Phase diagram and dynamic response functions of the Holstein-Hubbard model

W. Koller [a] D. Meyer [a] A. C. Hewson [a] Y. Ōno [b]

[a] *Department of Mathematics, Imperial College, London SW7 2AZ, U.K.*

[b] *Department of Physics, Niigata University, Ikarashi, Niigata 950-2181, Japan*

Abstract

We present the phase diagram and dynamical correlation functions for the Holstein-Hubbard model at half filling and at zero temperature. The calculations are based on the Dynamical Mean Field Theory. The effective impurity model is solved using Exact Diagonalization and the Numerical Renormalization Group. Excluding long-range order, we find three different paramagnetic phases, metallic, bipolaronic and Mott insulating, depending on the Hubbard interaction U and the electron-phonon coupling g. We contrast the behaviour of the one-electron spectral functions, local dynamic susceptibilities, and phonon spectra close to the transition from the metallic to the bipolaronic phase with the corresponding response functions for the Mott transition.

Key words:
strongly correlated electrons, electron-phonon coupling, Mott transition

Electron-phonon effects in strongly correlated electron systems are expected to be significant but have sofar received little theoretical attention. We study these effects here using the Holstein–Hubbard model[1,2] where a local Einstein phonon mode couples linearly to local charge fluctuations. The Hamiltonian is given by

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon(\boldsymbol{k})\, c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_i b^{\dagger}_i b_i + g \sum_i (b^{\dagger}_i + b_i)\big(n_{i\uparrow} + n_{i\downarrow} - 1\big)\,.$$

We use a semi-elliptical band of width $W = 4$ and focus on the particle-hole symmetric case at zero temperature. The phonon frequency is fixed to $\omega_0 = 0.2$. We calculate the phase diagram, in the absence of long-range order, using a number of local approximations (DMFT-NRG/ED [2], DIA [3]).

All methods agree on the phase diagram shown in the figure. It consists of a metallic region surrounded by two distinct gapped phases, a Mott insulator for large U and a bipolaronic phase, when the electron-phonon coupling g dominates. The transition to the Mott insulating phase is always continuous, as indicated by the grey boundary curve; the critical value of U is largely independent of g. In contrast, the transition to the bipolaronic phase is first order for $U \gtrsim 3$, as indicated by the full black line, but is also continuous for smaller values of U.

More of the physics of the interplay of the electron-phonon and electron-electron interactions is revealed in the spectra of the dynamic response functions. These were calculated using the DMFT-NRG [4]. Electron and phonon spectra are shown within the figure along different scans in the phase diagram. The results for the corresponding dynamic spin and charge susceptibilities are discussed in [1].

The two upper insets show the electron spectra $\rho_G(\omega)$. The left-hand scan for $U = 1$ and $g = 0.0, 0.4, 0.46, 0.5$ shows the continuous narrowing of the central resonance with increasing g and the subsequent opening of a gap at $g_c \approx 0.47$. Contrasting behaviour is seen in the upper right inset ($U = 5, g = 0.0, 0.6, 0.7, 0.75$) with an initial broadening of the

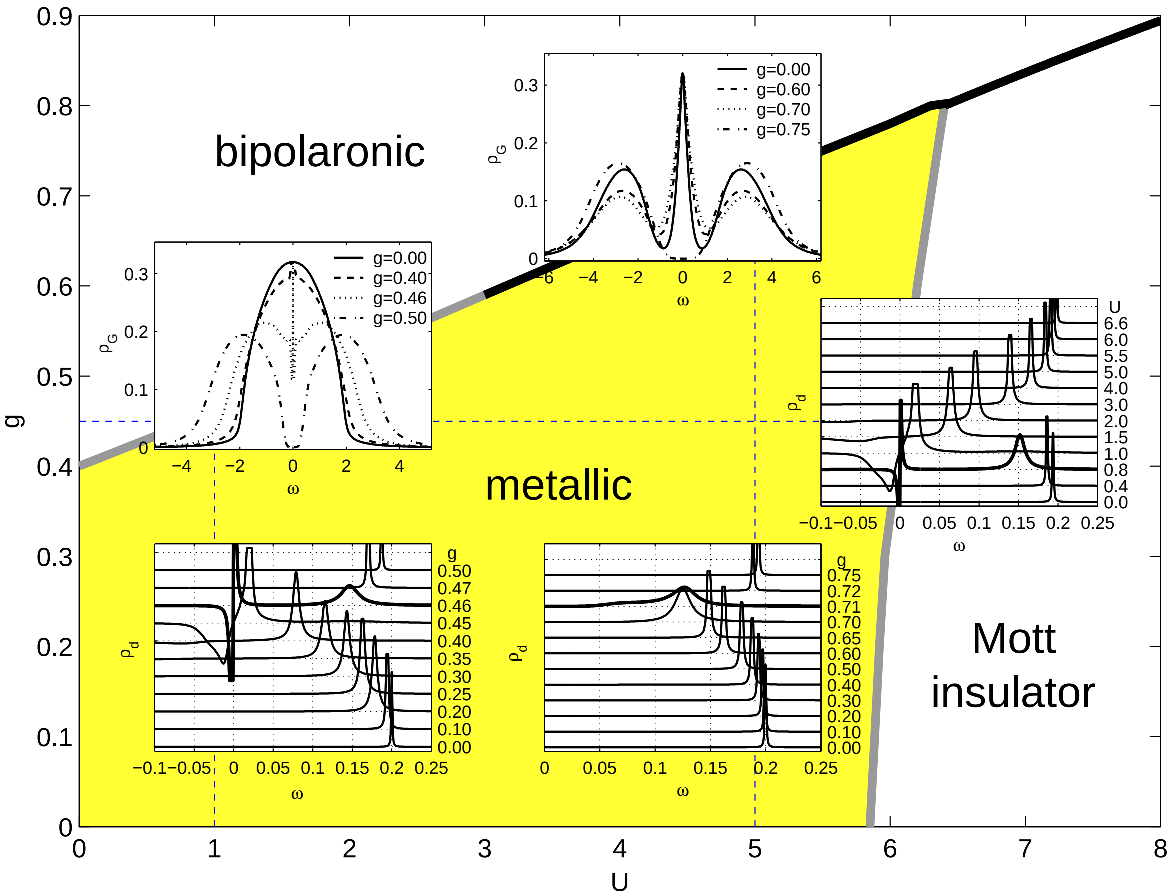

Fig. 1. Phase diagram for the particle-hole symmetric Holstein-Hubbard model at zero temperature for a semielliptical band of width $W = 4$ and a phonon frequency $\omega_0 = 0.2$. The insets show scans of the electron and phonon spectra, see text.

central peak followed by its sudden disappearance at a critical $g \approx 0.71$.

The two insets below the electron spectra show the behaviour of the corresponding phonon spectra $\rho_d(\omega) = -\frac{1}{\pi}\mathrm{Im}\langle\langle b_i ; b_i^\dagger\rangle\rangle_\omega$. For $U = 1$ we see with increasing g a complete softening of the phonon peak as the transition to the bipolaronic phase is approached. The increase of negative spectral weight for $\omega < 0$ indicates a growing number excited phonons. At $g_c \approx 0.47$ we observe a two-peak structure whose low energy peak vanishes and whose high-energy peak hardens back to ω_0 after the continuous transition. For $U = 5$ the softening of the phonons is much weaker due to suppression of charge fluctuations. There is no two-peak structure at the transition and again the peak hardens to ω_0 in the gapped phase.

Similar features can also be seen in the scan for a fixed $g = 0.45$ and increasing U, shown in the right-hand inset. The transition from the bipolaronic to the metallic phase is reflected by a two-peak structure. Increasing U further suppresses charge fluctuations and hardens the completely softened phonon peak until the Mott transition is approached and the peak arrives at the bare frequency ω_0.

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