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Peierls-insulator Mott-insulator transition in 1D

H. Fehske[a,*], G. Wellein[b], A. Weiße[a], F. Göhmann[a], H. Büttner[a], A.R. Bishop[c]

[a] *Physikalisches Institut, Universtät Bayreuth, Theoretische Physik I, Universitätsstrasse 30, 95440 Bayreuth, Germany*
[b] *RRZE, Universität Erlangen, 91058 Erlangen, Germany*
[c] *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

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 techniques.

Keywords: Electron–phonon systems; Peierls insulator; Mott insulator

In a wide range of quasi-one-dimensional materials, such as MX chains, conjugated polymers or ferroelectric perovskites, the itineracy 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 and charge-density-wave ground states, respectively. Hence, at half-filling, Peierls (PI) or Mott (MI) insulating phases are 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]. Furthermore, how is the crossover modified when phonon dynamical effects, which are known to be of particular importance in low-dimensional materials [2,3], are taken into account?

The paradigm in studies of this subject is the half-filled Holstein–Hubbard model (HHM), defined by the Hamiltonian

$$H = -t\sum_{i,\sigma}(c^{\dagger}_{i\sigma}c_{i+1\sigma} + \text{h.c.}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + g\omega_0\sum_{i,\sigma}(b^{\dagger}_{i} + b_i)n_{i\sigma} + \omega_0\sum_{i} b^{\dagger}_{i}b_i. \quad (1)$$

Here $c^{\dagger}_{i\sigma}$ creates a spin-σ electron at Wannier site i ($n_{i,\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$), $b^{\dagger}_{i}$ 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.

Applying basically exact numerical methods [4], we are able to diagonalize the HHM on finite chains, preserving the full dynamics of the phonons. In order to characterize the ground-state and spectral properties of the HHM in different parameter regimes, we have calculated the charge- and spin-structure factors at wave number $q = \pi$

$$S_{\rm c}(\pi) = \frac{1}{N}\sum_{j,\sigma\sigma'}(-1)^j(\langle n_{i\sigma}n_{i+j\,\sigma'}\rangle - \tfrac{1}{4}), \quad (2)$$

$$S_{\rm s}(\pi) = \frac{1}{N}\sum_{j}(-1)^j\langle S^z_i S^z_{i+j}\rangle \quad (3)$$

($S^z_i = (n_{i\uparrow} - n_{i\downarrow})/2$), the local magnetic moment $L = 3\langle (S^z_i)^2\rangle$, the kinetic energy $E_{\rm kin} = -t\langle \sum_{i,\sigma}(c^{\dagger}_{i\sigma}c_{i+1\sigma} + \text{h.c.})\rangle$, and the incoherent part of the optical conductivity

$$\sigma^{\rm reg}(\omega) = \frac{\pi}{N}\sum_{m\neq 0}\frac{|\langle\psi_0|\hat{j}|\psi_m\rangle|^2}{E_m - E_0}\,\delta(\omega - E_m + E_0), \quad (4)$$

where $\hat{j} = -iet\sum_{i,\sigma}(c^{\dagger}_{i\sigma}c_{i+1\,\sigma} - c^{\dagger}_{i+1\,\sigma}c_{i\sigma})$. Some typical results are shown in Figs. 1 and 2.

Our conclusions can be summarized as follows:

(i) At $U = 0$ the ground state is a Peierls distorted state in the adiabatic limit $\omega_0 \to 0$ for any finite EP coupling. As in the Holstein model of spinless fermions

*Corresponding author. Tel.: +49-921-55-3212; fax: +49-921-55-2991.

E-mail address: holger.fehske@uni-bayreuth.de (H. Fehske).

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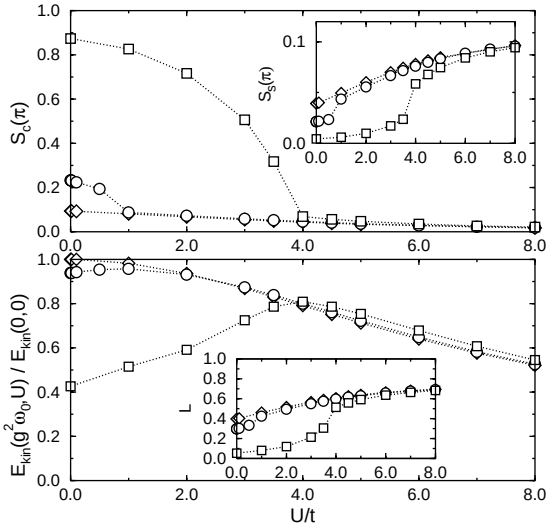

Fig. 1. Staggered charge- and spin-density correlations (upper panel), kinetic energy and local magnetic moment (lower panel) in the ground state of the Holstein–Hubbard model ($\omega_0/t = 1$; $N = 8$). Results are shown at $g^2\omega_0/t = 0$ ($\diamond$), 0.5 ($\circ$), and 2.0 ($\square$).

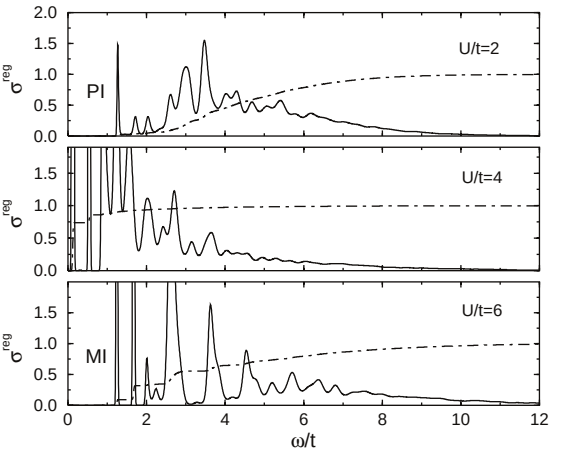

Fig. 2. Optical absorption in the HHM ($\omega_0/t = 1$; $N = 8$). Dashed lines give the integrated spectral weights $S^{\mathrm{reg}}(\omega) = \int_0^{\omega} \sigma^{\mathrm{reg}}(\omega')\,\mathrm{d}\omega'$ [normalized by $S^{\mathrm{reg}}(\infty)$].

[3], at $\omega_0 > 0$ quantum phonon fluctuations destroy the Peierls instability for small EP interaction strength g [2]. 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 charge-ordered bipolaronic insulator rather than a traditional Peierls band insulator. The PI regime is characterized by a large (small) charge (spin) structure factor, a strongly reduced kinetic energy, and an optical response that is dominated by multiphonon absorption and emission processes.

Table 1
Parity of the ground state of the HHM, $P|\psi_0\rangle = \pm|\psi_0\rangle$, where the site inversion symmetry operator P is defined by $Pc^{\dagger}_{i\sigma}P^{\dagger} = c^{\dagger}_{N-i\sigma}$ for $i = 0, 1, \ldots, N-1$. Charge and spin gaps, defined by $\Delta_c(N) = E_0(N/2+1, N/2) + E_0(N/2-1, N/2) - 2E_0(N/2, N/2)$ and $\Delta_s(N) = E_0(N/2+1, N/2-1) - E_0(N/2, N/2)$, respectively, where $E_0(N_\uparrow, N_\downarrow)$ denotes the ground-state energy of the system with $N_\uparrow$ spin-up and $N_\downarrow$ spin-down electrons. Note that Δ_c incorporates ground-state lattice relaxation effects and therefore differs from the optical gap [2]. In the infinite system, we expect that $\Delta_c = \Delta_s \geqslant 0$ for $U \leqslant U_c$, whereas $\Delta_c > \Delta_s = 0$ for $U > U_c$. Results are given at $g^2\omega_0 = 2$, $\omega_0/t = 1$

U/t	2	4	6
P	+	−	−
$\Delta_c(8)/t$	1.84	0.24	1.7
$\Delta_s(8)/t$	1.62	0.13	0.28

(ii) Increasing U at fixed g, the Peierls dimerization and the concomitant charge order are suppressed. Accordingly the system evolves from the PI to the MI regime. From our numerical data we found evidence for *only one* critical point U_c (cf., e.g., the development of the optical gap in the conductivity spectra shown Fig. 2). At U_c, in our finite system a site parity change of the ground state takes place from $P = +1$ (PI) to $P = -1$ (MI), and both the spin and the charge gaps are expected to vanish in the thermodynamic limit (cf. Table 1).

(iii) 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 Mott–Hubbard insulating regime the optical gap is by its nature a correlation gap. It is rapidly destroyed by doping the system away from half-filling [5].

(iv) Different from the case where the lattice vibrations are coupled to the transfer amplitudes of the electrons (SSH-type models), the HHM exhibits no spin-Peierls instability in the large-U limit of localized electrons interacting via an effective antiferromagnetic exchange interaction.

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