t=0.60\)
- \(\omega_0/t=0.1\)
- strong coupling: finite gap $\sim$ CDW insulator

![Graphs showing Photoemission Spectra III with different coupling regimes: weak, critical, and strong.](image)

- Weak coupling: 
  - $K=0$
  - $K=\pm \pi/4$
  - $K=\pm \pi/2$
  - $K=\pm 3\pi/4$
  - $N=8$ $M=32$
  - $\epsilon_p/t=1.6$
  - $\omega_0/t=0.1$

- Critical coupling: 
  - $K=\pi$
  - $N=8$ $M=28$
  - $\epsilon_p/t=0.6$
  - $\omega_0/t=0.1$

- Strong coupling: 
  - $N=8$ $M=12$
  - $\epsilon_p/t=0.1$
  - $\omega_0/t=0.1$
Renormalisation of phonon dispersion?

\[ D_Q(\omega) = 2\omega_0 \langle \langle x_Q; x_{-Q} \rangle \rangle_\omega \]

(with \( x_i = (b_i^\dagger + b_i)/\sqrt{2\omega_0} \); \( B_Q(\omega) = -\frac{1}{\pi} \text{Im} D_Q(\omega) \))

- weak coupling:

\[ \tilde{\omega}(Q) \simeq \omega_0 \]

- \( K = 0 \) “electron” state - phonon admixture
• $\lambda \to$ critical coupling:

- $\lambda = 0.7$
- $\alpha = 0.4$
- $N_c = 8$

- Zone boundary phonon becomes soft
- Redistribution of phonon spectral weight

**weak coupling:**

- $\lambda = 0.05$
- $\alpha = 0.4$
- $N_c = 8$ (CPT)
**strong coupling:** CDW insulator

- doubling of Brillouin zone
- phonon hardening sets in

\[ \lambda = 1.0 \]
\[ \alpha = 0.4 \]
\[ N_c = 6 \]

\[ \lambda = 0.05 \]
\[ \alpha = 0.4 \]
\[ N_c = 8 \text{ (CPT)} \]

\[ \lambda = 0.7 \]
\[ \alpha = 0.4 \]
\[ N_c = 8 \]
**Phonon Spectra - Anti-adiabatic Case**

**Weak Coupling**

\[ \lambda = 1 - g^2 = 0.5 \]
\[ \alpha = 4 \]
\[ N_c = 8 \]

- Signature of polaron band dispersion
- Precursor of softening?

**Strong Coupling**

\[ \lambda = 8 - g^2 = 4 \]
\[ \alpha = 4 \]
\[ N_c = 4 \]

- Almost perfect doubling
- Dispersionless signature at \( \omega_0 \)

Schematic phase diagram

Part II: Insulator-Insulator Transition

(Peierls vs Mott)

simplest model: 1D Holstein Hubbard model at half-filling

\[ H = \sum_{i\sigma} \epsilon_i n_{i\sigma} - t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - g \sum_{i\sigma} (b_{i\sigma}^{\dagger} + b_{i\sigma}) n_{i\sigma} + \omega_0 \sum_{i\sigma} b_{i\sigma}^{\dagger} b_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \]

N sites, \( N_{e\uparrow} = N_{e\downarrow} = N/2 \) electrons, i.e. \( n = 1 \), dispersionless phonons, \( T = 0 \)

parameters: \( g^2 = \epsilon_p/\omega_0; \lambda = \epsilon_p/2t, \alpha = \omega_0/t, \) and \( u = U/4t \)

Hardly any exact results!
Charge & Spin structure factors

- Suppression of CDW by Hubbard interaction?
- Increase of SDW? $S^z_i = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$

$$S_s(\pi) = \frac{1}{N^2} \sum_{i,j} (-1)^j \langle S^z_i S^z_{i+j} \rangle$$

Yes! Finite-size effects?

$g^2 = 2$
$\alpha = 1$
Phase transition? $N \to \infty! \sim$ DMRG finite-size scaling necessary

Critical ratio $u/\lambda$

Breaking of discrete symmetry

Peierls Insulator

U

Mott Insulator

$g$

SDW: no LRO

CDW: true LRO
**Phonon distribution**

- Phonon “contribution” to the ground state?

- MI: basically zero-phonon state (besides $Q = 0$ mode)

- QCP: increasing weight of multi-phonon states

- PI: Poisson-like distribution of phonons
Single-particle excitations?

Mott insulating regime $u/\lambda > 1$

- Mott-Hubbard correlation gap $\sim$ optical gap
- band renormalisation, phonon satellites
- “breather-like” excitations

Mott-to-Peierls transition $u/\lambda \simeq 1$

- gapless spin & charge excitations
- band width $\lesssim 4t$, broad (I)PE spectra
- uniform distribution of spectral weight
CDW regime?

**adiabatic case:** \( \alpha \ll 1 \)

- dispersion \( \propto \epsilon_k + \) gap feature
- phonon softening: \( \tilde{\omega}_\pi \rightarrow 0 \)

\( \rightarrow \) “normal” Peierls band insulator

**anti-adiabatic case:** \( \alpha \gg 1 \)

- low-weight dispersionless band
- \( \uparrow \downarrow \times \) + ordering

\( \rightarrow \) polaronic superlattice
Signatures of the PI-MI QPT in the optical conductivity?

EP coupling fixed ($\lambda = 1, \alpha = 1$) – increasing Hubbard interaction:

- $(u/\lambda)_c \sim$ optical gap $\Delta_{opt} = 0$, metal!?
- Drude-weight ill-defined!
### Many-body excitation gaps

- Proof of spin-charge separation? \(\sim\) DMRG finite-size scaling of

**Charge gap:**
\[
\Delta_c = E_0^{(N_{el}+1)}\left(\frac{1}{2}\right) + E_0^{(N_{el}-1)}\left(-\frac{1}{2}\right) - 2E_0^{(N_{el})}(0)
\]

**Spin gap:**
\[
\Delta_s = E_0^{(N_{el})}(1) - E_0^{(N_{el})}(0)
\]

(both including lattice relaxation!

![Graph showing the relationship between \(\Delta_c\) and \(\Delta_s\) with respect to \(1/N\) for different phases: PI, ~QCP, MI.](image)
QPT - SYMMETRY CONSIDERATIONS

• \((\mu/\lambda)_c\) – level crossing \(\iff\) symmetry change?

- HHM - invariant with respect to inversion at site \(i\)
  inversion symmetry (parity) operator: \(\hat{P}_{c_i\sigma}\hat{P}^\dagger = c_{N-i\sigma}\) \((i = 0, 1, \ldots, N-1)\)

- Hubbard model on finite lattices \((N = 4L; \text{PBC})\):
  \(P = 1\) for \(U = 0\) & \(P = -1\) \(\forall U > 0\)

- Holstein Hubbard model: \(\sigma^{\text{reg}}\) points parity change out!
  \(|\psi_0\rangle\) by ED \(\sim P = 1\) for \(U < U_c\)!

physical picture:

![Graph showing QPT and MI phases with \(U\) vs \(\Delta_{opt}\) and parity change]
Schematic phase diagram

Mott Insulator
\[ \Delta_c > \Delta_s = 0; P = -1 \]

SDW
\[ \downarrow \cdots \downarrow \cdots \downarrow \cdots \downarrow \cdots \downarrow \]

\[ \frac{u}{\lambda} \gg 1 \]

\[ \alpha \ll 1 \]

\[ \frac{u}{\lambda} \ll 1 \]

\[ \frac{\lambda}{\alpha} \gg 1 \]

\[ \frac{\lambda}{\alpha} \ll 1 \]

\[ g^2 \]

Band Insulator

Peierls Insulator
\[ \Delta_c = \Delta_s > 0; P = +1 \]

CDW
\[ \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \]

Peierls Insulator

Bipolaronic Insulator

HF, Wellein, Hager, Weiße, Bishop: Phys. Rev. B 69 , 165115 (2004), ...

Experimental relevance? \[ \sim \text{quasi-1D MX solids} \] (M=Pt,Pd,Ni - X=Cl,Br,I)!
Adiabatic limit

“Frozen phonons” ($\omega = 0$)?

schematic phase diagram:

$$H_{t-u} - \sum_{i \sigma} \Delta_i n_{i \sigma} + \frac{K}{2} \sum_i \Delta_i^2$$

Maybe two (continuous) transitions at weak EP couplings!?

Intrinsic localised vibrational modes

Pt-Cl MX-chain: CDW

Peierls-Hubbard model

\[ \propto \lambda_R (b_R + b_R^\dagger) (n_{e,2} - n_{e,4}) \]

non-linear dynamics!

IVCT gap \( \simeq 2.4 \) eV

EP-coupling

resonance raman spectra

JADA diagonalisation

\[ r_n = \frac{n \omega_R^{(1)} - \omega_R^{(n)}}{\omega_R^{(1)}} \]

redshift of overtones!

Swanson et al. PRL 82, 3288
HF et al PRB 63, 245121

\( r_n \)
Strongly correlated electron-phonon systems

~ remarkable variety of

interesting physical phenomena & theoretical problems

← great challenge!

• numerical study of simplified (but generic) model Hamiltonians on finite lattices ← powerful tool to address this field

• ground state and spectral properties of the 1D Holstein (Hubbard) model are understood to a large extent, but

• what about $0 < \eta < 1$ (including the spin degrees of freedom), $D > 1$, $T > 0$, ...?

There is still a lot of work to be done!