Nernst Coefficient and Magnetoresistance in High-T_c Superconductors: The Role of Superconducting Fluctuations

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In high-T_c cuprates, the Nernst coefficient (ν) as well as the magnetoresistance ($\Delta\rho/\rho$) increases drastically below the pseudogap temperature, T^*, which attracts much attention as a key phenomenon in the pseudogap region. We study these transport phenomena in terms of the fluctuation-exchange + T–matrix approximation. In this present theory, the d-wave superconducting (SC) fluctuations, which are mediated by antiferromagnetic (AF) correlations, become dominant below T^*. We especially investigate the vertex corrections both for the charge current and the heat one to keep the conservation laws. As a result, the mysterious behaviors of ν and $\Delta\rho/\rho$ are naturally explained as the reflection of the enhancement of the SC fluctuation, without assuming thermally excited vortices. The present result suggests that the pseudogap phenomena are well described in terms of the Fermi liquid with AF and SC fluctuations.

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In high-T_c cuprates, various transport phenomena in the normal state show striking non-Fermi-liquid(NFL)-like behaviors, such as resistivity (ρ) [1], Hall coefficient ($R_{\rm H}$) [2], magnetoresistance [(MR), $\Delta\rho/\rho$] [3–5], thermoelectric power [(TEP), S] [6], and Nernst coefficient (ν) [7,8]. Because it is impossible to understand these NFL-like phenomena in the framework of the relaxation time approximation (RTA), one may consider that the Landau-Fermi liquid picture—concept of the quasiparticle—is totally violated in high-T_c cuprates. However, before making a conclusion on this issue, one has to study the transport coefficients beyond the RTA, e.g., by the "conserving" approximation as Baym and Kadanoff [9].

In the past few years, we have studied $R_{\rm H}$ [10], $\Delta\rho/\rho$ [11,12], and S [13] in high-T_c cuprates above the pseudogap temperature (T^*) in terms of the conserving approximation: Owing to the vertex corrections (VC's) for currents, the total charge current with VC's, $\vec{J}_{\mathbf{k}}$, is no more perpendicular to the Fermi surface in the presence of strong antiferromagnetic (AF) fluctuations. This important mechanism of the VC, i.e., the "backflow" in the hydrodynamic regime, had been overlooked for years [10]. As a result, we succeeded to reproduce various NFL-like transport phenomena qualitatively as for $T > T^*$ [14].

In this Letter, we study transport phenomena below T^*. In the present stage, superconducting (SC) fluctuation is one of the promising origins of the pseudogap phenomena [15–18]. Based on this opinion, we combine the fluctuation-exchange (FLEX) approximation for describing the AF fluctuations [19] with the T-matrix approximation for describing the SC fluctuations (i.e., FLEX + T–matrix approximation) [16–18]. Next, we study the Nernst coefficient, $\nu \equiv S_{yx}/B = -E_y/B\partial_x T$, which is an off-diagonal TEP under the magnetic field $\mathbf{B} \parallel \mathbf{z}$. According to the linear response theory,

$$\nu = [\alpha_{xy}/\sigma - S\tan\theta_{\rm H}]/B, \tag{1}$$

where α_{xy} is the off-diagonal Peltier conductivity [$J_x = \alpha_{xy}(-\partial_y T)$], and $\tan\theta_{\rm H} \equiv \sigma_{xy}/\sigma$. In high-$T_c$ cuprates, ν increases divergently below T^*, which is sometimes interpreted as the evidence for the spontaneous vortexlike excitations in the pseudogap region [7,8]. [In the mixed state, ν takes a very large value in a clean 2D system, reflecting the high mobility of a vortex.] Contrary to such an exotic scenario, in the present work, we study ν due to the heat current carried by the quasiparticle motion. By considering the VC's due to strong AF and SC fluctuations, we obtain the results which are highly consistent with experiments. Thus, the nature of the pseudogap region is well described as the Fermi liquid with the strong AF + SC fluctuations.

In the self-consistent FLEX + T–matrix approximation, the full Green function and the self-energy are given by

$$G_{\mathbf{k}}(\epsilon_n) = [i\epsilon_n + \mu - \epsilon^0_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\epsilon_n)]^{-1}, \tag{2}$$

$$\Sigma_{\mathbf{k}}(\epsilon_n) = \Sigma^{\rm FLEX}_{\mathbf{k}}(\epsilon_n) + \Sigma^{\rm SCF}_{\mathbf{k}}(\epsilon_n), \tag{3}$$

where $\epsilon^0_{\mathbf{k}}$ is the tight binding dispersion and ϵ_n is a fermion Matsubara frequency. $\Sigma^{\rm FLEX}$ is given by the diagrams for the FLEX approximation, and $\Sigma^{\rm SCF}$ is given by the T-matrix approximation [16–18]. This is a kind of the one-loop approximation with respect to the AF and SC fluctuations. In the pseudogap region, $\Sigma^{\rm SCF}$ is approximately given by [15]

$$\Sigma^{\rm SCF}_{\mathbf{k}}(\epsilon_n) = -\Delta^2_{\rm pg}\psi^2_{\mathbf{k}} G_{\mathbf{k}}(-\epsilon_n), \tag{4}$$

$$\Delta^2_{\rm pg} = T \sum_{\mathbf{q}}{}' t_{\rm pg}(\mathbf{q}, \omega = 0), \tag{5}$$

where $\psi_{\mathbf{k}} = \cos k_x - \cos k_y$ and $\sum'_{\mathbf{q}} \equiv \sum_{\mathbf{q}} \theta(a - |\mathbf{q}|)$. The factor $a \ll 1$ is introduced not to overestimate the effect of SC fluctuations. We put $a = 0.03\pi$ in the present calculation, which would be smaller than the inverse of the SC coherent length. The result is not sensitive to its value, and this approximation becomes reasonable as $T \to T_c$, which is the favorite for the purpose of our study. $t_{\rm pg}(\mathbf{q}, \omega)$ is the T matrix for the $d_{x^2-y^2}$-wave channel, which is mediated by strong AF fluctuations.

To derive $t_{\rm pg}$, we solve the Eliashberg equation:

$$\lambda \phi_{\mathbf{k}}(\epsilon_n) = -T \sum_{\mathbf{k}', \epsilon_m} V^{\rm FLEX}_{\mathbf{k}-\mathbf{k}'}(\epsilon_n - \epsilon_m) |G_{\mathbf{k}'}(\epsilon_m)|^2 \phi_{\mathbf{k}'}(\epsilon_m),$$

where $V^{\rm FLEX}_{\mathbf{k}}$ is the effective interaction for a singlet pair within the FLEX approximation, which is given by Eq. (9) of Ref. [10] using the Green function in Eq. (2). λ is the eigenvalue of the equation which exceeds 1 below T_c. Hereafter, the eigenfunction ϕ is normalized as $\sum_{\mathbf{k},l} \phi^2_{\mathbf{k}}(\epsilon_l) = 1$. By using ϕ, we can approximate that

$$V^{\rm FLEX}_{\mathbf{k}-\mathbf{k}'}(\epsilon - \epsilon') \approx g \phi_{\mathbf{k}}(\epsilon) \phi_{\mathbf{k}'}(\epsilon'), \tag{6}$$

where $g \equiv \sum_{\epsilon,\epsilon'} \sum_{\mathbf{k},\mathbf{k}'} V^{\rm FLEX}_{\mathbf{k}-\mathbf{k}'}(\epsilon - \epsilon') \phi_{\mathbf{k}}(\epsilon) \phi_{\mathbf{k}'}(\epsilon')$. Then, the T matrix is given by

$$t_{\rm pg}(q, \omega_l) = g/[1 + g\bar{\chi}_{\mathbf{q}}(\omega_l)], \tag{7}$$

$$\bar{\chi}_{\mathbf{q}}(\omega_l) = T \sum_{\mathbf{k}, \epsilon_n} G_{\mathbf{k}}(\epsilon_n) G_{\mathbf{q}-\mathbf{k}}(\omega_l - \epsilon_n) \phi^2_{\mathbf{k}}(\epsilon_n), \tag{8}$$

where ω_l is a Matsubara frequency for boson. It is easy to see that $\lambda = -g\bar{\chi}_{\mathbf{q}=\mathbf{0}}(0)$ according to Eq. (6). In the FLEX + T–matrix approximation, we solve Eqs. (2)–(8) self-consistently. In this approximation, $\lambda < 1$ is satisfied in 2D systems at finite temperatures because a Kosterlitz-Thouless–type transition is not taken into account.

In the present numerical study for the Hubbard model, we put $U = 4.5$ and $(t, t', t'') = (-1, 0.15, -0.05)$ for $La_{2-x}Sr_xCuO_4$ (LSCO), where t, t', t'' are the nearest, the next-nearest, and the third-nearest neighbor hoppings, respectively. Figure 1 shows the obtained density of states (DOS); $\rho(\epsilon) = \frac{1}{\pi} \sum_{\mathbf{k}} {\rm Im} G_{\mathbf{k}}(\epsilon - i\delta)$. We see that a deep pseudogap emerges below $T^* \sim 0.03$, because SC fluctuations grow prominently below T^* [16–18]. In the present self-consistent calculation, $\lambda = 0.988$ and $\Delta_{\rm pg} = 0.147$ at $T = 0.02$.

Next, we calculate the Nernst coefficient by taking VC's into account. Based on the linear response theory for the thermoelectric transport phenomena [20], we can derive the general expression for α_{xy} in correlated electron systems by referring to the derivation for σ_{xy} by Kohno *et al.* [21]. The VC is uniquely given by the Ward identities associated with the local charge and energy conservation laws [22]. The obtained expression, which is exact with respect to $O(\gamma^{-2})$, is given by

$$\alpha_{xy} = B \cdot \frac{e^2}{T} \sum_{\mathbf{k}} \int \frac{d\epsilon}{2\pi} \left(-\frac{\partial f}{\partial \epsilon} \right) \times |{\rm Im} G_{\mathbf{k}}(\epsilon)| |G_{\mathbf{k}}(\epsilon)|^2 \cdot |\vec{v}_{\mathbf{k}}(\epsilon)| \gamma_{\mathbf{k}}(\epsilon) A_{\mathbf{k}}(\epsilon), \tag{9}$$

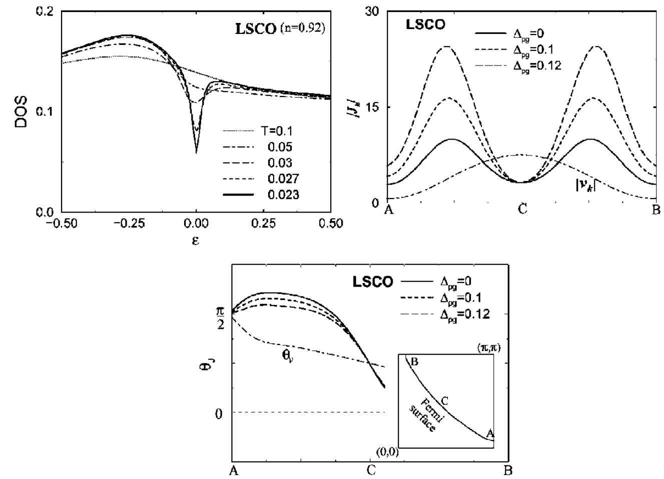

FIG. 1. (a) The DOS obtained by the self-consistent FLEX + T–matrix approximation. $T = 0.1$ corresponds to 300–400 K. (b),(c) $|\vec{J}_{\mathbf{k}}|$ and $\theta^J_{\mathbf{k}}$ obtained by the Bethe-Sapleter (BS) equation (13) for various $\Delta_{\rm pg}$.

$$A_{\mathbf{k}}(\epsilon) = \left(\vec{Q}_{\mathbf{k}}(\epsilon) \times \frac{\partial}{\partial k_\parallel} [\vec{J}_{\mathbf{k}}(\epsilon)/\gamma_{\mathbf{k}}(\epsilon)] \right)_z, \tag{10}$$

$$\vec{Q}_{\mathbf{k}}(\epsilon) = \vec{q}_{\mathbf{k}}(\epsilon) + \sum_{\mathbf{k}'} \int \frac{d\epsilon'}{4\pi i} \mathcal{T}_{\mathbf{k}\mathbf{k}'}(\epsilon, \epsilon') |G_{\mathbf{k}'}(\epsilon')|^2 \vec{Q}_{\mathbf{k}'}(\epsilon'), \tag{11}$$

$$\vec{J}_{\mathbf{k}}(\epsilon) = \vec{v}_{\mathbf{k}}(\epsilon) + \sum_{\mathbf{k}'} \int \frac{d\epsilon'}{4\pi i} \mathcal{T}_{\mathbf{k}\mathbf{k}'}(\epsilon, \epsilon') |G_{\mathbf{k}'}(\epsilon')|^2 \vec{J}_{\mathbf{k}'}(\epsilon'), \tag{12}$$

where $k_\parallel$ is the momentum along the Fermi surface, $\vec{v}_{\mathbf{k}}(\epsilon) \equiv \vec{\nabla}[\epsilon^0_{\mathbf{k}} + {\rm Re}\Sigma_{\mathbf{k}}(\epsilon)]$, and $\vec{q}_{\mathbf{k}}(\epsilon) \equiv \epsilon \cdot \vec{v}_{\mathbf{k}}(\epsilon)$. $\mathcal{T}$ is the irreducible VC introduced by Eliashberg as $\mathcal{T}^{(0)}_{22}$ [23].

Next, we calculate the total charge current $\vec{J}$ and the heat one $\vec{Q}$ numerically. Here, we take only the infinite series of the Maki-Thompson(MT)–type VC's due to the AF and SC fluctuations although the Ward identity gives other terms, because they are expected to be most important when the fluctuations are strong [10,17]. In the present FLEX + T–matrix approximation, the Bethe-Salpeter equation (12) is simply written as

$$\vec{J}_{\mathbf{k}}(\epsilon) = [\gamma_{\mathbf{k}}(\epsilon)/\gamma^{\rm FLEX}_{\mathbf{k}}(\epsilon)] \times \left[\vec{v}_{\mathbf{k}}(\epsilon) + \sum_{\mathbf{k}'} \int \frac{d\epsilon'}{4\pi i} \mathcal{T}^{\rm FLEX}_{\mathbf{k},\mathbf{k}'}(\epsilon, \epsilon') \times |G_{\mathbf{k}'}(\epsilon')|^2 \vec{J}_{\mathbf{k}'}(\epsilon') \right], \tag{13}$$

where $\mathcal{T}^{\rm FLEX}$ represents the MT terms due to the AF fluctuations, whose functional form is given by Eq. (A9) of Ref. [10]. Note that the factor $\gamma_{\mathbf{k}}/\gamma_{\mathbf{k}}^{\rm FLEX}$ comes from the MT terms due to the SC fluctuations, which becomes unity if $\Delta_{\rm qp} = 0$. Performing a similar discussion as in Sec. V of Ref. [10] and using the relation $\gamma_{\mathbf{k}}^{\rm FLEX} = \sum_{\mathbf{k}'} \int \frac{d\epsilon}{4\pi} \mathcal{T}_{\mathbf{k},\mathbf{k}'}^{\rm FLEX}(0,\epsilon) {\rm Im} G_{\mathbf{k}'}^{\rm A}(\epsilon)$, the following approximate relation is derived from Eq. (13) [24]:

$$\vec{J}_{\mathbf{k}} \approx (\gamma_{\mathbf{k}}/\gamma_{\mathbf{k}}^{\rm FLEX}) \vec{J}_{\mathbf{k}}^{[\Delta_{\rm qp}=0]}, \tag{14}$$

where $\vec{J}_{\mathbf{k}}^{[\Delta_{\rm qp}=0]}$ is given by the FLEX approximation without $\Sigma_{\mathbf{k}}^{\rm SCF}$ and $\mathcal{T}^{\rm SCF}$ $(= \mathcal{T} - \mathcal{T}^{\rm FLEX})$, whose behavior was analyzed in Ref. [10] in detail.

Figure 1 shows the numerical solution for the Bethe-Sapleter equation (13) for various $\Delta_{\rm pg}$ at $T = 0.02$ [10,17]. As $\Delta_{\rm pq}$ increases, $|\vec{J}_{\mathbf{k}}|$ is prominently enhanced except for the cold spot (C), whereas $\theta_{\mathbf{k}}^{J} = \tan^{-1}(J_{\mathbf{k}x}/J_{\mathbf{k}y})$ is affected only slightly. The result is consistent with Eq. (14) because $\gamma_{\mathbf{k}}/\gamma_{\mathbf{k}}^{\rm FLEX} \approx 1 + b\psi_{\mathbf{k}}^2$, where $b > 0$ and b increases as T approaches to T_c. As a result, owing to the MT terms by the $d_{x^2-y^2}$-SC fluctuations, $|J_{\mathbf{k}}|$ is enhanced if $\Delta_{\rm pq}$ is large, except for the cold spot where $\psi_{\mathbf{k}} = 0$. A more detailed discussion will be given in a future publication [24]. In contrast, we can show that $\vec{Q}_{\mathbf{k}}(\epsilon) \sim \vec{q}_{\mathbf{k}}(\epsilon)$ because the effect of the VC for the heat current, which is not conserved by the electron-electron N processes, is small in general [22,24]. This means that $\vec{Q}_{\mathbf{k}}$ is no more parallel to $\vec{J}_{\mathbf{k}}$ in the presence of strong AF fluctuations. This fact is important for understanding the Nernst effect as will be explained.

Now we calculate transport coefficients by using the self-consistent solutions of Eqs. (11) and (12). Figure 2 shows the resistivity, the Hall coefficient, and the TEP obtained by the FLEX + T–matrix approximation, $\rho_{\rm AF+SC}$, $R_{\rm H}^{\rm AF+SC}$ and $S_{\rm AF+SC}$, for the filling $n = 0.92$. For reference, $\rho^{\rm AF}$, $R_{\rm H}^{\rm AF}$, and $S_{\rm AF}$ are given by the FLEX approximation. We see that both $R_{\rm H}^{\rm AF+SC}$ and $S_{\rm AF+SC}$ start to decrease below the pseudogap temperature $T^* \sim 0.03$, which is consistent with experiments [2,6], whereas $R_{\rm H}^{\rm AF}$ and $S_{\rm AF}$ increase monotonously as T decreases because both quantities are enhanced due to the VC's created by the AF fluctuations [10,13]. The reason why both $R_{\rm H}^{\rm AF+SC}$ and $S_{\rm AF+SC}$ decrease below T^* is that the AF fluctuations are suppressed in the pseudogap region, which was at first discussed in Refs. [10,13] and shown numerically in Ref. [17] for $R_{\rm H}$.

On the contrary, the drastic enhancement of the Nernst coefficient below T^* is a very mysterious and intriguing phenomenon in the pseudogap region [7,8]. Here, we show that it is naturally explained as a quasiparticle transport phenomenon, without assuming thermally excited vortices. Based on the AF + SC fluctuation theory, we calculate α_{xy} given by Eq. (9): Fig. 3 shows the Nernst coefficient obtained by the FLEX + T–matrix method, $\nu_{\rm AF+SC}$, with full MT-type VC's due to AF + SC fluctuations. We see that $\nu_{\rm AF+SC}$ starts to increase below T^*, and its magnitude is consistent with experimental values. In contrast, $S\tan\theta_{\rm H}$ decreases at lower temperatures, reflecting the suppression of the AF fluctuations.

Here we discuss the reason why ν is enhanced in the presence of AF and d-SC fluctuations: The factor $\gamma_{\mathbf{k}} A_{\mathbf{k}}$ in Eq. (9) is rewritten as

$$\vec{Q}_{\mathbf{k}} \cdot \vec{J}_{\mathbf{k}} \frac{\partial \theta_{\mathbf{k}}^{J}}{\partial k_{\parallel}} + (\vec{Q}_{\mathbf{k}} \times \vec{J}_{\mathbf{k}})_z \frac{\partial}{\partial k_{\parallel}} \log(|\vec{J}_{\mathbf{k}}|/\gamma_{\mathbf{k}}). \tag{15}$$

According to Fig. 1(b), the second term with the factor $\frac{\partial}{\partial k_{\parallel}} |\vec{J}_{\mathbf{k}}|$ should cause the enhancement of ν in the pseudogap region: It does survive because $\vec{J}_{\mathbf{k}}$ is not parallel to $\vec{Q}_{\mathbf{k}}$ due to the VC's by strong AF fluctuations. In contrast,

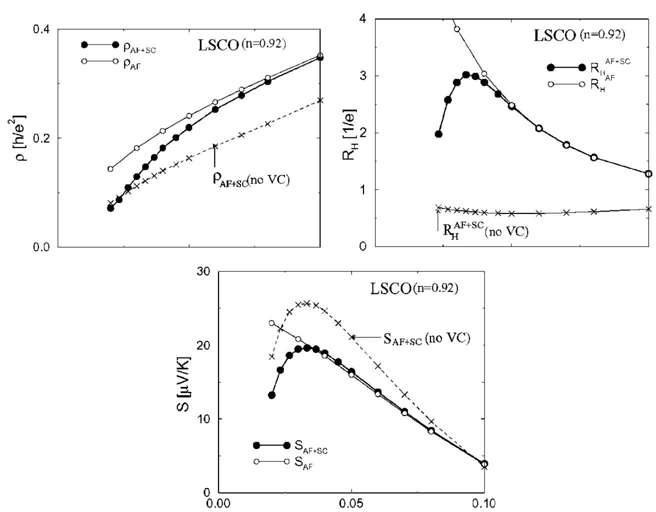

FIG. 2. Transport coefficients per one layer studied by the FLEX + T–matrix approximation with VC's (AF + SC). $h/e^2 = 1.3 \times 10^6\ \Omega$.

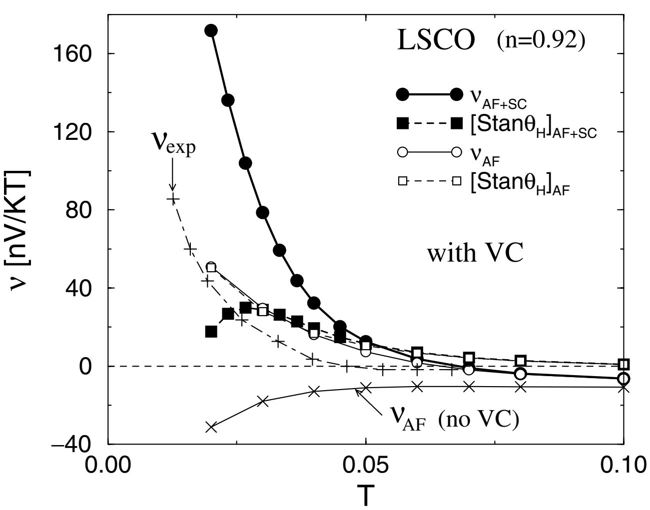

FIG. 3. $\nu_{\rm AF+SC}$ and $[S\tan\theta_{\rm H}]_{\rm AF+SC}$ studied by the FLEX + T–matrix approximation with VC's. $\nu_{\rm exp}$ is the experimental data reported in Ref. [2] for LSCO ($x = 0.07$), assuming that $T = 0.1$ corresponds to 300 K.

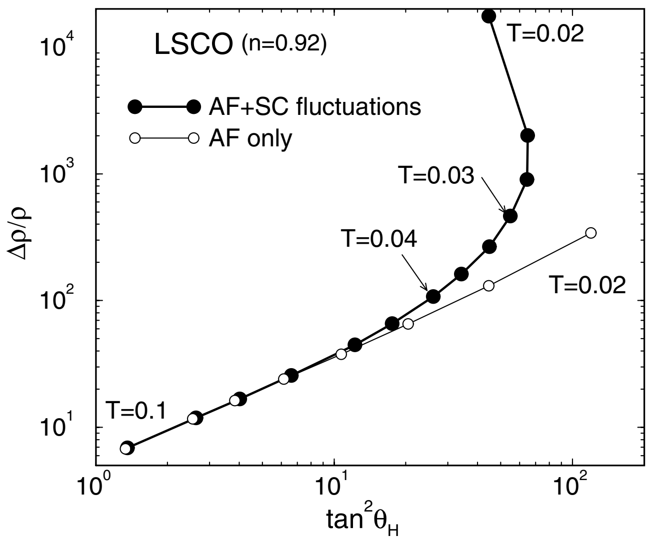

FIG. 4. $\Delta\rho/\rho$ by the FLEX + T−matrix approximation increases drastically in the pseudogap region.

this term vanishes identically within the RTA because of $\vec{v}_{\mathbf{k}} \parallel \vec{q}_{\mathbf{k}}$.

Finally, we discuss the MR, $\Delta\rho/\rho$, in the pseudogap region. Figure 4 shows the calculated $\Delta\rho/\rho$ vs $\tan^2\theta_H = (\sigma_{xy}/\sigma)^2$ for the filling $n = 0.92$. First, in the FLEX approximation (AF only), $\Delta\rho/\rho \propto \tan^m\theta_H$ and $m \approx 1.5$ is approximately satisfied. Note that $m \approx 2$ is obtained for $n \sim 0.85$ by the FLEX approximation [12], which is called the modified Kohler rule observed in high-T_c cuprates for $T > T^*$ [3–5]. In contrast, according to the present FLEX + T−matrix approximation where the effect of SC fluctuations is involved (AF + SC), the relation $\Delta\rho/\rho \propto \tan^m\theta_H$ is prominently violated in the pseudogap region: As shown in Fig. 4, $\Delta\rho/\rho$ starts to increase abruptly below $T^* \sim 0.03$, while the suppression of $\tan\theta_H$ starts at the same time. The obtained result is very well consistent with experiments [3–5].

Now, we discuss why $\Delta\rho/\rho$ increases drastically below T^*: The expression for magnetoconductance ($\Delta\sigma_{xx}$), which is given by Eq. (7) of Ref. [12], has a term proportional to $(\frac{\partial}{\partial k_\parallel}|J_{\mathbf{k}}|)^2$. As discussed before, this factor causes the drastic increase of $\Delta\rho/\rho$ below T^* [see Fig. 1(b)]. As a result, we find the reason why both ν and $\Delta\rho/\rho$ are enhanced in the pseudogap region. In the meanwhile, other quantities such as ρ, R_H, and S decrease below T^* because of the lack of the factor $\frac{\partial}{\partial k_\parallel}|J_{\mathbf{k}}|$.

We note that the positive MR below T^* is frequently ascribed to the magnetic field suppression of the transport due to SC fluctuations, which is theoretically expressed as the Aslamazov-Larkin term. However, one has to assume a rather large coherent length in the underdoped region ($\lesssim 40$ Å) to fit the observed huge MR [5]. Instead, the present work naturally explains the increase of $\Delta\rho/\rho$ below T^*, as well as ν, in terms of the quasiparticle transport phenomena, which is expressed as the infinite series of MT terms.

In summary, we studied the origin of the transport anomaly in the pseudogap region using the FLEX + T−matrix approximation. Below T^* in hole-doped compounds, the resistivity, the TEP, and the Hall coefficient decrease moderately, whereas the Nernst coefficient and the MR increase drastically. In the present study, we could reproduce the characteristic behaviors of these coefficients satisfactorily. Especially, the drastic increase of ν and $\Delta\rho/\rho$ below T^* is naturally explained as the quasiparticle origin, by taking the VC's due to the AF and SC fluctuations correctly. Thus, unusual transport properties of high-T_c cuprates are well explained as the quasiparticle transport phenomena.

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