Phase diagram of Holstein-Kondo lattice model at half-filling

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Abstract

We study the Kondo lattice model which is modified by the Holstein term, involving both the Kondo exchange coupling and the electron-phonon coupling constants, characterized by $J$ and $g$, respectively. The model is solved by employing the dynamical mean-field theory in conjunction with exact diagonalization technique. A zero temperature phase diagram of symmetry unbroken states at half filling is mapped out which exhibits an interplay between the two interactions and accounts for both spin and charge fluctuations. When the Kondo exchange coupling is dominant the system is in Kondo insulator state. Increasing $g$ for small values of $J$ leads to a Kondo insulator-metal transition. Upon further enhancement of $g$ a transition to the bipolaronic insulating phase takes place. Also a small region with non-Fermi liquid behavior is found near the Kondo insulator-metal transition.
There has been a continued interest in a class of compounds called heavy fermion semiconductors, which exhibit a spin and a charge gap at low temperatures typically ranging between 1 and 100 meV [1, 2]. In contrast to the ordinary band insulators, these two gaps are different, indicating a separation of the spin and charge degrees of freedom brought about by correlation effects. The gap formation in heavy fermion semiconductors is attributed to the renormalized hybridization between a broad band of conduction electrons and a nearly flat band of strongly correlated f-electrons.

The Kondo lattice model (KLM) at half-filling is considered to be a good starting point for investigating the properties of the heavy fermion semiconductors. In this model, at each lattice site a local moment interacts with the spin of a conduction electron, and thus, results in complex correlation effects between them. In fact, a conduction and a localized electron with antiparallel spins undergo a spin-flip process, causing itinerant electrons to leave a trace of their spin exchange at each localized spin site. As a result, the direction of a localized spin is affected by the history of the electrons passing through it. There are similar correlation effects in the periodic Anderson model due to the dynamical aspects of the localized electrons.

Experiments involving the Kondo insulators at high magnetic fields indicate the closure of the Kondo insulating gap, exemplifying a transition from the Kondo insulator to a correlated metal [3, 4]. It is expected that the electron-phonon (e-ph) interaction leads to similar results. Many experiments suggest that the e-ph effects are important in describing a number of observations such as the existence of an unusual phonon softening in the Kondo lattice, CeCu$_2$, which is indicative of coupling between electrons and phonons [5]. Furthermore, the lattice plays an important role in some heavy fermion compounds, called 14-1-11, where various properties can be altered through isoelectronic substitutions [6]. In fact, it is believed that the coupling between phonon modes and the Kondo effect could manifest new material properties, such as non-Fermi liquid behavior and unconventional superconductivity [7, 8, 9].

Even less studies has been devoted to the role played by lattice vibrations in these compounds. The role of the lattice vibrations is not trivial, but if, on general grounds, the minimal effect of e-ph coupling is a phonon-retarded attraction between conduction electrons with opposite spins, then the spin excitation has a gap while the charge excitation, depending on the strength of the e-ph coupling, can be either gap-full or gapless. Therefore, there arises a competition between the spin- and the charge-fluctuations whose behavior is determined, on the one hand, by the relative strength of the Kondo exchange between the conduction electrons and the localized moments and,
on the other hand, by the conduction electron-phonon coupling leading to a complicated phase diagram.

It is the goal of this paper to investigate the dynamical competition between the e-ph and Kondo interactions. A natural way of incorporating the e-ph coupling in the KLM is to add the Holstein coupling term to its hamiltonian. In the Holstein coupling the phonon variables are coupled to the local density of the conduction electrons. In this paper, we will present the zero temperature phase diagram of the Holstein-Kondo lattice model (H-KLM) at half-filling. The focus is on the transition between the unbroken symmetry ground state as the e-ph and Kondo interactions parameters, $J$ and $g$, are varied.

The H-KLM Hamiltonian is defined by:

$$H = - t \sum_{(i,j)\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{c.c.}) + \frac{J}{2} \sum_{i,\alpha\beta} S_i \cdot (c_{i\sigma}^\dagger \sigma_{\alpha\beta} c_{i\sigma}) + g \sum_i (n_i - 1) (b_i^\dagger + b_i) + \Omega_0 \sum_i b_i^\dagger b_i,$$  

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) and $b_i$ ($b_i^\dagger$) are, respectively, destruction (creation) operators for itinerant electrons with spin $\sigma$ and local vibrons of frequency $\Omega_0$ on site $i$, $n_i$ is the electron density on site $i$, $S_i$ is the spin operator for the localized spin on site $i$, $\sigma$ is a pseudo-vector represented by Pauli spin matrices, $t$ stands for the itinerant electrons hopping matrix elements between the nearest-neighbor sites, $J$ is the coupling strength between itinerant electrons and localized spins, and $g$ denote the electron-phonon coupling. We do not consider the coulomb repulsion term between itinerant electrons, because it tends to suppress the double occupation of sites and in our model the exchange coupling, $J$, already does the same thing.

Our calculations are based on the dynamical mean field theory [10], a powerful, non-perturbative tool to study the properties of strongly correlated systems, which allows us to treat, on equal footing, the two kinds of interactions present in our model. This technique, which becomes exact in the limit of infinite coordination number, reduces the full lattice many-body problem to a local impurity embedded in a self-consistent effective bath of free electrons, mimicking the effect of the full lattice on the local site. A self consistency condition links the effective impurity model to the original lattice problem. Adopting a semi-circular density of states (DOS) $\rho_0(\epsilon) = (2/\pi D) \sqrt{D^2 - \epsilon^2}$ of the noninteracting system, corresponding to a Bethe lattice with the
half bandwidth $D$, the self-consistency relation imposed on the DMFT solution is given by

$$\frac{D^2}{4} G(i\omega_n) = \sum_k \frac{V_k^2}{i\omega_n - \epsilon_k},$$

(2)

where $\epsilon_k$ and $V_k$ are the energies and the hybridization parameters of the effective impurity model (bath parameters). We use exact diagonalization (ED) technique to solve the effective impurity model [11]. This solver allows us to access the ground state properties of the system with a finite energy resolution. The ED technique consists of restricting the sum in Eq. (2) to a small number of levels, and moreover, it truncates the infinite phonon Hilbert space. The ground state and the Green’s function of our discretized model are determined via the Lanczos procedure and the self-consistency equation in turn allows us to derive a new set of bath parameters. The process is iterated until convergence is reached. In the theory of Mott transition, the investigation of the paramagnetic (PM) phase has been very fruitful providing a lucid understanding of the finite temperature state, above the magnetic order in many compounds. We pursue a similar approach in our investigation and study the PM state. We force the system to be in a paramagnetic state by averaging the spin up and spin down to study the underlying normal state. In all our calculations presented here the convergence of truncation has been checked.

Fig. 1 shows the $T = 0$ phase diagram of the half-filled H-KLM in the parameter space of $J$ and $g$ with $\Omega_0/t = 0.2$. All types of long-range order are excluded. Three different phases are distinguished: metallic phase and the bipolaronic and Kondo insulating phases. In what follows, a detailed discussion of the phase diagram of these systems will be presented. The Kondo lattice model ($g = 0$) and Holstein model ($J = 0$), which are special limiting cases of the H-KLM, have been extensively studied using the DMFT. The ground state of KLM is the Kondo insulating phase with a spin and a charge gap for all $J$ values [12]. For the Holstein model, the ground state is metallic. The metallic phase is found to be a Fermi liquid, in the sense that, the Luttinger sum rule $\rho(0) = 2\rho_0(0)$ for the spectral function $\rho(\omega) = -\text{Im}G(\omega + i0^+)/\pi$, or equally stated, the limit of $\text{Im}G(i\omega_n) \rightarrow -1$ as $\omega_n \rightarrow 0$, is satisfied ($\omega_n$ is the Matsubara frequency). Upon increasing $g$, the conduction electrons lose their mobility, eventually acquiring polaronic character, in which the presence of an electron is associated with a finite lattice distortion. Also, the same e-ph coupling can cause any two polarons to attract and form a bound pair in real space, called bipolaron [14]. In the absence of pair hopping, the bipolaron formation would cause the system to undergo a first order metal to bipolaronic insulating phase transition at the critical coupling $g_c$ [15, 16]. Meyer et al. have reported that there is a coexistence region near $g_c$, which is reduced as the phonon
FIG. 1: Zero temperature phase diagram of the unbroken symmetry Holstein-Kondo lattice model at half-filling. The model shows three different phases: metallic, bipolaronic and Kondo insulating phase. A narrow region with non-Fermi liquid character is seen near the Kondo insulator-metal transition.

frequency $\Omega_0$ is decreased and disappears for $\Omega_0 \leq 0.10D$ [17]. The bipolaron formation may be accommodated by reconstructing the system into a phase separated state [18] or a charge ordered state in which the doubly occupied and empty sites alternate in real space [19].

At small fixed $J$-values, with increasing e-ph coupling, a continuous transition to a metallic state occurs at a critical coupling $g_{1c}(J)$, whose value increases with increasing $J$. This behavior is physically expected. An increase in $J$ leads to a larger insulating gap, and this in turn, leads to the suppression of the charge fluctuations which would otherwise couple to phonons. As a result a transition to metallic state occurs at larger e-ph coupling. We also find that the metallic phase near $g_{1c}$ shows non-Fermi liquid character. Further increase of $g$ causes a metal-bipolaronic phase transition taking place at a critical coupling $g_{2c}$. As it can be distinguished, a Holstein coupling is weakly affected by exchange coupling between conduction electrons with local spins. The metallic state becomes more correlated as $g$ or $J$ is increased. This is reflected in the decreasing behavior of the quasiparticle weight $z = 1/[1 - Im \Sigma(i\omega_0)/\omega_0]$ when $g$ or $J$ is increased (Fig. 2).

Fig. 3 shows the imaginary part of electron self-energy, $Im \Sigma(i\omega_n)$, for $J = 0.1$ and several
values of $g$ in the vicinity of both phase transitions. For small $g$ values, the imaginary part of the self-energies diverge as $\omega_n \to 0$, indicating the presence of a charge gap (See panel a). Increasing $g$ causes the system to change its phase from an insulator to a bad metal in the sense that its self-energy extrapolates to a finite value $\text{Im} \Sigma(i0^+) \equiv \Gamma(J) \neq 0$ for $g \geq g_{1c}$. Hence, a finite lifetime is found at the Fermi level for a narrow range of e-ph couplings near the $g_{1c}$, indicating that well defined quasiparticles do not exist in this range. The violation of the Luttinger sum rule in this region is also seen from $\text{Im} G(i\omega_n)$, which tends to a negative constant $c < 0$ in the limit of $\omega_n \to 0$, with $c < \pi \rho_0(0) = 1$. Although the discretness of the spectra obtained in the exact diagonalization technique does not allow us to unambiguously identify the non-Fermi liquid region, we believe that the spectral function at $g = 0$ displays a narrow insulating gap, whose width is proportional to the value of $J$, with two peaks on each side. For a fixed $J$, increasing $g$ causes the low-energy spectrum widen and are also suppressed. If these peaks overlap before being damped completely, a narrow pseudogap forms near the Fermi level, $E_F$. With further enhancement of $g$, there is a rapid shallowing of the pseudogap till finally a quasiparticle peak forms at $E_F$. At this stage, the system will have a Fermi-liquid character. Upon increasing $g$ further, there is a weakly narrowing of quasiparticle peak until it disappears at the second critical value of e-ph coupling $g_{2c}$ where a gap opens. A more detailed results on the spectra might be obtained by the numerical renormalization group technique. The inset of panel (b) shows double occupancy $d = \langle n_\uparrow n_\downarrow \rangle$ as a function of $g$. There is no signature of the Kondo insulator-metal transition in the double occupancy, but at $g_{2c}$ the double occupancy jumps suddenly to $d \approx 1/2$, indicating a discontinuous transition to bipolaronic phase.
FIG. 3: Imaginary part of electron self-energy, $Im \Sigma(i\omega_n)$, obtained at different values of $g$ in the vicinity of both phase transitions, with fixed $J = 0.1$. Panel (a): $Im \Sigma(i\omega_n)$ in the vicinity of the transition from the Kondo insulator state to the metallic state. Changing the $Im \Sigma(i\omega_n)$ behavior as $\omega_n \to 0$ from diverging to extrapolating to zero shows the insulator-matallic phase transition. Panel (b): $Im \Sigma(i\omega_n)$ in the vicinity of the transition from the metallic state to bipolaronic state. Inset: the double occupancy $d = <n_\uparrow n_\downarrow>$ as a function of $g$. The transition from the metallic state to bipolaronic state is clearly visible by observing when the double occupancy’s jump to $\approx 1/2$ begins to set in.
Fig. 4(a) shows the phonon spectral function, $\rho_{\text{ph}}(\omega) = -Imd(\omega + i0^+)/\pi$, for $J = 0.1$ as a function of e-ph interaction strengths. The phonon Green’s function is defined by $d(\omega) = \ll b_i; b_i^\dagger \gg \omega$. The figure illustrates how the phonon mode is softened with increasing $g$. The softening phonon mode is a manifestation of a lattice instability as in structural phase transitions. A stability is restored by the condensation of the unstable mode. It results in a nonzero expectation value of the phonon operator ($\langle b \rangle \neq 0$) or in large average number of excited phonons in the ground state. The appearance of negative spectral function for $\omega < 0$, when the bipolaronic state is approached implies that there is a large increase in the lattice displacement. In the bipolaronic state, the phonon mode hardens back to the bare mode as $g$ assumes values greater than $g_{c2}$. This is due to the fact that screening is not effective in an insulating state. This is the same behavior which had already been seen for pure Holstein model [20]. Panel (b) of Fig. 4 shows the phonon spectral function for $g = 0.2$ and various values of $J$. The phonon mode gradually hardens back to $\Omega_0$, as the $J$-values increase. We observe no signature of a transition to Kondo insulator in the phonon spectrum. The effect of increasing $J$ is to suppress continuously the charge fluctuations which results in a decoupling of electrons and phonons causing the phonon peak to exhibit hardening. In contrast to the Holstein-Hubbard model results, where softening is absent in Mott insulator phase and phonons are effectively decoupled from electrons [20], here the hardening of the phonon peak takes place very slowly.

In conclusion, we have studied the Holstein-Kondo lattice model at half-filling. We find that the model presents the physics of the Kondo insulator when the exchange coupling, $J$, plays a dominant role and a transition to correlated metal takes place for small $J$ and intermediate e-ph coupling, $g$. Moreover, a bipolaronic-metal insulator takes place for small $J$ and large $g$. We also find a small region with non-Fermi liquid character near the Kondo insulator-metal transition. The remaining interesting questions will be how the phase diagram and nature of transitions will change as $\Omega_0$ or electron density is changed. It is also interesting to study the symmetry breaking states such as the antiferromagnetic and superconducting states. Works in this direction are in progress and will be reported in a separate publication.
FIG. 4: Phonon spectral function for different values of $g$. The bare phonon frequency is $\Omega_0 = 0.2$ and a Lorentzian broadening with the full width at half maximum of 0.02 has been implemented. Panel (a): Spectral function for $J = 0.1$ and various values of $g$. A considerable phonon softening is seen upon approaching the transition to the bipolaronic insulator. Panel (b): Spectral function for $g = 0.2$ and various values of $J$. The transition to Kondo insulator does not obviously affect the phonon spectral function.
Acknowledgments

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