Periodic Anderson model with electron-phonon correlated conduction band

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This paper reports dynamical mean field calculations for the periodic Anderson model in which the conduction band is coupled to phonons. Motivated in part by recent attention to the role of phonons in the $\gamma$-$\alpha$ transition in Ce, this model yields a rich and unexpected phase diagram which is of intrinsic interest. Specifically, above a critical value of the electron-phonon interaction, a first order transition with two coexisting phases develops in the temperature-hybridization plane, which terminates at a second order critical point. The coexisting phases display the familiar Kondo screened and local moment character, yet they also exhibit pronounced polaronic and bipolaronic properties, respectively.

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The Periodic Anderson Model (PAM) and its impurity variant have played pivotal roles in elucidating the nature of Kondo screening as the techniques of many-body theory have improved. Perhaps its most noted application has been the Kondo Volume Collapse scenario for understanding the unique isostructural $\gamma$-$\alpha$ transition in Ce, with its very large 15% volume change. The relative merits of this perspective versus the Mott transition scenario are still under debate, although both have played pivotal roles in elucidating the nature of this transition scenario. The focus on critical phase transitions are still under debate, although both perspectives versus the Mott transition versus the Kondo screened and local moment character, yet they also exhibit pronounced polaronic and bipolaronic properties.

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is present at large temperatures. Therefore the data we show are for \( n_f \sim 1.0 \) and \( n_c \sim 0.8 \). The Continuous Time Quantum Monte Carlo (CTQMC) \(^{26}\), generalized for electron-phonon coupling \(^{27}\), is employed as the impurity solver.

Fig. 1 displays the local hybridization factor \( \Gamma = \langle c_{\uparrow}^\dagger f_0 + h.c. \rangle \) (here \( 0 \) denotes the impurity site) as a function of \( V \) for \( g^2/2k = 1.0 \) and different values of inverse temperature, \( \beta \). As the temperature decreases, the slope of the \( \Gamma \) vs. \( V \) curve becomes progressively larger, which indicates the system is approaching a critical point. Interestingly, the curves approximately cross for a critical value of the electron-phonon coupling \( \beta \). As the temperature decreases, the crossing disappears. This indicates that the corresponding susceptibility reaches a plateau as a function of the temperature and the critical behavior is lost. We believe that \( g^2/2k = 0.49 \) is a lower bound for the critical value of the electron-phonon coupling.

The inset of Fig. 1 shows \( \Gamma \) vs. \( V \) at \( g^2/2k = 0.49 \). Notice that for this value of the coupling the slope does not become steeper as the temperature decreases, and the crossing disappears. This indicates that the corresponding susceptibility reaches a plateau as a function of the temperature and the critical behavior is lost. We believe that \( g^2/2k = 0.49 \) is a lower bound for the critical value of the electron-phonon coupling.

When the temperature is further decreased to \( T = 0.0167 \) (\( \beta = 60 \)), \( \Gamma \) vs. \( V \) displays a hysteresis loop as shown in Fig. 2. The red line is obtained by starting at the large \( V \) side (\( V = 1.2 \)), and using the output self-energy to initiate the simulation for the next smaller \( V \). On the other hand, we obtain the black line by starting at \( V = 0.8 \) and using the output self-energy as the input for the next larger value of \( V \). The coexistence of two solutions for the same value of \( V \) at \( T = 0.0167 \) is a direct evidence of a first order phase transition. The absence of such a hysteresis at higher temperatures indicates that the first order transition ends at a second order terminus \( (V_c, T_c) \).

For the same parameters, \( V = 0.96, g^2/2k = 1.0, \omega_0 = 0.01, \) and \( U = 4.0 \), we also perform a series of isothermal scans on the chemical potential to study the relationship between the total electron density \( n = n_e + n_f \) and the chemical potential \( \mu \). As long as the temperature is not below \( T = 0.0167 \), the compressibility \( \frac{dn}{d\mu} \) shows no tendency to diverge. This indicates the phase transition here is not compressibility driven.

In Fig. 2 we show the temperature times the local f-orbital spin susceptibility, \( T \cdot \chi^{f}_{ff} \), versus temperature. As \( T \) approaches zero \( T \cdot \chi^{f}_{ff} \) is roughly constant for \( V = 0.8 \), while it goes to zero for \( V = 1.2 \). This indicates that at \( V = 0.8 \) the \( f \)-electrons display a robust local moment and paramagnetic local susceptibility with \( 1/T \) dependence, while at \( V = 1.2 \) the \( f \) local moments are quenched. The inset of Fig. 2 shows the \( f \)-orbital density of states (DOS) at \( T = 0.01 \). Notice that at \( V = 0.8 \) there is a gap across the Fermi level, while at \( V = 1.2 \) a Kondo resonance peak appears. The screening of the local moment in the large \( V \) region is a consequence of the singlet formation between \( c \) and \( f \)-electrons.

The main panel of Fig. 3 shows the occupancy distribution histogram of the \( c \)-electrons, \( P(n_c) \), at \( T = 0.0167 \). \( P(n_c) \) has been used to illustrate bipolaron formation \(^{27}\). At \( V = 0.8 \) the \( c \)-orbital electrons are in a bipolaronic state, which is characterized by the oscillation between zero and double occupancy. While for \( V = 1.2 \), the \( c \)-electrons are in a polaronic state, where the occupancy oscillates between zero and one. For the PAM, without electron-phonon coupling, the structure of \( P(n_c) \) is totally different. Here there is only one peak at roughly the \( c \)-electron filling \( n_c = 0.8 \), and \( P(n_c) \) quickly decays to zero for \( n_c \) away from this filling. In the inset, the quasi-particle fraction \( Z \) is plotted as a function of temperature. The quasi-particle fraction is calculated...
exact at zero temperature. As \( T \to 0 \) converges to a finite value for Fermi liquid formation.

For \( V = 1.2 \) (red line), \( T \cdot \chi_{ff}^{\sigma \sigma} \) converges to zero indicating the local moment is screened. Inset: The \( f \)-electron DOS at \( T = 0.01 \). The Kondo peak found for \( V = 1.2 \) (red line), but absent for \( V = 0.8 \) (black line) is consistent with the screening and unscreening scenarios in the main panel.

for the lower quasiparticle band at the Fermi level using a generalization of the single band formulation \[28\]. The main component of this approach is to make the replacement

\[
\frac{d \text{Re} \Sigma(\omega)}{d\omega} |_{\omega=0} \approx \frac{\text{Im} \Sigma(i\pi T)}{\pi T},
\]

which becomes exact at zero temperature. As \( T \to 0 \), \( Z \) goes to zero for \( V = 0.8 \) indicating non-Fermi liquid behavior, while it converges to a finite value for \( V = 1.2 \), the signature of Fermi liquid formation.

The isothermal \( \Gamma \) vs. \( V \) curves still cross and their slopes diverge at a critical value of the hybridization, \( V_c \), as the temperature is decreased. We also find that \( V_c \) changes roughly linearly with \( g^2/2k \).

In Fig. 3(a) the time integrated local \( f \)-orbital spin-spin correlation function, \( \chi_{ff}^{\sigma} \), is plotted as a function of temperature for \( V = 1.1, 1.2 \) and \( 1.3 \). We identify the Kondo scale \( T_K \) as the energy where \( \chi_{ff}^{\sigma} \) falls to around half of its low temperature value. We find that \( T_K \) changes very little as \( V \) increases, so the line \( V \) vs. \( T_K \) should have a large slope. Fig. 3(b) shows the time integrated local \( c \)-orbital spin-spin correlation function, \( \chi_{cc}^{\sigma} \) vs. \( V \), at different temperatures, where large values reflect the \( c \)-electron spin degeneracy in the polaronic state in contrast to the small susceptibility for the spinless bipolarons. For \( V < 0.96 \) the curves almost overlap for all \( T < 0.1 \). In fact, the corresponding \( c \)-electron occupancy histograms (not shown) show an obvious bipolaronic double peak feature even at relatively high temperatures like \( T = 0.1 \). If we define \( T^* \) as the energy where bipolaron formation begins, then the line \( T^* \) vs. \( V \) must be nearly horizontal.

We have also calculated the renormalized phonon frequency. At \( T = 0.025 \) it is roughly constant for hybridization \( V > 0.96 \); however, it drops precipitously for \( V < 0.96 \), decreasing by half when \( V = 0.8 \). This behavior softens with increasing temperature, e.g., a more gradual decrease begins for \( V < 1.2 \) at \( T = 0.1 \). This indicates an important temperature dependence of the phonons properties. Indeed the analysis in \[13\] for Ce found that the temperature dependence of the phonons was a critical factor for obtaining a significant phonon contribution to the entropy change across the \( \gamma \rightarrow \alpha \) transition \[12\].

Fig. 4 is a schematic summary of our findings. Two phases, local moment-bipolaron and Kondo singlet-polaron, are separated by a first order transition line, which terminates at a second order critical point \( (V_c, T_c) \). The positive slope of the \( V \) vs. \( T \) first order transition line is a consequence of a Clausius-Clapeyron-like relation where hybridization \( V \) is the intensive analog of pressure. There is no broken symmetry between these two phases.
FIG. 6: (color online) Schematic $V$ vs. $T$ phase diagram. The solid black line represents the first order phase transition which separate the local moment-bipolaron phase for small $V$ from the Kondo singlet-polaron phase for large $V$. This first order phase terminates at a second order critical point. The red dashed line coming out of the critical point represents the Kondo scale $T_K$ and the green dashed line the bipolaron energy scale $T^\ast$. as we can move adiabatically from one to another by wandering around the critical point. Both phases are destroyed by increasing the temperature. In order to have such a first order phase transition, the electron-phonon coupling on the c-band must be larger than a certain critical value. The fact that the critical temperature is a function of electron-phonon coupling implies that the critical point touches zero temperature at some $g_c$, where the first order phase transition becomes a quantum phase transition tuned by $V$.

In conclusion, when the conduction band of the periodic Anderson model is coupled to phonons, one obtains a rich and unexpected phase diagram. Above a critical strength of the electron-phonon coupling a first order transition with two coexisting phases develops in the temperature-hybridization plane. This transition terminates at a second order critical point. These coexisting phases correspond to the familiar Kondo screened and bipolaronic behavior, respectively. While the PAM and its impurity variant exhibit pronounced polaronic and bipolaronic behavior, the Kondo temperature, which measures the critical energy scale of hybridization between $4f$ and valence electrons, has a roughly exponential volume dependence leading to an order of magnitude increase from $\gamma$- to $\alpha$-Ce [3, 4]. This scale is comparable to that of the lattice vibrations (Debye temperature) only in the $\gamma$ phase of Ce, and so it is no accident that the present work finds the most dramatic manifestations of the electron-phonon interaction, a bipolaronic state with significant phonon softening, in this local moment region.

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