Temperature and doping dependence of the singlet and triplet pair susceptibilities in the one-band Hubbard model based on the dynamical mean-field theory

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Abstract. The superconductivity in the one-band Hubbard model on a Bethe lattice is investigated on the basis of the dynamical mean-field theory (DMFT) in which the irreducible vertex function has no \(k\)-dependence and then only the s-wave superconductivities with the spin-singlet even-frequency and the spin-triplet odd-frequency pairings are possibly realized. We calculate the pair susceptibility by solving the Bethe-Salpeter equation with the use of the linearized DMFT and find that the spin-singlet pair susceptibility is suppressed by the on-site Coulomb interaction \(U\) especially for the region near the Mott transition. On the other hand, the spin-triplet pair susceptibility is apparently enhanced by \(U\) in the strong correlation regime at very low temperatures where the effective interaction for the triplet pairing is considered to be attractive and then the triplet superconductivity is expected to be realized.

1. Introduction
The Hubbard model has a long history of research as the fundamental model for describing electron correlation effects in magnetism and Mott metal-insulator transition. Especially after the discovery of high-\(T_c\) cuprate superconductors, it is actively used for the studies as a fundamental model which describes superconductivity by electron correlation effects. The Dynamical mean-field theory (DMFT) [1], which can take into account local electron correlation effects non-perturbatively, has been developed for many studies in the Hubbard model including superconductivity, because it becomes exact in infinite spacial dimensions and is expected to be a good approximation in three dimensions. In the previous DMFT studies, both the singlet and triplet superconductivities have not been observed in the one-band Hubbard model [2,3] in contrast to the case with the two-band Hubbard model where the singlet and/or triplet superconductivities are found to be realized [3,4,5]. However, the detailed results of the pair susceptibilities for superconductivity over the whole parameter regime including quite low temperatures where the superconductivity is expected to be realized were not been explicitly shown there [2,3].

In the present paper, we calculate the singlet and triplet pair susceptibilities in the one-band Hubbard model for a wide range of parameters: the electron number per site \(n\), the temperature \(T\) and the on-site Coulomb interaction \(U\). The singlet (triplet) pair susceptibility is constructed by ladder diagrams of the particle-particle channel with respect to the singlet (triplet) irreducible vertex function \(\Gamma_s (\Gamma_t)\) which corresponds to an effective interaction leading singlet (triplet) pairing and is obtained by solving the Bethe-Salpeter equation with the use of the linearized DMFT [6] developed for describing the electronic state close to the Mott transition.
2. Model and formulation

We consider the one-band Hubbard model on a Bethe lattice with infinite connectivity $Z = \infty$. The Hamiltonian is given by

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + U \sum_i n_i^\dagger n_i,$$

where $c_{i\sigma}$ is the annihilation operator of an electron with spin $\sigma (= \uparrow, \downarrow)$ at site $i$ and $n_i = c_{i\uparrow}^\dagger c_{i\uparrow}$, $n_i = c_{i\downarrow}^\dagger c_{i\downarrow}$, $U$ is the on-site Coulomb interaction and $t_{ij} = t/\sqrt{Z}$ is the transfer integral between the nearest-neighbor sites and we set $t = 1$ eV resulting in the bare band width of 4 eV. To solve the model eq. (1), we use the DMFT in which the lattice model is mapped onto an impurity Anderson model embedded in an effective medium which is determined so as to satisfy the self-consistency condition for the single-particle Green’s functions [1].

The s-wave pair susceptibilities with the spin-singlet even-frequency and the spin-triplet odd-frequency pairings $\chi_s$ and $\chi_t$ are respectively given by

$$\chi_s = \sum_{m,l} \chi_s(y_m, y_l)$$

and

$$\chi_t = \sum_{m,l} \chi_t(y_m, y_l)$$

with the frequency-dependent pair susceptibilities defined by

$$\chi_{\alpha\beta}(i\nu_m, i\nu_l) = \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 e^{-i\nu_1\tau_1} e^{i\nu_2\tau_2} e^{-i\nu_3\tau_3}$$

$$\times \sum_{kk'} \left[ \langle T_{\tau_1} [c_{k\uparrow}(\tau_1)c_{-k\downarrow}(\tau_3)c_{k\downarrow}(\tau_3)] \rangle - \langle T_{\tau_2} [c_{k\uparrow}(\tau_2)c_{-k\downarrow}(\tau_3)c_{k\downarrow}(\tau_3)] \rangle \right]$$

where $\nu_m = (2m + 1)\pi/\beta$ is an odd Matsubara frequency with the inverse temperature $\beta = 1/k_B T$. As shown in Figure 1, the singlet (triplet) pair susceptibility $\chi_s(\chi_t)$ is constructed by ladder diagrams of the particle-particle channel with respect to the singlet (triplet) irreducible vertex function $\Gamma_s(\Gamma_t)$ which corresponds to an effective interaction leading singlet (triplet) pairing and is obtained by solving the Bethe-Salpeter equation. Within the DMFT, $\Gamma_s(\Gamma_t)$ has no $k$-dependence and can be obtained by solving the Bethe-Salpeter equation in the effective impurity Anderson model. For numerical simplicity, we calculate $\Gamma_s(\Gamma_t)$ by employing the linearized DMFT developed for describing the electronic state close to the Mott transition [6].

Figure 1. Diagrammatic representation for the pair susceptibility $\chi$ constructed by ladder diagrams with respect to irreducible vertex function $\Gamma$, where solid lines represent the single-particle Green’s functions.
3. Results

Figure 2 (a) shows the $T$ dependence of the spin-singlet pair susceptibility $\chi_s$ which is negative and then the absolute value $|\chi_s|$ is plotted there. We see that $\chi_s$ is suppressed by the repulsion $U$ especially at half-filling $n = 1$, where $n$ is the number of electrons per site. We plot the $U$ dependence of $\chi_s$ at $T = 10K$ in Fig. 2 (b) and find that $\chi_s$ is suppressed by $U$ especially for the region near $U = 6eV$ where the Mott transition takes place at $n = 1$ within the linearized DMFT [6]. From these results, it is considered that the $s$-wave superconductivity with the spin-singlet even-frequency pairing is not realized for $U > 0$ as consistent with the previous DMFT studies [2,3].

The $T$ dependence of the spin-triplet pair susceptibility $\chi_t$ is shown in Fig. 3 (a). We see that the divergent property of $\chi_t$ down to $T = 1K$ for $U = 5.3eV$ is enhanced as compared to that for $U = 0$.

![Figure 2](image1.png)

**Figure 2.** Absolute values of the spin-singlet pair susceptibilities $|\chi_s|$ as functions of $T$ for several values of $n$ and $U$ (a), and those as functions of $U$ for several values of $n$ at $T = 10K$.

![Figure 3](image2.png)

**Figure 3.** The spin-triplet pair susceptibilities $\chi_t$ as functions of $T$ for several values of $n$ and $U$ (a), and those as functions of $U$ for several values of $n$ at $T = 1K$. 


where $\chi_t$ diverges with $T \to 0$. We plot the $U$ dependence of $\chi_t$ at $T = 1K$ in Fig. 3 (b) and find that $\chi_t$ is enhanced by $U$ especially for the region just below the Mott transition $U_c = 6eV$ in contrast to the case with $\chi_s$ which is suppressed by $U$ as shown in Fig. 2 (b). These results suggest that, in the region just below the Mott transition, $\chi_t$ diverges at a finite temperature $T_c(< 1K)$ below which the $s$-wave superconductivity with the spin-triplet odd-frequency pairing is expected to be realized. To be more conclusive, we need further calculations of $\chi_t$ at very low temperatures by using the full DMFT.

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