Nature of the Peierls- to Mott-Insulator Transition in One Dimension

H. Fehske[1,2], G. Wellein[3], A. P. Kampf[4], M. Sekania[4], A. Weiße[2], F. Göhmann[2], H. Büttner[2], & A. R. Bishop[5]

Universities [1]Greifswald, [2]Bayreuth, [3]Erlangen, [4]Augsburg (Germany) & [5]Los Almos National Laboratory (U.S.A.)

Abstract

In an attempt to clarify the nature of the crossover from a Peierls band insulator to a Mott-Hubbard insulator, we analyze ground-state and spectral properties of the one-dimensional half-filled Holstein-Hubbard model using exact diagonalization and density matrix renormalization group techniques.

Motivation

In a wide range of quasi-one-dimensional materials, such as MX chains, conjugated polymers or ferroelectric perovskites, the itinerancy of the electrons strongly competes with electron-electron and electron-phonon (EP) interactions, which tend to localize the charge carriers by establishing spin-density-wave (SDW) and charge-density-wave (CDW) ground states (GSs), respectively. Other sources for CDW formation are finite range Coulomb interactions or staggered (atomic) potentials. Hence, at half-filling, Peierls (PI) or Mott (MI) insulating phases are usually energetically favored over the metallic state.

An interesting and still controversial question is whether or not only one quantum critical point separates the PI and MI phases at $T = 0$ [1, 2].

Furthermore, how is the crossover modified when phonon dynamical effects, which are known to be of particular importance in low-dimensional materials [3, 4], are taken into account?

1D Model Hamiltonians

Holstein-Hubbard model:

$$
\begin{aligned}
H_{HHM} &= H_{t-U} + H_{e-ph} + H_{ph} \\
H_{t-U} &= -t \sum_{i,\sigma} (c_{i\sigma}^{\dagger} c_{i+1\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \\
H_{e-ph} &= -g\omega_0 \sum_{i,\sigma} (b_i^{\dagger} + b_i) n_{i,\sigma} \\
H_{ph} &= \omega_0 \sum_i b_i^{\dagger} b_i \quad \text{with} \quad g^2 = \varepsilon_p/\omega_0
\end{aligned}
$$

Here $c_{i\sigma}^{\dagger}$ creates a spin-σ electron at Wannier site i ($n_{i,\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$), $b_i^{\dagger}$ creates a local phonon of frequency ω_0, t denotes the hopping integral, U is the on-site Hubbard repulsion, g is a measure of the EP coupling strength, and the summation over i extends over a (periodic) chain of N sites.

Adiabatic Holstein-Hubbard model:

$$
H_{AHHM} = H_{t-U} - \sum_{i,\sigma} \Delta_i n_{i\sigma} + \frac{K}{2} \sum_i \Delta_i^2
$$

Here the elastic energy of the lattice is included via the "stiffness constant" $K(\varepsilon_p)$. $\Delta_i = (-1)^i \Delta$ is a measure of a staggered density modulation.

Ionic Hubbard model:

$$
H_{IHM} = H_{t-U} + \sum_{i,\sigma} (-1)^i \frac{\Delta}{2} n_{i\sigma}
$$

Only the half-filled band case is considered.

Symmetry considerations:
Since the Hamiltonian of the HHM is invariant with respect to inversion at site i, any nondegenerate eigenstate $|\psi_m\rangle$ of H must obey $P|\psi_m\rangle = \pm|\psi_m\rangle$ ($P^2 = 1$), where the site inversion symmetry operator P (parity) is defined by $P c_{i\sigma}^{\dagger} P^{\dagger} = c_{N-i\sigma}^{\dagger}$ for $i = 0, 1, \ldots, N-1$ (and $P|0\rangle = |0\rangle$ holds for the electron vacuum state).

Defining criteria for insulating phases:

Band insulator (BI)	$\Delta_c = \Delta_s > 0$
Mott insulator (MI)	$\Delta_c > 0, \Delta_s = 0$
Correlated insulator (CI)	$\Delta_c > \Delta_s > 0$

Charge gap:

$$\Delta_c(N) = E_0(\tfrac{N}{2}+1, \tfrac{N}{2}) + E_0(\tfrac{N}{2}-1, \tfrac{N}{2}) - 2E_0(\tfrac{N}{2}, \tfrac{N}{2})$$

Spin gap:

$$\Delta_s(N) = E_0(\tfrac{N}{2}+1, \tfrac{N}{2}-1) - E_0(\tfrac{N}{2}, \tfrac{N}{2})$$

Note that Δ_c is distinct from the optical gap, Δ_{opt}, which corresponds to the minimal excitation energy $(E_m - E_0)$ in the same particle number sector.

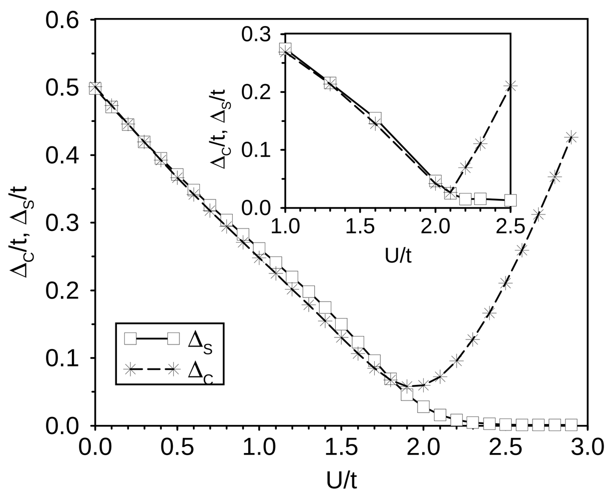
Selection rule for optical transitions: $\langle 0|\hat{j}|m\rangle \neq 0$ only if $|m\rangle$ and $|0\rangle$ have different parities.

Numerical Results

Ionic Hubbard model

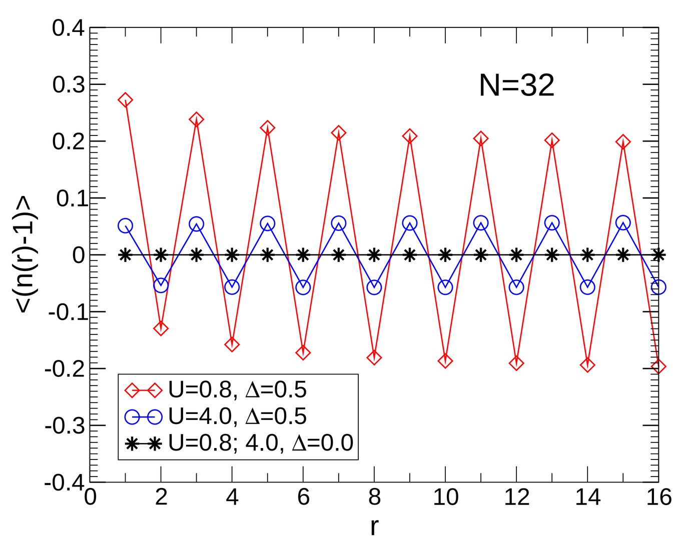
DMRG calculations were performed for $\Delta = 0.5$, on open chains with $N = \{30, 40, 50, 60\}$ (main plot) $N = \{30, 40, 50, 60, 200, 300\}$ (inset), and extrapolated to the limit of infinite chain length.

Charge- (Δ_c) and spin- (Δ_s) excitation gaps:



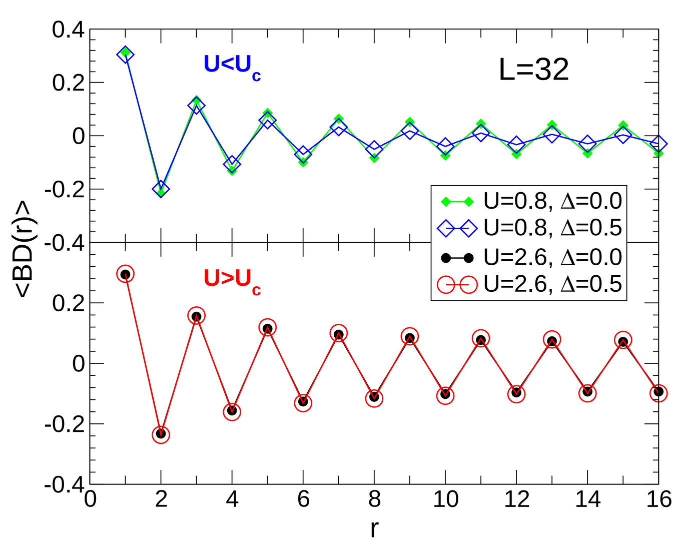
Existence of a single insulator-insulator transition point with $\Delta_c > 0$ at $U_c(\Delta)$.
Origin of the transition: level crossing of different site-parity sectors [5, 6] $\rightsquigarrow$ $\Delta_{opt} = 0$ at $U_c(\Delta)$.

Density distribution (open chain; $N = 32$):



For finite Δ the CDW persists for arbitrary finite U.

Bond-charge-density distribution:



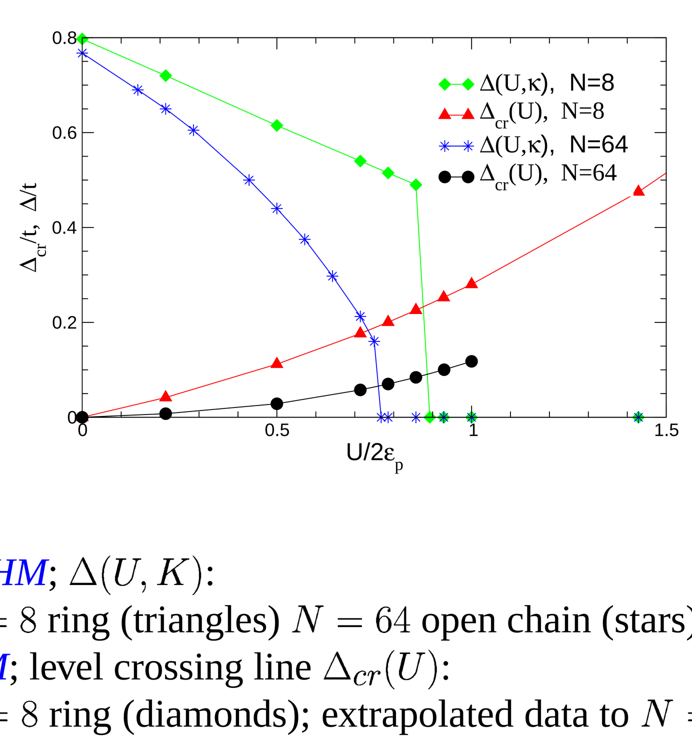
Open boundaries lead to strong Friedel-like oscillations of the bond-charge-density-wave (BCDW).

$$
BD(r) = \frac{\sum_\sigma \langle c_{r,\sigma}^{\dagger} c_{r+1,\sigma} + H.c.\rangle}{\frac{1}{L}\sum_{r,\sigma}\langle c_{r,\sigma}^{\dagger} c_{r+1,\sigma} + H.c.\rangle} - 1
$$

$U < U_c$ – (BI): reduction of BCDW oscillation.
$U > U_c$ – (CI): enhancement of BCDW oscillation.
$\rightsquigarrow$ possible bond-order wave (BOW) in the CI phase [7, 8].

Adiabatic Holstein-Hubbard model

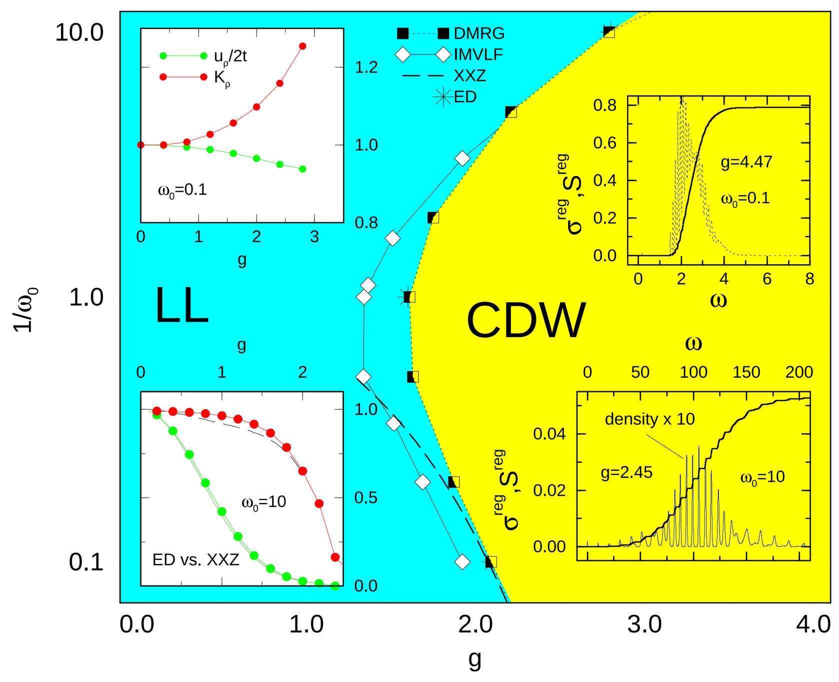
$\Delta(U, K)$ and $\Delta_{cr}(U)$:



AHHM; $\Delta(U, K)$:
$N = 8$ ring (triangles) $N = 64$ open chain (stars)
IHM; level crossing line $\Delta_{cr}(U)$:
$N = 8$ ring (diamonds); extrapolated data to $N = 64$ from $N = 8, 10, 12, 14$ ring (circles)

Holstein model of spinless fermions

Phase diagram:



GS phase diagram at half filling ($N_e = N/2$), showing the boundary between the Luttinger liquid (LL) and charge-density-wave (CDW) states obtained by exact diagonalization (ED) and density matrix renormalization group (DMRG) [9] approaches (dashed line - asymptotic result for the XXZ model). Left insets show the LL parameters u_ρ and K_ρ in the metallic regime, obtained to leading order from the scaling relations

$$
\begin{aligned}
E_0(N)/N &= \epsilon_\infty - \pi u_\rho/(6N^2) \\
E_0(N \pm 1) - E_0(N) &= \pi u_\rho/(2K_\rho N)
\end{aligned}
$$

Right insets display the regular part of the optical conductivity

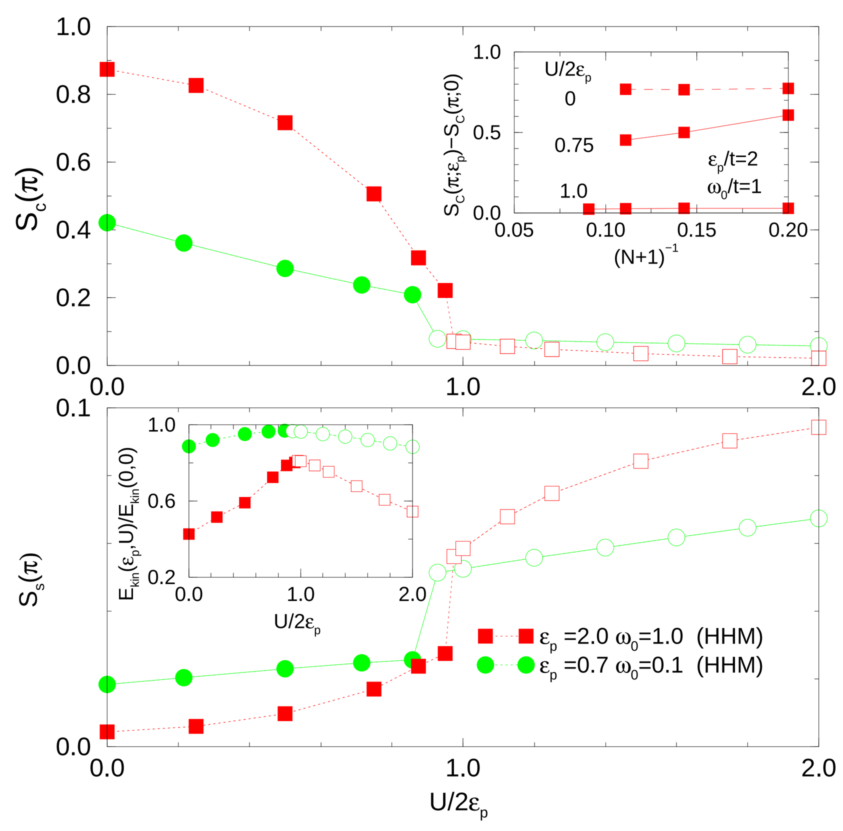
$$\sigma^{\text{reg}}(\omega) = \frac{\pi}{N}\sum_{m\neq 0} \frac{|\langle\psi_0|\hat{j}|\psi_m\rangle|^2}{E_m - E_0}\,\delta(\omega - E_m + E_0)$$

with $\hat{j} = -\text{i}et\sum_{i\sigma}(c_{i\sigma}^{\dagger} c_{i+1\sigma} - c_{i+1\sigma}^{\dagger} c_{i\sigma})$, and the integrated spectral weight $S^{reg}(\omega) = \int_0^\omega d\omega' \sigma^{reg}(\omega')$ in the CDW region.

Holstein-Hubbard model

Rescaled parameter: $u = U/4t$, $\lambda = \varepsilon_p/2t$, $\alpha = \omega_0/t$

Charge- and spin structure factor ($U = 0$; $N = 8$):

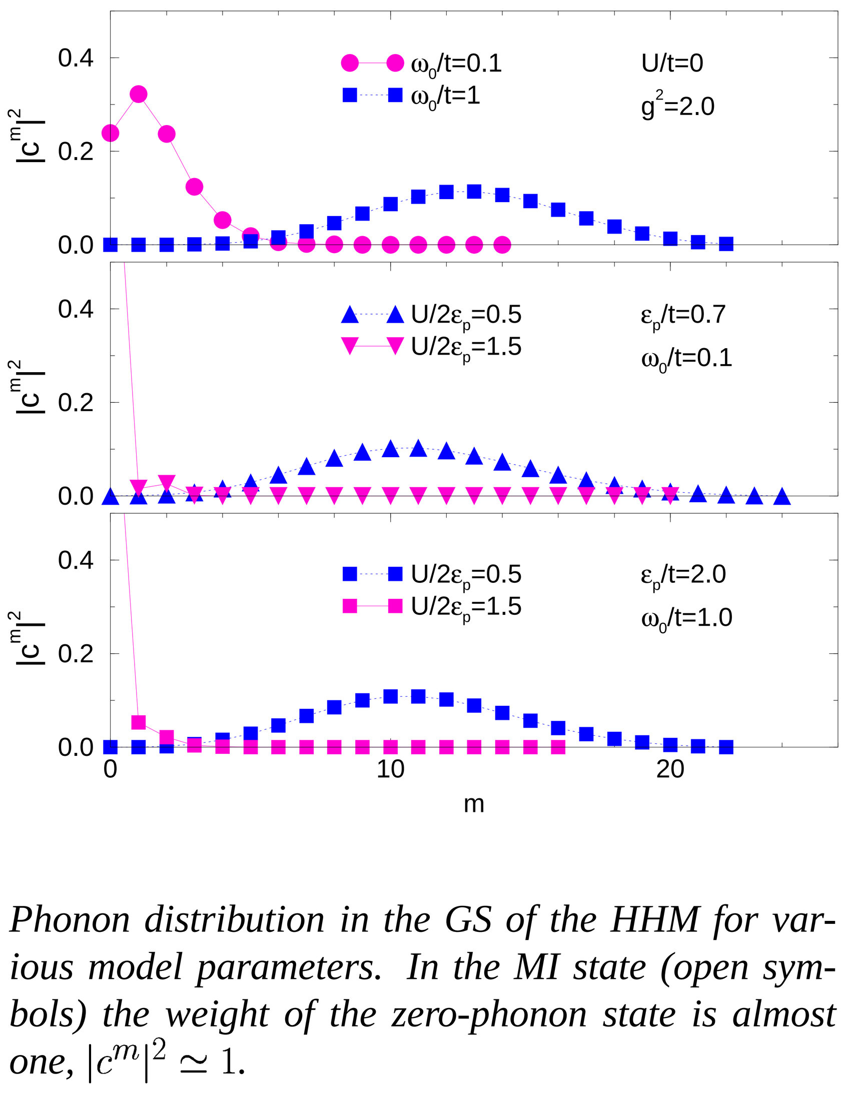


Staggered charge- and spin-structure factors,

$$
\begin{aligned}
S_c(\pi) &= \tfrac{1}{N}\textstyle\sum_{j,\sigma\sigma'}(-1)^j \langle (n_{i\sigma} - \tfrac{1}{2})(n_{i+j,\sigma'} - \tfrac{1}{2})\rangle \\
S_s(\pi) &= \tfrac{1}{N}\textstyle\sum_j (-1)^j \langle S_i^z S_{i+j}^z\rangle\ , \quad S_i^z = \tfrac{1}{2}(n_{i\uparrow} - n_{i\downarrow})\ ,
\end{aligned}
$$

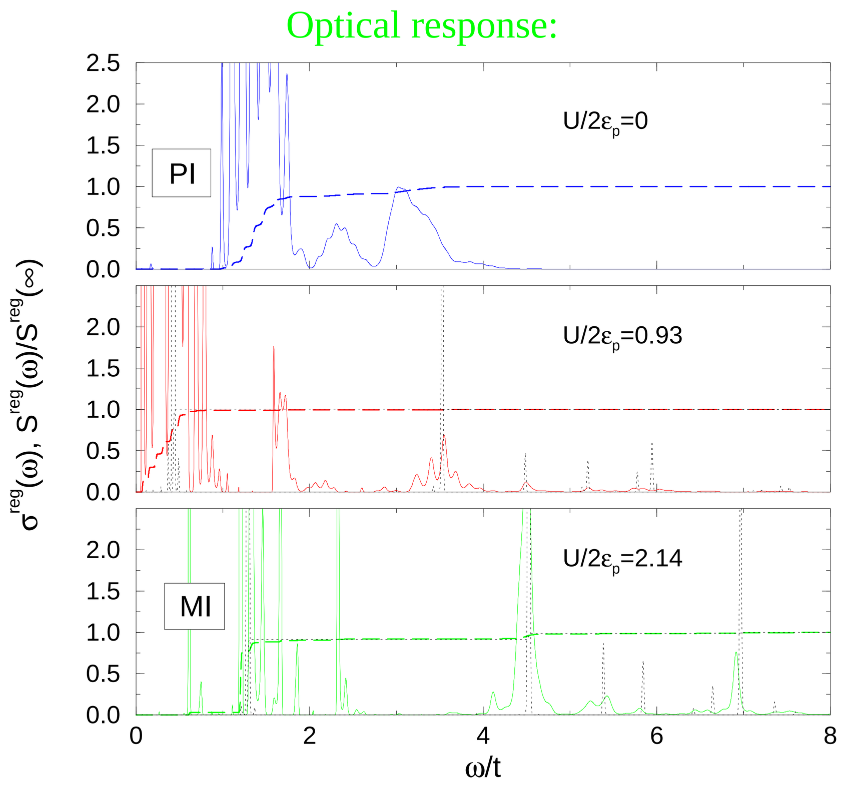
vs. the rescaled Hubbard interaction $U/2\varepsilon_p$. Lanczos results for the HHM on an 8-site ring are given in the adiabatic (triangles) and non-adiabatic (squares) regimes. Upper inset: finite-size scaling of $S_c(\pi)$ for various U; lower inset: U-dependence of the kinetic energy E_{kin}. Open (closed) symbols belong to GSs with $P = -1$ (+1).

Phonon distribution function:



Phonon distribution in the GS of the HHM for various model parameters. In the MI state (open symbols) the weight of the zero-phonon state is almost one, $|c^m|^2 \simeq 1$.

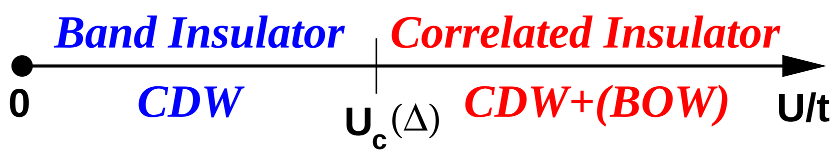
Optical response:



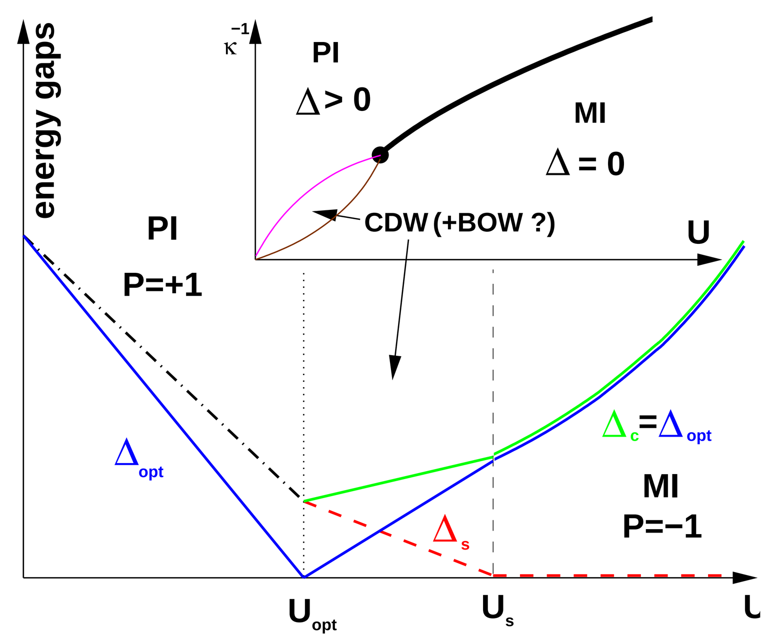
Optical conductivity in the 8-site HHM for $\omega_0 = 0.1t$ and $g^2 = 7$. Top panel: PI phase for $U = 0$; middle panel: near criticality $U \sim U_{opt}$; lower panel: MI phase for $U = 3t$. Dashed lines give the normalized integrated spectral weights $S^{reg}(\omega)$. The lower two panels include σ^{reg} for $g = 0$ (dotted lines), i.e. for the pure Hubbard chain.

Schematic Phase Diagrams

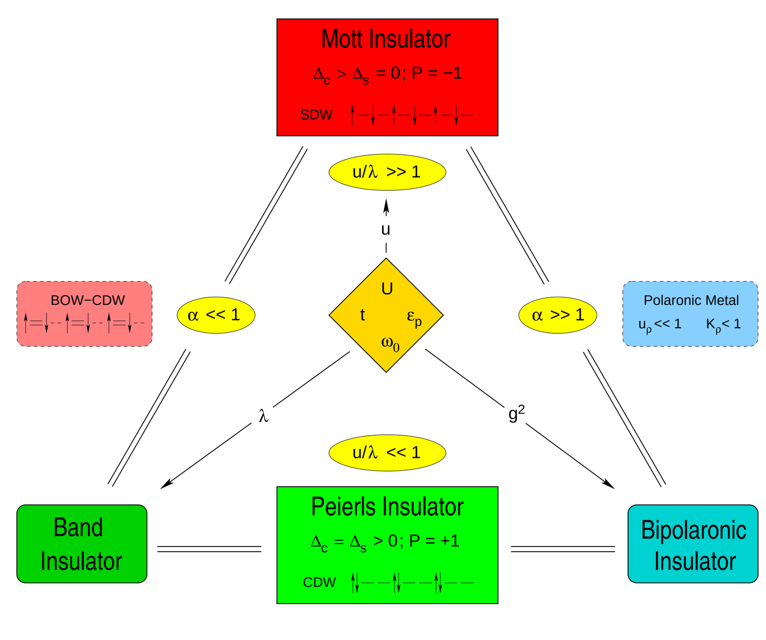
Ionic Hubbard model:



Adiabatic Holstein-Hubbard model



Holstein-Hubbard model :



At $U = 0$ and $\omega_0 = 0$ the GS is a Peierls distorted state $\forall\ \varepsilon_p > 0$. As in the Holstein model of spinless fermions, at $\omega_0 > 0$ quantum phonon fluctuations destroy the Peierls instability for small g. Above a critical threshold $g_c(\omega_0)$, the HHM describes a PI with gapped spin and charge excitations. In the non-adiabatic strong EP coupling regime, the system is typified by a CDW bipolaronic insulator rather than a traditional Peierls BI.

Increasing U at fixed g, the dimerization and the concomitant CDW are suppressed. As a result the system evolves from the PI to the MI. At U_c the parity of the GS of our finite system undergoes a change from $P = +1$ (PI) to $P = -1$ (MI).

Above U_c, in the MI phase, the low-energy physics of the system is governed by gapless spin and massive charge excitations. In the MI regime the optical gap is by its nature a correlation gap.

References

[1] M. Fabrizio, A. O. Gogolin, and A. A. Nersesyan, Phys. Rev. Lett. **83**, 2014 (1999); S. Qin, J. Lou, T. Xiang, Z. Su, and G.-S. Tian, arXiv:cond-mat/0004162.

[2] P. Brune, G. I. Japradize, and A. P. Kampf, arXiv:cond-mat/0106007 v2.

[3] E. Jeckelmann, C. Zhang, and S. R. White, Phys. Rev. B **60**, 7950 (1999).

[4] H. Fehske, M. Holicki, and A. Weiße, Adv. Sol. State Phys. **40**, 235 (2000).

[5] N. Gidopoulos, S. Sorella, and E. Tosatti, Eur. Phys. J. B **14**, 217 (2000).

[6] Y. Anusooya-Pati, Z.G. Soos, and A. Painelli, Phys. Rev. B **63**, 205118 (2001).

[7] R. Resta and S. Sorella, Phys. Rev. Lett. **74**, 4738 (1995).

[8] T. Wilkens and R. M. Martin, Phys. Rev. B **63**, 235108 (2001).

[9] R. J. Bursill, R. H. McKenzie, and C. J. Hamer, Phys. Rev. Lett. **80**, 5607 (1998); A. Weiße and H. Fehske, Phys. Rev. B **58**, 13562 (1998).