Superfluid state in the periodic Anderson model with attractive interactions

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Abstract. We investigate the periodic Anderson model with attractive interactions. By combining dynamical mean-field theory (DMFT) with a continuous-time quantum Monte Carlo impurity solver, we study the competition between the superfluid state and the paramagnetic Kondo insulating state. It is found that both the particle and hole doping of the Kondo insulating state yields a phase transition to the superfluid state, and induces low energy in-gap states in the density of states. The phase diagram of the model is determined.

1. Introduction
Ultracold atoms have attracted considerable interest [1, 2] since the successful realization of Bose-Einstein condensation in a bosonic $^{87}$Rb system [3]. One of the most active topics in this field is the study of fermionic optical lattice systems, which are formed by loading ultracold fermions into a periodic potential [4, 5, 6, 7]. Due to the high controllability of the lattice structure and onsite interactions, fermionic optical lattice systems are sometimes regarded as quantum simulators of the Hubbard model. Recent papers have suggested the possible realization of optical lattice systems described by a multi-component model [8, 9, 10] and the Kondo lattice model [11, 12, 13]. This motivates us to investigate the periodic Anderson model (PAM) with itinerant and localized bands [14]. The PAM may provide a stage to discuss quantum phase transitions in optical lattice systems, since quantum critical behavior is expected to occur in both the repulsive and attractive models. In our previous paper [15], we have investigated the PAM with attractive interactions to clarify how the chemical potential affects the competition between the Kondo insulating state and the superfluid state at low temperatures. It is also instructive to clarify the doping dependence of low temperature properties in the PAM model. This topic was beyond the scope of our previous paper, but it may be important for the investigation of quantum critical behavior in optical lattice systems.

We study here the PAM with attractive interactions by combining dynamical mean-field theory (DMFT) [16, 17, 18, 19] with the continuous-time quantum Monte Carlo (CTQMC) approach [20]. We then discuss the competition between the superfluid state and the Kondo insulating state and determine the phase diagram. By examining dynamical properties, we clarify that the particle or hole doping of the Kondo insulating state yields a phase transition to the superfluid state, which induces low energy in-gap states in the density of states.
The paper is organized as follows: In Sec. 2, we introduce the model Hamiltonian and briefly summarize our theoretical approach. We demonstrate how the superfluid state competes with the Kondo insulating state at low temperatures in Sec. 3. A brief summary is given in the last section.

2. Model and Method

We consider the periodic Anderson model with conduction and localized bands, which is described by the following Hamiltonian,

\[
H = -t \sum_{\langle i,j \rangle \sigma} c_{i \sigma}^\dagger c_{j \sigma} + V \sum_{i \sigma} \left( c_{i \sigma}^\dagger f_{i \sigma} + f_{i \sigma}^\dagger c_{i \sigma} \right) + E_f \sum_{i \sigma} n_{i \sigma}^f - U \sum_i \left[ n_{i \uparrow}^f n_{i \downarrow}^f - \frac{1}{2} \left( n_{i \uparrow}^f + n_{i \downarrow}^f \right) \right],
\]

where \( c_{i \sigma} \) (\( f_{i \sigma} \)) annihilates a fermion in the conduction (localized) band on the i-th site with spin \( \sigma \), and \( n_{i \sigma}^a = a_{i \sigma}^\dagger a_{i \sigma} \) \( (a = c, f) \). \( t \) is the nearest-neighbor hopping matrix for the conduction band, \( V \) is the hybridization between the two bands, \( U \) is the attractive interaction, and \( E_f \) is the energy level for the localized band. In this model, the hybridization between the conduction and localized bands favors the formation of a local Kondo singlet state, and stabilizes the Kondo insulating state around half filling. On the other hand, the attractive interaction enhances pairing correlations. This tends to stabilize the superfluid state, which should be the Kondo insulating state at low temperatures in Sec. 3. A brief summary is given in the last section.

To discuss how the superfluid state competes with the Kondo insulating state, we make use of DMFT, where local particle correlations can be taken into account precisely. In DMFT, the lattice Green’s function is obtained via a self-consistency condition imposed on the impurity problem. The non-interacting Green’s function for the lattice model is given as

\[
\hat{G}_0^{-1}(k, i\omega_n) = \begin{pmatrix}
(i\omega_n + h_c)\sigma_0 + (\mu_c - \epsilon_k) \sigma_z & -V \sigma_z \\
-V \sigma_z & (i\omega_n + h_f)\sigma_0 + (\mu_f - E_f) \sigma_z
\end{pmatrix},
\]

where \( \epsilon_k \) is the dispersion relation of the conduction band, \( \sigma_z \) is the z component of the Pauli matrix, \( \sigma_0 \) is the identity matrix, \( \omega_n = (2n + 1)\pi T \) is the Matsubara frequency, and \( T \) is the temperature. Here, the Green’s function is represented in the Nambu formalism to enable a description of the superfluid state. The lattice Green’s function is then given in terms of the self-energy \( \tilde{\Sigma}(i\omega_n) \) as,

\[
\hat{G}(i\omega_n) = \begin{pmatrix}
G_{cc}(i\omega_n) & G_{cf}(i\omega_n) \\
G_{fc}(i\omega_n) & G_{ff}(i\omega_n)
\end{pmatrix} = \int dk \left[ \hat{G}_0^{-1}(k, i\omega_n) - \tilde{\Sigma}(i\omega_n) \right]^{-1},
\]

\[
\tilde{\Sigma}(i\omega_n) = \begin{pmatrix}
0 & 0 \\
0 & \Sigma_f(i\omega_n)
\end{pmatrix}.
\]

The self-energy for the localized band \( \Sigma_f \) is given as,

\[
\Sigma_f(i\omega_n) = \begin{pmatrix}
\Sigma_{f\uparrow}(i\omega_n) & S_f(i\omega_n) \\
S_f(i\omega_n) & -\Sigma_{f\downarrow}(i\omega_n)
\end{pmatrix},
\]

where \( \Sigma_{f\uparrow}(i\omega_n) \) [\( S_f(i\omega_n) \)] is the normal (anomalous) part of the self-energy for the localized band. In DMFT, the self-consistency condition is given by \( G_{ff}(i\omega_n) = G_{imp}(i\omega_n) \), where \( G_{imp} \) (2011) 012040 doi:10.1088/1742-6596/302/1/012040
is the Green’s function of the effective impurity model. The effective medium for each site is given by \( G^{-1}(i\omega_n) = [G_{\text{imp}}(i\omega_n)]^{-1} + \Sigma_f(i\omega_n). \)

In the PAM with attractive interactions, it is necessary to accurately treat different energy scales such as the hybridization gap and the superfluid gap. To this end, we make use of the CTQMC method, which has recently been developed \([20, 21]\) and has successfully been applied to general classes of models such as the Hubbard model \([22, 23, 24, 25, 26, 27]\), the PAM \([15, 28]\), the Kondo lattice model \([29]\), and the Holstein-Hubbard model \([30]\). Here, we use the continuous-time auxiliary field version of the weak-coupling CTQMC method \([31]\) extended to the Nambu formalism, which allows us to directly access the superfluid state at low temperatures \([26]\). In our CTQMC simulations, we measure normal and anomalous Green’s functions on a grid of one thousand points. In the following, we set \( \mu = \mu_c = \mu_f, \ h = h_c = h_f = 0, \) and \( E_f = 0 \) for simplicity.

3. Results

We consider the PAM on the hypercubic lattice. The bare density of states for the conduction band is given by a Gaussian with bandwidth \( t^* \): \( \rho(x) = \exp[-(x/t^*)^2]/\sqrt{\pi t^*}. \) In the paper, we use \( t^* \) as the unit of energy. Here, we focus on a system with \( V = 0.4 \) and \( U = 1.0, \) which is in the Kondo insulating state at half filling, at least, down to \( T = 0.005. \) To clarify how the superfluid state is realized by the particle doping, we calculate the pair potential for each band, as shown in Fig. 1. It is found that when \( n_f = 0.5 \), the pair potentials are zero and the hybridization stabilizes the Kondo insulating state. In fact, the density of states is symmetric, with a hybridization gap, as shown in Fig. 2. The introduction of the chemical potential leads to an increase in the number of the particles. At a certain critical value \( n_f = n_{fc1}, \) a phase transition to the superfluid state occurs and the pair potential is induced. The simulation gives \( n_{fc1} \approx 0.54 (T = 0.02) \) and \( 0.503 (T = 0.01). \) An in-gap state is simultaneously induced below the Fermi level inside the hybridization gap, as shown in Fig. 2. This low energy peak is associated with the superfluid state, since it is always located in the vicinity of the Fermi level as long as the system is in the superfluid state. If we further increase the total particle number, the pair potential goes through a maximum and finally vanishes at \( n_f = n_{fc2}, \) where \( n_{fc2} \approx 0.75 \)}
Figure 2. Density of states for the conduction (left) and localized (right) band of the system with $U = 1$ and $V = 0.4$ at $T = 0.01$. The data are for the following particle numbers in the localized band: $n_f = 0.5, 0.503, 0.575, 0.732, 0.823, \text{ and } 0.858$ (from the bottom to the top).

$T = 0.02$ and $0.85 (T = 0.01)$. The second phase transition is to the normal metallic state and marked by the collapse of the superfluid gap, as shown in Fig. 2. We also note that the small increase in the total number of particles (the chemical potential) is associated with an increase in the number of particles in the localized band $n_f$, while a slight decrease is observed in the other band, as shown in the inset of Fig. 1. This behavior is not sensitive to the temperature, in contrast to the the pair potential and the density of states, as shown in the inset of Fig. 1. Therefore, we conclude that this charge transfer does not originate from the realization of the superfluid state, but is simply a consequence of the attractive interactions, which favor doubly occupied states at each site.

By performing similar calculations, we obtained the phase diagram shown in Fig. 3. At low temperatures, the introduction of holes or particles in the Kondo insulating state immediately induces a phase transition to the superfluid state. Therefore, we find that the Kondo insulating state is realized only around $n_f \sim 0.5$, while the superfluid state is stable in a wide region of parameter space. This phase diagram may be useful in understanding the low temperature properties of optical lattice systems with a confining potential, where the local particle number depends on the location of the sites.

4. Summary
We have investigated the periodic Anderson model with attractive interactions on the hypercubic lattice. By combining DMFT with the CTQMC method based on the Nambu formalism, we have studied quantitatively how the superfluid state is stabilized at low temperatures. It has been found that a low-energy state characteristic of the superfluid phase appears in the hybridization gap when particles are doped into the Kondo insulating state.

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Figure 3. Phase diagram for the system with $U = 1.0$ and $V = 0.4$. Open (solid) circles indicate the state with (without) pair potentials. The phase boundary is a guide to eyes.

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