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Dynamical properties of ultracold fermions with attractive interactions in an optical lattice

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Abstract. We study dynamical properties of ultracold fermions with attractive interactions by means of dynamical mean-field theory and a continuous-time quantum Monte Carlo method. By calculating the pair potential and the density of states, we discuss the stability of the superfluid state. We also show that when holes are doped into the fermionic optical lattice system with intermediate interaction strength, the quasi-particle peak smears and a gap structure instead appears in the dilute system.

Ultracold atomic systems have attracted wide-spread interest in the physics community since the demonstration of Bose-Einstein condensation (BEC) in a Rb atom system [1]. Interesting topics in the field are the nature of the superfluid state in fermionic systems, including the BCS-BEC crossover [2, 3, 4], and the recently observed pseudogap behavior [5, 6]. These experimental observations stimulate theoretical investigations on the superfluid state and related phenomena in ultracold atomic systems.

Two-component Fermi gas systems have been studied theoretically in much detail and it has been clarified that a pseudogap phenomenon indeed appears in the BCS-BEC crossover region above the critical temperature [7, 8, 9, 10]. On the other hand, in fermionic optical lattice systems, such dynamical properties at finite temperatures have not been discussed. In our previous paper, we have studied the attractive Hubbard model to clarify how the superfluid state is stabilized and how the gap structure appears at finite temperatures [11]. It is also instructive to systematically study the doping dependence of dynamical properties. This topic was beyond the scope of our previous paper, but it may be interesting to investigate how the introduction of the lattice potential changes low energy properties of the Fermi gas system.

To clarify this, we consider the infinite-dimensional attractive Hubbard model and discuss how the particle density affects dynamical properties at low temperatures. The model Hamiltonian is given as $\hat{\mathcal{H}} = \sum_{ij,\sigma} (-t_{ij} - \mu \delta_{ij}) c_{i\sigma}^{\dagger} c_{j\sigma} - U \sum_{i} n_{i\uparrow} n_{i\downarrow}$, where $c_{i\sigma} (c_{i\sigma}^{\dagger})$ annihilates (creates) a fermion on the *i*th site with spin $\sigma(=\uparrow,\downarrow)$, and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. U is the onsite attractive interaction, t_{ij} is the transfer integral between sites, and μ is the chemical potential. The low-energy properties have been studied in one dimension [17, 18, 19, 20], two dimensions [21, 22, 23, 24] and higher dimensions [11, 25, 26, 27, 28, 29]. It is known that the superfluid ground state is always realized in two and higher dimensions. Here, we focus on the BCS-BEC crossover region to study how dynamical properties are affected by the particle density and temperature. To this end, we make use of DMFT [12, 13, 14, 15]. In DMFT, the original lattice model is mapped to an effective impurity model, where local particle correlations are taken into account precisely. The lattice Green's function is obtained via a self-consistency condition imposed on the impurity problem. This treatment is formally exact in the limit of infinite spatial dimensions. The self-consistency condition of our model [30] is given by $\hat{G}_0^{-1}(i\omega_n) = i\omega_n\hat{\sigma}_0 + \mu\hat{\sigma}_z - \left(\frac{D}{4}\right)^2\hat{\sigma}_z\hat{G}(i\omega_n)\hat{\sigma}_z$, where $\hat{G}_0(i\omega_n)$ [$\hat{G}(i\omega_n)$] is the non-interacting [interacting] Green's function for the impurity model, $\omega_n = (2n+1)\pi T$ is the Matsubara frequency, and T is the temperature. $\hat{\sigma}_0$ is the identity matrix and $\hat{\sigma}_z$ is the z-component of the Pauli matrix. We have used the semi-circular density of states, $\rho_0(x) = \frac{2}{\pi D}\sqrt{1-\left(\frac{x}{D}\right)^2}$, where D is the half bandwidth. In the DMFT framework, an impurity solver is necessary to obtain the local Green's

In the DMFT framework, an impurity solver is necessary to obtain the local Green's function from the effective impurity model. Here we use the CTQMC technique [16], which has successfully been applied to a wide variety of models such as the Hubbard model [11, 31, 32, 33, 34], the periodic Anderson model [35, 36], the Kondo lattice model [37], and the Holstein-Hubbard model [38, 39]. In this paper, using a CTQMC method in the hybridization expansion formulation [31, 32, 40] extended to the Nambu formalism [11], we directly compute how the superfluid state is realized in the system.

To discuss the stability of the superfluid state, we first calculate the pair potential $\Delta = \langle c_{i\uparrow}c_{i\downarrow} \rangle$ in the system with U = 2D and n = 0.5, 0.25 and 0.125, where $n = \sum_{\sigma} \langle n_{i\sigma} \rangle / 2$, as shown in Fig. 1 (a). At high temperatures, the pair potential is zero and the normal state is realized.



Figure 1. (a) Pair potential as a function of temperature in the system with U = 2D. (b) Phase diagram of the attractive Hubbard model. Solid circles, squares, and triangles represent results for the system at half, quarter, and one-eighth filling. Open circles represent the phase boundary at zero temperature where the first-order pairing transition occurs [29].

As the temperature is decreased, a phase transition occurs to the superfluid state at a critical temperature T_c , where the pair potential is induced. We find that the decrease of the particle density reduces the critical temperature. By examining the critical behavior $\Delta \sim |(T - T_c)/D|^{\beta}$ with the exponent $\beta = 1/2$, we determine the critical temperatures $T_c \sim 0.10D$ (n = 0.5), 0.094D (n = 0.25), and 0.084D (n = 0.125).

By performing similar calculations, we obtain the phase diagram, as shown in Fig. 1 (b). In the small U case, weakly coupled Cooper pairs are formed and the BCS-type superfluid state is realized. In the large U case, the strong attraction tightly couples the fermions, and hence a BEC-type superfluid state is realized. In this case, the superfluid critical temperature is scaled by the effective hopping for paired bosons $\sim t^2/U$. The BCS-BEC crossover, which may be characterized by the maximum of the critical temperature, occurs in the intermediate region $(U \sim 2D)$. Fig. 1 (b) shows that the decrease in the particle density results in only a small shift of the BCS-BEC crossover region, at least for $n \ge 0.125$. Nevertheless, a drastic change appears in the density of states around the BCS-BEC crossover at $T = T_c$. The density of



Figure 2. Density of states of the attractive Hubbard model with U = 2D at $T = T_c$ (a) and T = 0.05 (b) when n = 0.5, 0.33, 0.25, 0.125 and 0.05.

states is calculated by means of the maximum entropy method [41, 42, 43], using the classic algorithm and a Gaussian default model. We find in Fig. 2 (a) a quasi-particle peak near the Fermi level for n > 0.25, while a gap structure appears in the case n < 0.125. This may originate from the pairing transition, which is realized only in the normal state. It has already been clarified that when the system is restricted to be paramagnetic, the pair transition as a function of the attractive interaction takes place between the heavy metallic Fermi liquid state and the insulating bound pairs state [29]. Note that this transition occurs in systems with arbitrary fillings, in contrast to the Mott transition in the repulsive Hubbard model. The zerotemperature phase boundary is shown by the open circles in Fig. 1 (b). It is found that the phase boundary crosses the U = 2D line around $n \sim 0.125$. At the finite temperature we consider here $(T = T_c)$, the crossover behavior between the metallic and insulating states appears at a slightly smaller interaction, compared to the transition point at T = 0. Therefore, in the system with U = 2D, the decrease of the particle density induces a change from heavy metallic behavior to insulating behavior. Once the system is in the superfluid state (T = 0.05D), the pairing transition does not affect the low energy properties. Instead, the superfluid gap opens in the vicinity of the Fermi level, as shown in Fig. 2 (b).

We comment on the difference of low energy properties between the dilute lattice system and the Fermi gas system. It has already been clarified that in the Fermi gas system, a pseudogap behavior appears around the BCS-BEC crossover region [7, 8, 9, 10]. In the lattice model, either a metallic behavior or a gap behavior appears, depending on the interaction strength and the particle density. Therefore, a competition between these incompatible behaviors should appear in dynamical properties when the lattice potential is gradually introduced in the Fermi gas system.

We have investigated the attractive Hubbard model in infinite spatial dimensions. By combining dynamical mean-field theory with the strong-coupling version of the continuous-time quantum Monte Carlo method, we have directly dealt with the superfluid phase in the system. By calculating the pair potential and the density of states of the system at different band fillings, we have clarified that a gap behavior indeed appears in the density of states when the system is far away from half filling.

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