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Two-Particle Excitations of the Kondo Insulator around the Critical Point

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The spin and the charge excitations of the Kondo insulator are investigated based on the periodic Anderson model at half-filling. We employ the self-consistent fluctuation approximation, where the two-particle correlation functions and the effective irreducible vertices are determined self-consistently to satisfy the Pauli principle. When the system approaches the antiferromagnetic critical point with the strong electron correlation, the spin excitation spectrum is enhanced while the charge excitation spectrum is suppressed. The characteristic energy of the spin excitation is more strongly renormalized than that of the charge one.

KEYWORDS: Kondo insulator, two-particle excitations, self-consistent fluctuation approximation

1. Introduction

The periodic Anderson model (PAM) at half-filling is known to exhibit an insulating behavior at low temperatures as an ordinary non-interacting band insulator. Since the gap opens at the Fermi level in the model as decreasing temperature, it is often considered as a fundamental theoretical model of the Kondo insulator [1, 2], i.e., a renormalized band insulator in heavy fermions. Since the hybridization gap of the PAM is adiabatically connected to that of the non-interacting limit, at first glance, there were no distinctions of the indirect gap magnitudes in the charge and spin channels as an ordinary insulator, in which particle-hole pairs across the gap contribute similarly to both excitations. However, the strong correlation must change the character of the charge and the spin excitations, individually, and the difference could be most prominent near the quantum critical point of the magnetically ordered phase. In the present study, we investigate two-particle excitation spectra of the PAM at half-filling to elucidate the character of the charge and the spin excitations of the Kondo insulator around the magnetic quantum critical point. Moreover, it is considered that the self-consistent renormalization (SCR) theory [3–6] and its equivalents [7,8] well describe the system around the quantum critical point. However, in the presence of the excitation gap in the renormalized quasiparticle bands, it is a nontrivial issue since there exists no infinitesimally small excitation continuum. Motivated by these questions, we adopt the self-consistent fluctuation (SCF) approximation, and address how the charge and spin spectra behave with taking account of various fluctuations.

2. Model and Method

We consider the PAM on the square lattice,

$$\mathcal{H} = \sum_{k\sigma} \left\{ (\varepsilon_{\boldsymbol{k}} - \mu) c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + (\varepsilon^{f} - \mu) f^{\dagger}_{\boldsymbol{k}\sigma} f_{\boldsymbol{k}\sigma} + V (c^{\dagger}_{\boldsymbol{k}\sigma} f_{\boldsymbol{k}\sigma} + f^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}) \right\} + U \sum_{i} f^{\dagger}_{i\uparrow} f_{i\uparrow} f^{\dagger}_{i\downarrow} f_{i\downarrow},$$

$$\varepsilon_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y), \qquad (1)$$

where the nearest-neighbor hopping on the square lattice is assumed and a lattice constant is set to be unity. Hereafter, the hopping energy t of the conduction electron is used as an energy unit. Under the particle-hole symmetric condition $\varepsilon^f + U/2 = \mu = 0$ among the f level ε^f, the on-site Coulomb energy U and the chemical potential μ, the system is always insulating at ground state for arbitrary strength of U.

To investigate charge and spin excitations of the system, we adopt the SCF approximation [9]. The SCF approximation treats various two-particle fluctuations self-consistently on an equal footing by enforcing the crossing symmetry, i.e., a fully anti-symmetric nature of the full vertex functions. In this scheme, the local and instantaneous renormalized couplings for the irreducible vertices in the charge and the spin channels are introduced and they are denoted by Λ_c and Λ_s, respectively. According to Ref. 9, the charge (c) and the spin (s) correlation functions are expressed as

$$\chi_c(q) = \frac{\chi_0(q)}{1 + \Lambda_c\chi_0(q)}, \qquad \chi_s(q) = \frac{\chi_0(q)}{1 - \Lambda_s\chi_0(q)}, \tag{2}$$

where q indicates a set of valuables for a wave vector $\boldsymbol{q}$ and the bosonic Matsubara frequency $\mathrm{i}\omega_m$; $q = (\boldsymbol{q}, \mathrm{i}\omega_m)$. Note that the renormalized coupling and the corresponding correlation function in the even-parity Cooper channel are the same as Λ_c and χ_c at half-filling. Following Ref. 9, the SCF equations are now expressed under the particle-hole symmetry as

$$\begin{aligned} &\Lambda_c = U - \frac{1}{2\chi_{02}}(f_c - 3f_s), \qquad \Lambda_s = U - \frac{1}{2\chi_{02}}(3f_c - f_s), \\ &f_{c(s)} = -\sum_q (\chi_0(q))^2\,\Phi_{c(s)}(q), \qquad \chi_{02} = \sum_q (\chi_0(q))^2, \qquad \Phi_{c(s)}(q) = -\Lambda_{c(s)}^2\chi_{c(s)}(q), \end{aligned} \tag{3}$$

where $\sum_q \equiv (T/N)\sum_{\boldsymbol{q}}\sum_m$ with the number N of the lattice points at temperature T. The proper part $\chi_0(q)$ of the two-particle correlation function is given by the non-interacting (or equivalently Hartree) f-electron Green's function $G_0^{ff}(k)$, and they are expressed for the present model under the particle-hole symmetry as

$$\begin{aligned} \chi_0(q) &= -\sum_k G_0^{ff}(k)G_0^{ff}(k+q), \\ G_0^{ff}(k) &= \cfrac{1}{\mathrm{i}\varepsilon_n - \cfrac{V^2}{\mathrm{i}\varepsilon_n - \varepsilon_{\boldsymbol{k}}}}, \end{aligned} \tag{4}$$

where $k = (\boldsymbol{k}, \mathrm{i}\varepsilon_n)$ with the fermionic Matsubara frequency, ε_n. Solving the above equations self-consistently, we obtain the effective irreducible vertices Λ_c and Λ_s, and the corresponding charge and spin correlation functions.

3. Results

In the present study, we have solved the self-consistent equations given in Sec. 2 in the first Brillouin zone with equally spaced mesh of 64 × 64 and on 2048 Matsubara-frequency points. We have adopted the Padé approximation to obtain the real-frequency spectrum. In the results shown below, the hybridization strength V is fixed as $V/t = 0.5$.

First, we show the U dependence of the effective irreducible vertices at $T/t = 0.1$ in Fig. 1. With increasing U, Λ_s is strongly suppressed as compared with Λ_c, The values of $\Lambda_s\chi_0(\boldsymbol{Q}, 0 + \mathrm{i}\eta)$ approaches 1 and the antiferromagnetic spin fluctuation is enhanced for larger values of U. When the value of $\Lambda_s\chi_0(\boldsymbol{Q}, 0 + \mathrm{i}\eta)$ reaches 1 for an antiferromagnetic vector $\boldsymbol{Q} = (\pi, \pi)$, the system shows the antiferromagnetic order. Although the magnetic order should not occur in the two-dimensional system at finite temperature according to the Mermin-Wagner theorem [10], it is shown that $\Lambda_s\chi_0(\boldsymbol{Q}, 0 + i\eta)$ approaches 1 as temperature decreases and the system approaches the antiferromagnetic critical point as shown in Fig. 2.

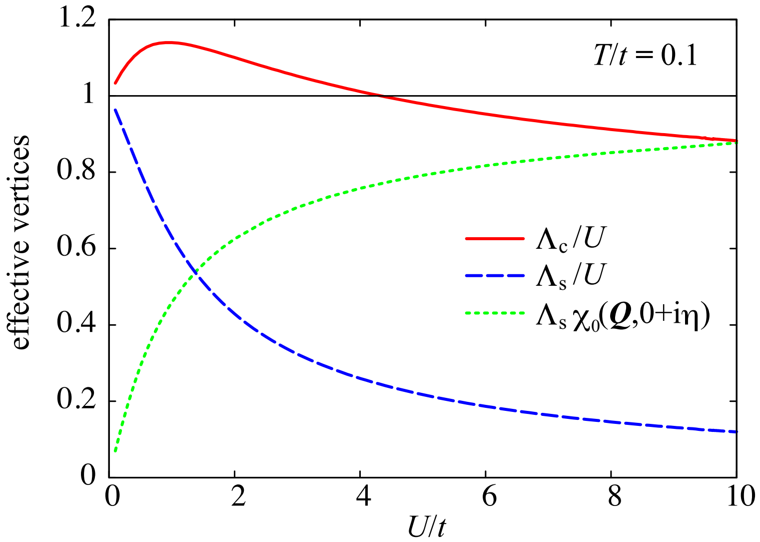

Fig. 1. (Color online) U dependence of the effective irreducible vertices Λ_c and Λ_s at $T/t = 0.1$. The parameter $\Lambda_s\chi_0(\boldsymbol{Q}, 0 + i\eta)$ indicates a measure toward the antiferromagnetic instability (see text).

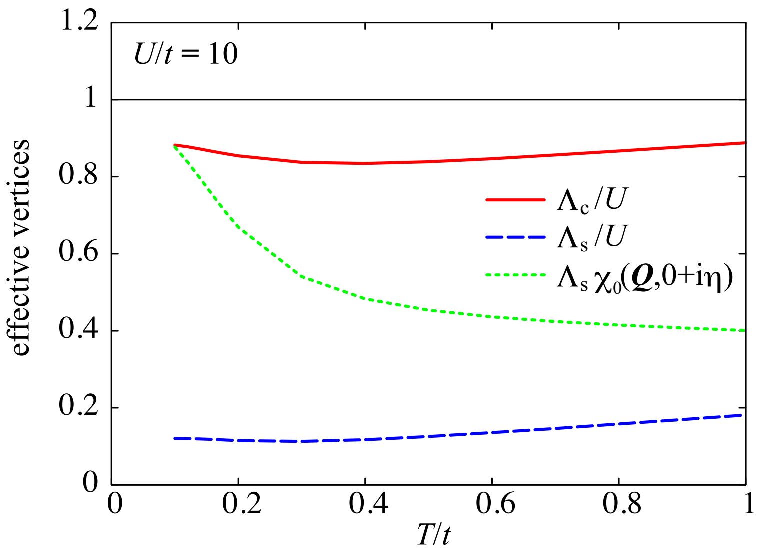

Fig. 2. (Color online) Temperature dependence of the effective irreducible vertices Λ_c and Λ_s for $U/t = 10$.

Figure 3 shows a contour map of the imaginary part of the dynamical spin susceptibility, Im $\chi_s(\boldsymbol{q}, \omega + i\eta)$, along the high-symmetry line. Owing to the existence of the hybridization gap at the Fermi level, $\Delta^*/t \simeq 0.2$, the intensity of the spectrum is cut below $\omega/t \lesssim 0.2$ (this disappearance of the intensity may be an artifact of the frequency independent vertices used in the present approximation). The lowest-energy excitation is located at the M point ($\boldsymbol{q} = \boldsymbol{Q}$), and the dominant weight of the intensity is distributed around the renormalized energy, $\omega/t \simeq 0.3$. On the other hand, in the charge excitation, the most of the spectral weight is distributed around $\omega/t \simeq 3$ as shown in Fig. 4.

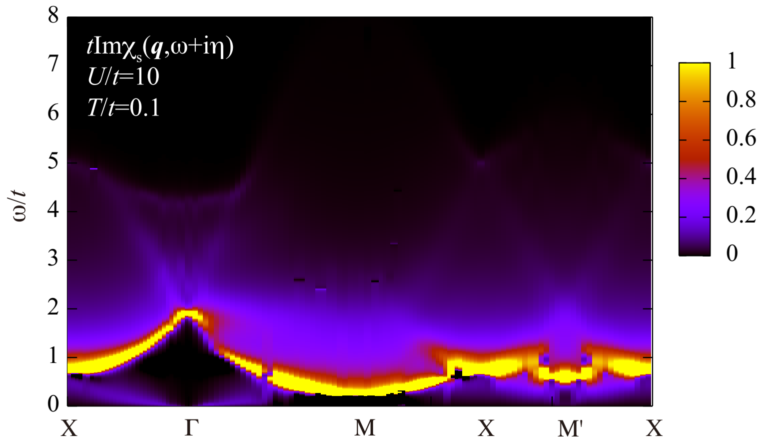

Fig. 3. (Color online) Contour map of the imaginary part of the dynamical spin susceptibility, $t\,\mathrm{Im}\chi_{\mathrm{s}}(\boldsymbol{q}, \omega + \mathrm{i}\eta)$, for $U/t = 10$ at $T/t = 0.1$ along the high-symmetry line. X : $\boldsymbol{q}_{\mathrm{X}} = (\pi, 0)$, Γ : $\boldsymbol{q}_{\Gamma} = (0, 0)$, M : $\boldsymbol{q}_{\mathrm{M}} = (\pi, \pi)$, and M′ : $\boldsymbol{q}_{\mathrm{M}'} = (\pi/2, \pi/2)$.

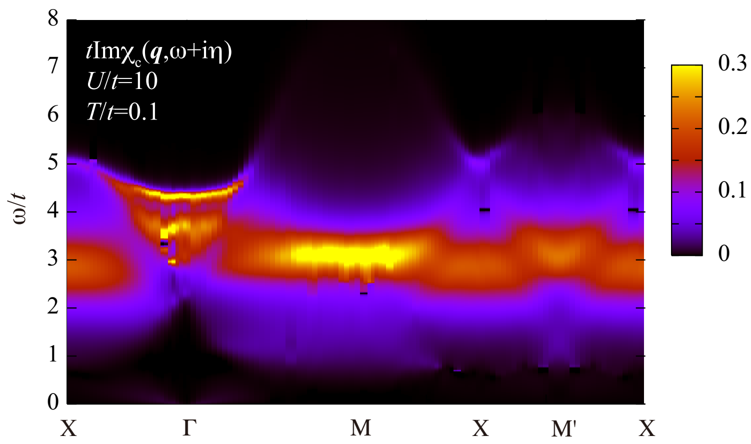

Fig. 4. (Color online) Contour map of the imaginary part of the dynamical charge susceptibility, $t\,\mathrm{Im}\chi_{\mathrm{c}}(\boldsymbol{q}, \omega + \mathrm{i}\eta)$, for $U/t = 10$ at $T/t = 0.1$ along the high-symmetry line.

We compare the spin and charge excitation spectra in Fig. 5. The spin excitation spectrum is strongly enhanced because of the electron correlation and the sharp peak develops at lower energy near the excitation gap [11]. On the other hand, the charge excitation spectrum is suppressed and the peak slightly moves toward higher energy. In the spectra at high temperature ($T/t = 0.5$), the gap structure vanishes due to the disappearance of the hybridization gap.

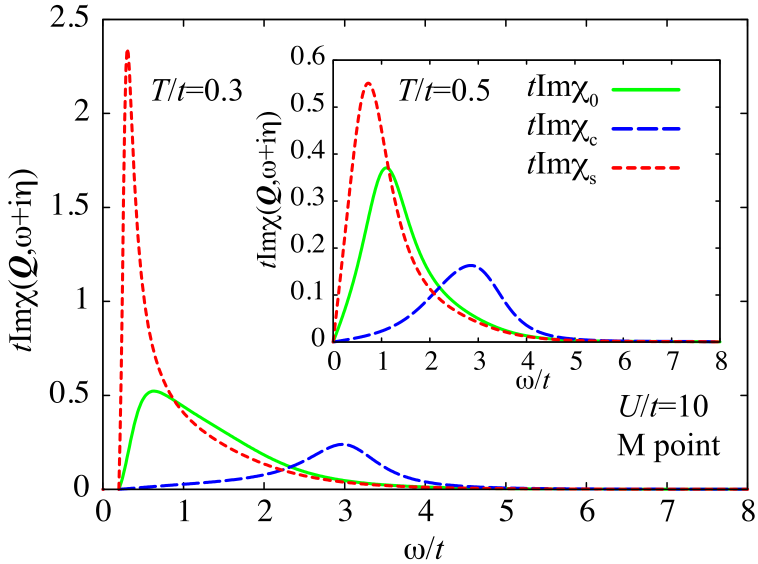

Fig. 5. (Color online) Imaginary parts of the spin and charge correlation functions at $\boldsymbol{Q}$ for $U/t = 10$ at $T/t = 0.3$. The inset shows those at higher temperature, $T/t = 0.5$.

4. Summary and Discussions

In the present study, we have investigated the charge and spin excitations of the Kondo insulator by taking account of the strong antiferromagnetic fluctuation. We have adopted the self-consistent fluctuation approximation for the periodic Anderson model at half-filling on the square lattice. As U increases, the effective irreducible vertex in the spin channel is strongly renormalized, while that in the charge channel is hardly suppressed. For large U, the antiferromagnetic fluctuation is enhanced with decreasing temperature. In this situation, the spin excitation spectrum at lower energy is strongly enhanced. The charge excitation spectrum is suppressed and the peak of the spectrum slightly moves toward higher energy. The spin excitation energy scale is smaller than the charge one at finite temperature. Let us consider more about the spin gap at zero temperature. In the present scheme, the spin excitation spectrum is expressed as

$$\mathrm{Im}\chi_{\mathrm{s}}(\boldsymbol{q},\omega+\mathrm{i}\eta) = \frac{\mathrm{Im}\chi_0(\boldsymbol{q},\omega+\mathrm{i}\eta)}{(1-\Lambda_{\mathrm{s}}\mathrm{Re}\chi_0(\boldsymbol{q},\omega+\mathrm{i}\eta))^2 + (\Lambda_{\mathrm{s}}\mathrm{Im}\chi_0(\boldsymbol{q},\omega+\mathrm{i}\eta))^2}. \tag{5}$$

The energy dispersion of the spin excitation (paramagnon) is determined by the condition, $\Lambda_{\mathrm{s}}\,\mathrm{Re}\,\chi_0(\boldsymbol{q},\omega+\mathrm{i}\eta) = 1$, and its minimum corresponding to the spin gap should approach to zero when the system approaches to the magnetic instability. However, the intensity of the spin excitation is cut below the energy gap determined by the proper (bare) part $\mathrm{Im}\chi_0(\boldsymbol{q},\omega+\mathrm{i}\eta)$ due to the factor in the numerator. The true spin gap should be determined by the gap in the paramagnon dispersion as mentioned above, which has been obscured by the bare gap of χ_0. This is the reason why the excitation gap is almost unchanged with increasing U in Fig. 5. In reality, the numerator should depend on U and the true spin gap would show up. This could be achieved by more sophisticated approximations.

Nevertheless, the effective irreducible vertices Λ_{s} and Λ_{c} themselves reflect the characteristic energy scales corresponding to the spin and charge gaps, respectively. In fact, the U dependence of the spin and charge gaps for the 1D PAM by the numerical diagonalization method [12] are very similar to those obtained by the present scheme. Thus, an improvement of the proper correlation function would yield a better behavior of the magnetic excitation spectra.

References

[1] G. Aeppli and Z. Fisk : Comments Condens. Matter Phys. **16** (1992) 155.
[2] P. Riseborough : Adv. Phys. **49** (2000) 257.
[3] T. Moriya and A. Kawabata : J. Phys. Soc. Jpn. **34** (1973) 639; T. Moriya and A. Kawabata : J. Phys. Soc. Jpn. **35** (1973) 669.
[4] T. Moriya : *Spin Fluctuations in Itinerant Electron Magnetism* (Springer, Heidelberg,1985).
[5] A. Kawabata : J. Phys. F **4** (1974) 1477.
[6] T. Moriya and T. Takimoto : J. Phys. Soc. Jpn. **64** (1995) 960.
[7] J. A. Hertz : Phys. Rev. B **14** (1976) 1165.
[8] A. J. Millis : Phys. Rev. B **48** (1993) 7183.
[9] H. Kusunose : J. Phys. Soc. Jpn. **79** (2010) 094707; H. Kusunose: J. Phys. Soc. Jpn. **80** (2011) SA137.
[10] N. D. Mermin and H. Wagner : Phys. Rev. Lett. **17** (1966) 1133.
[11] Spectra $t\,\mathrm{Im}\,\chi_0$ and $t\,\mathrm{Im}\,\chi_\mathrm{s}$ at $T/t = 0.3$ have small negative values below $\omega/t \lesssim 0.2$, which are the artifact of the Padé approximation, and they have been omitted in drawing of Fig. 5.
[12] T. Nishino and K. Ueda : Phys. Rev. B **47** (1993) 12451.