Hybrid theory of the dynamical mean field and the spin-fluctuations in strongly correlated electron systems

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Abstract

In order to take account of the spatial fluctuation beyond the dynamical mean field theory (DMFT), the two-particle self-consistent theory is carefully reinvestigated and is proved to be unable to reproduce the correct low energy scale in the strong correlation limit. An improved theory is proposed which starts from DMFT and is combined with the spin-fluctuation theory (SFT) in a phenomenological form. The present theory therefore encompasses DMFT and SFT, and describes the quantum critical behavior properly with the same exponent as SFT. The local quantum dynamics is fully taken into account as in DMFT in contrast to the phenomenological treatment in SFT.

Key words: dynamical mean field theory, two-particle self-consistent theory, spin-fluctuation theory, strongly correlated electron systems

The most powerful method for the description of the strongly correlated electron systems (SCES) may be the dynamical mean-field theory (DMFT).[1] It, however, lacks the effect of intersite spin fluctuations, which becomes important, e.g. in the vicinity of the quantum phase transitions.[2] Several methods were proposed to overcome this deficiency of DMFT by taking account of the cluster instead of the effective impurity in DMFT,[3,4] but none of them has succeeded in the description of the quantum critical phenomena (QCP) because of the use of the finite size of the cluster. The extended DMFT is proposed by Si and Smith[5] for the fermion-boson model, which can describe the properties at QCP. The other successful approachs to QCP are the spin fluctuation theories (SFT's).[6,2] The SFT by Moriya was further developped

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in a form which is more phenomenological but flexible in use.[9] The two-particle self-consistent theory (TPSC)[7] has been proposed to improve SFT. We, however, recently proved that TPSC cannot reproduce the correct low energy scale in the strong correlation limit of the single impurity Anderson model (SIAM), and therefore cannot be a good candidate for an improved theory.[8] The proof proceeds as follows. For the symmetric case of SIAM, the TPSC equation for the spin sector

$$T\sum_{\omega}\frac{2\Pi_0(\mathrm{i}\omega)}{1-U_s\Pi_0(\mathrm{i}\omega)}=n-2\langle n_\uparrow n_\downarrow\rangle, \tag{1}$$

reads as

$$1-\frac{U_s}{2U}\simeq\frac{2}{\pi^2}\log\frac{\omega_c}{\Delta-U_s/\pi}, \tag{2}$$

where ω_c denotes a cutoff frequency of the order $O(\Delta)$ (resonance width), and we have used the low energy form for the poralization function $\Pi_0(\omega)$. The above equation determines the effective interaction U_s in the spin channel and the static susceptibility $\chi_s = 1/2(\pi\Delta - U_s) = 1/4T_K$. However, the above equation (2) yields the Kondo temperature $T_{\mathrm{K}} \to (\pi/2)\omega_c \exp(-\pi^2/2)$ for $U \to \infty$ which is finite and does not vanish.

We then propose a theory which avoids the above defect and combines both DMFT and SFT. This is done first by introducing the effective vertex $\Gamma(\omega) = U/[1 + U\Pi_0(\omega)]$ and expressing the local dynamical susceptibility approximately as ($g\mu_B = 1$)

$$\chi_L(\omega)=\frac{\frac{1}{2}\Pi_0(\omega)}{1-\Gamma(\omega)\Pi_0(\omega)}, \tag{3}$$

where $\Pi_0(\mathrm{i}\omega) = -T\sum_\epsilon G(\mathrm{i}\epsilon)G(\mathrm{i}\epsilon + \mathrm{i}\omega)$ and the Green's function $G(\mathrm{i}\epsilon)$ is the solution of DMFT. $\chi_L(0)$ diverges when and only when $U \to \infty$ at $T = 0$, which is the desired property for impurity. Actually, we modify this as

$$\tilde{\chi}_L(\omega)=\frac{1}{\chi_L(\omega)^{-1}-\mathrm{i}C\omega}, \tag{4}$$

and determine the parameter C by the sum rule, eq.(1), to correct the low energy scale as a fine tuning.

Next task is to construct the wave-vector-dependent dynamical susceptibility $\chi(q, \omega)$ by taking account of the $1/d$ corrections. In $d \to \infty$ limit, $\chi(q, \omega)$ can

be calculated from the knowledge of the effective impurity[1] as

$$\chi(q, \mathrm{i}\omega) = \sum_{\epsilon\epsilon'} \left[\frac{\chi_q^0(\mathrm{i}\omega)}{1 - \Gamma(\mathrm{i}\omega)\chi_q^0(\mathrm{i}\omega)} \right]_{\epsilon\epsilon'}, \tag{5}$$

where

$$\chi_q^0(\mathrm{i}\omega)_{\epsilon\epsilon'} = -\sum_k G(k, \mathrm{i}\epsilon) G(k+q, \mathrm{i}\epsilon' + \mathrm{i}\omega)\delta_{\epsilon\epsilon'}, \tag{6}$$

and $\Gamma(\mathrm{i}\omega)_{\epsilon\epsilon'} = \Gamma(\mathrm{i}\epsilon, \mathrm{i}\epsilon', \mathrm{i}\omega) = [\chi_L^0(\mathrm{i}\omega)^{-1} - \chi_L(\mathrm{i}\omega)^{-1}]_{\epsilon\epsilon'}$ is the vertex function which is local and the matrix of the Matsubara frequencies ϵ, ϵ' and $\chi_L(\mathrm{i}\omega) = \sum_{\epsilon\epsilon'} \chi_L(\mathrm{i}\omega)_{\epsilon\epsilon'}$. $G(k, \mathrm{i}\epsilon)$ is the Green's function in $d \to \infty$.

For $d < \infty$, the calculation of $\chi(q, \omega)$ is not easy, but it has a general form as

$$\chi(q, \omega) = [\chi_{\mathrm{L}}(\omega)^{-1} - J(q, \omega)]^{-1}. \tag{7}$$

Therefore, we rather adopt Moriya's approach[9] and use the approximate long-wavelength expansion form around the ordering vector Q:

$$\chi(Q + q, \omega) = [\tilde{\chi}_{\mathrm{L}}(\omega)^{-1} - J_Q(T) + Aq^2]^{-1}, \tag{8}$$

and determin $J_Q(T)$ by the sum rule similar to [1] but including the wave-vector sum. If $J_Q(T = 0)$ is chosen so that $\chi(Q, \omega = 0, T = 0)^{-1} = \tilde{\chi}_L(\omega = 0, T = 0)^{-1} - J_Q(T = 0) = 0$ (QCP), the specific heat, staggered susceptibility and resistivity show $T^{3/2}$ behaviors at low temperatures[10] in accord with the SFT.[9] An example for the Hubbard model[10] is shown in Fig. 1.

The present theory thus encompasses DMFT[1] and SFT[9], and describes the quantum critical behavior properly with the same exponent as SFT.[8] The local quantum dynamics is fully taken into account as in DMFT in contrast to the phenomenological treatment in SFT. It could acquire a microscopic basis if one would be able to calculate $J(q, \omega)$ microscopically up to $O(1/d)$. Furthermore, a formula for calculating the self-energy from $\chi(q, \omega)$ is not yet established in the case of strong correlation except for the fermion-boson model.[12] For $d \to \infty$, the self-energy can be calculated with a rather good accuracy by using the iterative perturbation theory[11]. An extension of it to the case with orbital degeneracy would be a future issue[13].

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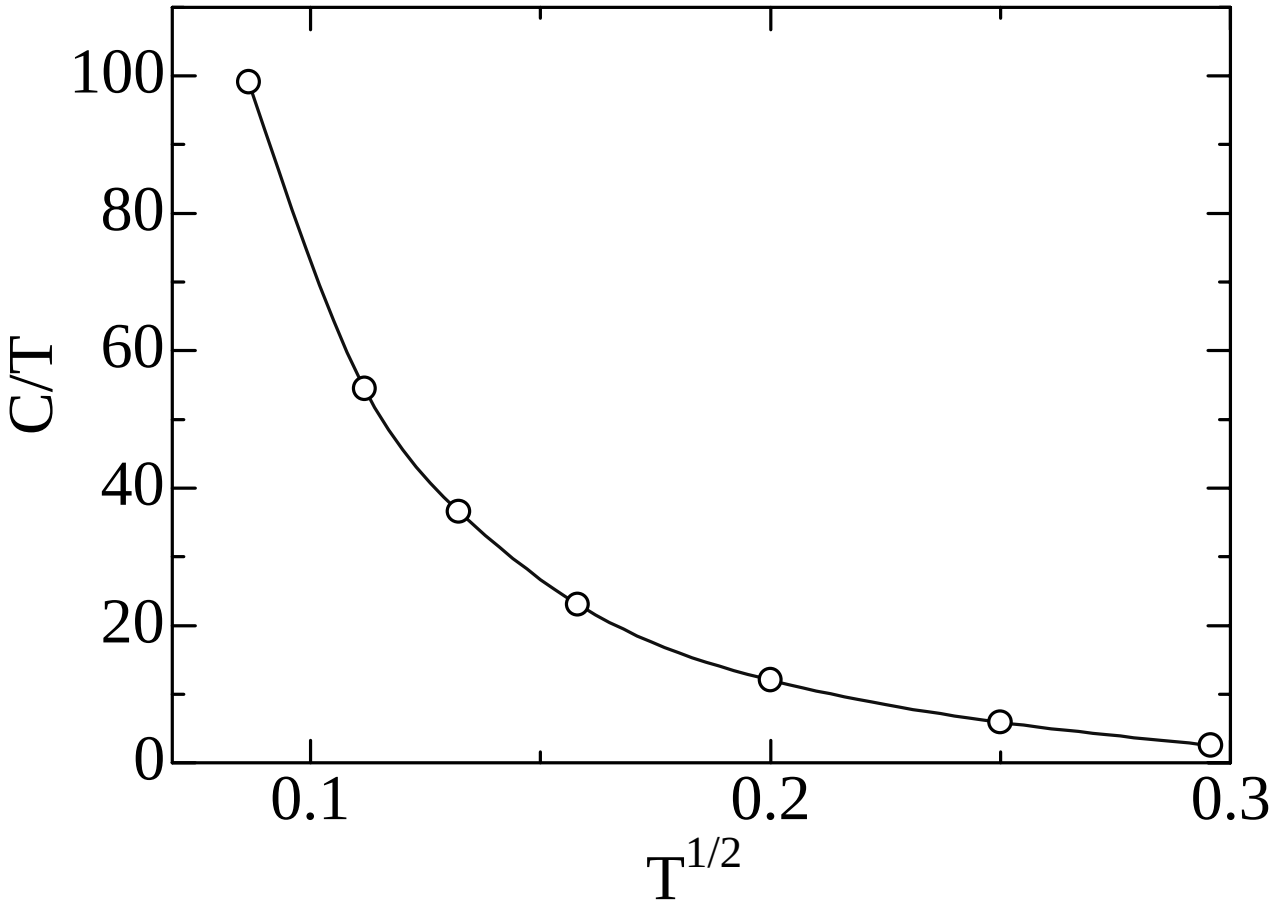

Fig. 1. Temperature dependence of $C(T)/T$ of the Hubbard model at QCP is plotted.