GAP FORMATION IN THE HOLSTEIN MODEL*

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We investigate the Holstein model, which describes the coupling of a local phonon mode to a band of conduction electrons, in $d = \infty$. In the limit of large phonon frequency ω_0, this model can be mapped onto a Hubbard model with effective attractive electron–electron interaction. The latter model is known to exhibit a metal–insulator transition at half filling for large enough coupling strengths. We show that the system with small phonon frequencies also develops a gap as function of the electron–phonon coupling. The physics of the gap formation differs for small and large phonon frequencies, *e.g.* the "hysteresis" seen for large ω_0 disappears for smaller values.

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The simplest model to describe the coupling between electronic and lattice degrees of freedom is the Holstein model [1]. Here a local non-degenerate phonon mode is coupled to the electron density of a single conduction band,

$$H = \sum_{\vec{k}\sigma} \varepsilon(\vec{k}) c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_i \omega_0 b^{\dagger}_i b_i + \sum_i g(b^{\dagger}_i + b_i) \sum_{\sigma} (n_{i\sigma} - \tfrac{1}{2}) \,. \qquad (1)$$

The phonon frequency is given by ω_0, the electron–phonon coupling strength g. We are interested in the particle-hole symmetric situation and consider the model in the limit of infinite dimensions. Despite its simplicity this model is not exactly solvable for finite electron density.

Contrary to previous calculations which take the static limit [2], we treat the phonons quantum mechanically. Also since perturbative approaches (*e.g.* Migdal–Eliashberg) are known to break down at strong coupling [3, 4], we apply a combination of the dynamical mean-field theory (DMFT) [5]

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and the numerical renormalization group (NRG) [6]. The DMFT maps the Holstein model onto the Anderson–Holstein impurity model [7]. This mapping becomes exact in the limit of infinite spatial dimensions ($d = \infty$) [8]. The application of the NRG to the Anderson–Holstein model is presented in Ref. [7].

In the limit of $\omega_0 \to \infty$ one can map the Holstein model onto the attractive Hubbard model with an effective interaction strength $|U| = 2g^2/\omega_0$ [9]. This model can subsequently be mapped onto the repulsive Hubbard model with the charge and spin channels exchanged. When anti-ferromagnetism is suppressed in that model, it is known to show a Mott–Hubbard metal–insulator transition in $d = \infty$. The properties of this transition are well understood [5,10]. Therefore, at least in this limit such a metal–insulator transition is also to be expected in the Holstein model if charge order is suppressed.

One of the aims of this paper will be to clarify the range of validity of the mapping of the Holstein to the Hubbard model and investigate how the physical properties evolve from those of the Hubbard model as ω_0 is decreased. Here we want focus on the gap formation in the electronic spectral density as function of coupling strength g.

In our numerical evaluations, we take the non-interacting conduction band to be semielliptical with the bandwidth $W = 1$ defining the energy unit. Typical phonon frequencies are much smaller than W, though in some cases (Fullerides) [11] the phonon frequencies can be as large as $0.2W$. To clarify the relation to the Hubbard model, we have extended the calculations to include the regime $\omega_0 > W$.

In Fig. 1, we have plotted the electronic spectral density for the Holstein model for various phonon frequencies ω_0 and coupling strengths g. For all phonon frequencies the low-energy properties show a number of common features: For weak electron–phonon coupling g, the system is a Fermi liquid with the spectral function pinned at the Fermi energy $E_{\mathrm{F}} = 0$. The spectra for all ω_0 develop a narrow low-energy resonance when most of the spectral weight shifts to higher energies. Above a critical coupling g_{c}, a gap opens at the Fermi energy. The quasiparticle weight vanishes continuously for all values of ω_0. The energy scale of the gap formation depends strongly on ω_0.

The structure of the high-energy sub-bands differs for the various values of ω_0. For small ω_0, only two sub-bands emerge, for larger ω_0 four. The lower-energy ones can be termed "bipolaron bands" and are positioned at the *bipolaron binding energy* $\lambda = 2g^2/\omega_0$. The higher-energy features positioned roughly at $\pm\omega_0$ are "multi-phonon peaks" known from the atomic limit [7]. Only for $\omega_0 = 3$ these are totally split off from the other sub-bands and not visible on the plotted scale. Also their weight vanishes with increasing ω_0 (see Ref. [7]). For very large $\omega_0 \sim 3$, they can be neglected, and the system

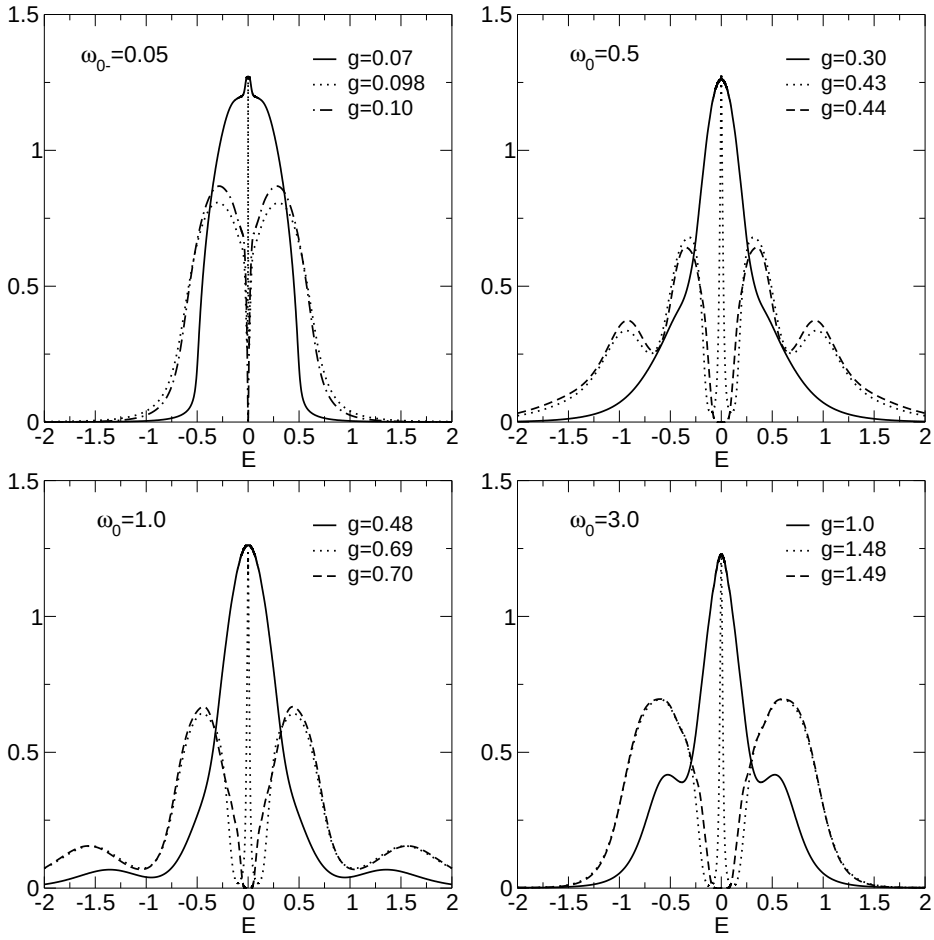

Fig. 1. Electron spectral functions for different ω_0 and g as indicated. The chosen values of g correspond to $0.7\,g_c$, $0.99\,g_c$ and $1.01\,g_c$, respectively, with g_c denoting the critical value where the quasiparticle weight vanishes and the gap in the spectral function opens for each value of ω_0.

can be described by two sub-bands separated by the bipolaron binding energy λ which becomes the effective attractive Hubbard interaction. Only in this limit is the mapping onto a Hubbard model precise.

The Mott metal–insulator transition in the Hubbard model shows a co-existence regime, where both the metallic and insulating solutions exist ("hysteresis"). For large ω_0, the gap formation in the Holstein model should correspond to this, and also show this hysteresis. This can be seen in Fig. 2, where the upper and lower values for the critical coupling strength are plotted. On reducing ω_0, the critical coupling strength rapidly moves to

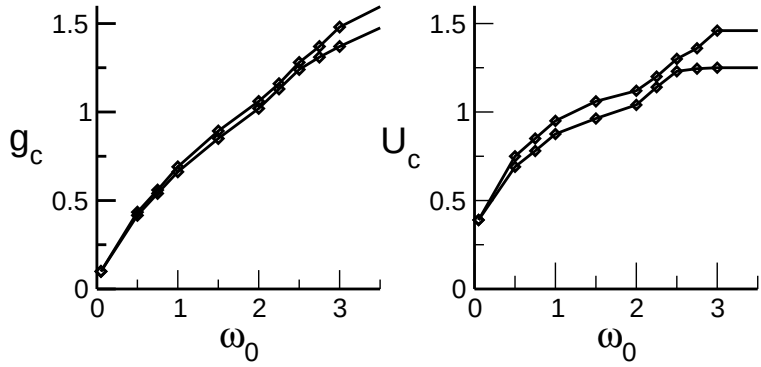

Fig. 2. Critical values of the coupling strength g_c and $|U| = 2g_c^2/\omega_0$ for the metal–insulator transition in the Holstein model. The two lines show the upper and lower boundary of the co-existence region of metallic and insulating solution. The increase in slope around $\omega_0 \approx 2$ coincides with the separation of bipolaron- and multiphonon subbands. For $\omega_0 > 3$ both the lower and the upper critical value of U are constant.

lower values and simultaneously the size of the co-existence regime shrinks. Finally, for the (physically most relevant) case of $\omega_0 = 0.05$, we do not see any hysteresis at all. Due to the numerical nature of our investigation, we cannot strictly rule out the existence of an extremely narrow coexistence region for these small values of ω_0, but, if existing, it would need to be very small.

Using the NRG technique in conjunction with the DMFT we have examined the Holstein model for all coupling strengths and ranges of phonon frequency. A more extensive presentation of the electronic and phonon response functions and a more detailed discussion of the physics involved will be published elsewhere.

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