Nonlocal Effect of Local Nonmagnetic Impurity in High-$T_c$ Superconductors: Induced Local Moment and Huge Residual Resistivity

Hiroshi Kontani a,∗, Masanori Ohno a

aDepartment of Physics, Nagoya University, Furo-cho, Nagoya 464-8602, Japan.

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Abstract

We study a Hubbard model with a strong onsite impurity potential based on an improved fluctuation-exchange (FLEX) approximation, which we call the GV$^I$-FLEX method. We find that (i) both local and staggered susceptibilities are strongly enhanced around the impurity. By this reason, (ii) the quasiparticle lifetime as well as the local density of states (DOS) are strongly suppressed in a wide area around the impurity (like a Swiss cheese hole), which causes the “huge residual resistivity” beyond the radius of the AF correlation length. These results by the GV$^I$ method naturally explains the various impurity effects in HTSC’s in a unified way, which had been a long-standing theoretical problem.

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In under-doped high-$T_c$ superconductors (HTSC’s), nonmagnetic impurities (such as Zn) causes nontrivial widespread change of the electronic states. For example, both the local and the staggered spin susceptibilities are strongly enhanced around the impurity, within the radius of the AF correlation length $\xiAF$. This behavior was experimentally observed in the site-selective $^{89}$Y NMR measurements for Zn-doped YBCO [1]. Moreover, a small concentration of Zn causes a huge residual resistivity, much beyond the $s$-wave unitary scattering limit [2]. These nontrivial impurity effects had been frequently considered as the evidence of the breakdown of the Fermi liquid state in under-doped HTSC’s.

Pure HTSC’s samples also show various intrinsic non-Fermi liquid (NFL) behaviors free from impurity effects. Many of them had been explained based on the spin fluctuation theories like the SCR theory and the fluctuation-exchange (FLEX) approximation [3]. For example, Curie like behavior of the Hall coefficient $R_H$ is naturally understood if one take the current vertex correction (CVC) due to AF fluctuations into account [4]. Anomalous transport phenomena in the pseudo-gap region, such as a drastic increment of the Nernst coefficient, are also reproduced by taking account of CVC on the basis of the FLEX+T-matrix approximation [5].

In the present paper, we study a single impurity problem in a $(N \times N)$ square lattice Hubbard model (with $N = 64$). In general, it is not easy to obtain an appropriate solution for this model because two different kinds of strong interactions have to be taken into account on the same footing. To overcome this difficulty, we develop the GV$^I$-method, which is a powerful method of calculating the electronic states in real space. Based on the GV$^I$-method, we succeed in explaining nontrivial impurity effects in HTSC’s in a unified way within the scheme of the spin fluctuation theory, without assuming any exotic mechanisms.

In the present model, the self-energy $\Sigma(r-r',\epsilon)$ is not a function of $r-r'$ because of the absence of translational invariance. Therefore, the self-energy in the site representation is expressed in a matrix form $N^2 \times N^2$, $\Sigma(\epsilon)$. In the present model, the self-energy is divided into three parts; $\Sigma^0(\epsilon)$, impurity potential $I$, and $\delta\Sigma(\epsilon)$. The first term corresponds to the self-energies only by the Hubbard interaction $U$, and the last term is the cross-term between $U$ and $I$.

In the GV$^I$-method [6], $\Sigma^0$ is given by the FLEX approximation. $\delta\Sigma_{i,j}(\epsilon)$ is given by $T \sum_\omega G_{i,j}(\epsilon + \omega)V^T_{i,j}(\omega) - \Sigma^0$, where $\hat{G} = (\hat{G}^0)^{-1} - \Sigma^{-1}$ and $\hat{G}^0(\epsilon)$ is the noninteracting Green function. Moreover, $V^T = V^{\text{FLEX}}[\hat{G}^I]$, which is...
Here, we put \((t', t)\) results of the spin susceptibility given by the fluctuations. In the RPA, the AF-order is suppressed by thermal and quantum fluctuation effect. In the FLEX approximation, the AF-order is highly consistent with NMR measurements [1].

\(U\) neighbor hopping integrals, respectively. We assume the breakdown of the Fermi liquid state. Qualitatively, these obtained numerical results are very similar for YBCO, LSCO and NCCO. We succeeds in explaining the upturn effect of \(\rho\) for YBCO, LSCO and NCCO. We assume the breakdown of the Fermi liquid state. Qualitatively, these obtained numerical results are very similar for YBCO, LSCO and NCCO. We succeeds in explaining the upturn effect of \(\rho\) for YBCO, LSCO and NCCO. We succeed in explaining the upturn effect of \(\rho\) for YBCO, LSCO and NCCO. We succeed in explaining the upturn effect of \(\rho\) for YBCO, LSCO and NCCO. We succeed in explaining the upturn effect of \(\rho\) for YBCO, LSCO and NCCO. We succeed in explaining the upturn effect of \(\rho\) for YBCO, LSCO and NCCO. We succeed in explaining the upturn effect of \(\rho\) for YBCO, LSCO and NCCO.

Hereafter, we take the unitary limit \(I = \infty\). Numerical results of the spin susceptibility given by the \(GV^I\)-method in site representation, \(\chi^I_s(\mathbf{r}, \mathbf{r})\), are explained in Ref. [6]. Here, we present the local susceptibility \(\chi^I_s(\mathbf{r}, \mathbf{r})\) in Fig. 1, around the impurity site (at \((0, 0)\)) along the \(x\)-direction. Here, we put \((t', t, t'') = (-1, 1/6, -1/5)\), where \(t', t\), and \(t''\) are the nearest, the next nearest, and the third nearest neighbor hopping integrals, respectively. We assume \(U = 8\) for hole-doped system (YBCO) and \(U = 5.5\) for electron-doped system (NCCO). \(T = 0.02\) corresponds to 80K in real systems. At \(\mathbf{r} = (7, 0)\), \(\chi^I_s(\mathbf{r}, \mathbf{r})\) takes almost an bulk value without impurity. However, it decreases gradually as one approach the impurity. The temperature dependence of \(\chi^I_s(\mathbf{r}, \mathbf{r})\) away from the impurity is moderate. On the other hand, it increases drastically around the impurity as temperature decreases. At the same time, the radius of the enlargement of \(\chi^I_s(\mathbf{r}, \mathbf{r})\) increases. The obtained result is highly consistent with NMR measurements [1].

Here, we discuss the physical reason for the obtained impurity effect. In the FLEX approximation, the AF-order (in the RPA) is suppressed by thermal and quantum fluctuations. In the \(GV^I\)-method, the reduction of fluctuations due to an impurity gives rise to the enhancement of susceptibility. However, this mechanism is absent in the RPA. Therefore, the enhancement of susceptibility is tiny within the RPA.

Next, we discuss the transport phenomena in the presence of dilute impurities on the basis of the \(GV^I\)-method [6]. Figure 2 shows the resistivity \(\rho\) for NCCO with \(n_{imp} = 0, 0.01\) and 0.02. The obtained result shows a huge parallel shift of resistivity at finite temperatures (\(\Delta \rho\)) due to impurities, far beyond the s-wave unitary scattering limit. As \(T\) decreases, nonmagnetic impurities cause a “Kondo-like upturn” of \(\rho\) below \(T_x\), reflecting an extremely short quasiparticle lifetime around the impurities. We see that \(T_x\) decreases as \(n_{imp}\) does. The obtained Kondo-like upturn of \(\rho\) strongly suggests that the insulating behavior of \(\rho\) observed in under-doped HTSC’s is caused by residual disorder in the CuO2-plane, or residual apical oxygen in NCCO.

The present study reveals that a single impurity strongly affects the electronic states in a wide area around the impurity in the vicinity of the AF-QCP. Here, we developed the \(GV^I\)-FLEX method, which is a powerful method to study the impurity effect in strongly correlated systems. Using the \(GV^I\) method, characteristic impurity effects in under-doped HTSC’s are well explained in a unified way, without introducing any exotic mechanisms which assume the breakdown of the Fermi liquid state. Qualitatively, these obtained numerical results are very similar for YBCO, LSCO and NCCO. We succeeds in explaining nontrivial impurity effects in HTSC’s in a unified way in terms of a spin fluctuation theory, which strongly suggests that the ground state of HTSC is a Fermi liquid. We expect that novel impurity effects in other metals near AF-QCP, such as heavy fermion systems and organic metals, could be explained by the \(GV^I\)-method.

Fig. 1. Local spin susceptibility obtained by the \(GV^I\)-method around the impurity site (at \((0, 0)\)).

Fig. 2. Temperature dependence of \(\rho\) for NCCO with dilute impurities given by the \(GV^I\)-method.

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