

Chapter 2

Fluctuation Theory

2.1 Phenomenological Spin Fluctuation Model

Here, we discuss the phenomenological dynamical spin susceptibility $\chi_{\mathbf{q}}^s(\omega)$ in nearly AF metals. We use the unit $c = \hbar = k_B = 1$ hereafter. This is the most important physical quantity in such metals since it is the origin of various non-Fermi liquid behaviors in HTSCs. The functional form of $\chi_{\mathbf{q}}^s(\omega)$ is given by [1–5]

$$\chi_{\mathbf{q}}^s(\omega) = \sum_{\mathbf{Q}} \frac{\chi_Q}{1 + \xi_{\text{AF}}^2(\mathbf{q} - \mathbf{Q})^2 - i\omega/\omega_{\text{sf}}}, \quad (2.1)$$

where $\mathbf{Q} = (\pm\pi, \pm\pi)$ is the antiferromagnetic (AF) wavevector, and ξ_{AF} is the AF correlation length. This is referred to as the Millis-Monien-Pines model [4]. These parameters can be obtained by using NMR/NQR spectroscopy and the neutron diffraction measurement. In HTSCs above the pseudo-gap temperature T^* , both χ_Q and $1/\omega_{\text{sf}}$ are scaled by ξ_{AF}^2 as follows [6]:

$$\xi_{\text{AF}}^2 \approx \alpha_0/(T + \Theta), \quad (2.2)$$

$$\chi_Q \approx \alpha_1 \cdot \xi_{\text{AF}}^2, \quad 1/\omega_{\text{sf}} \approx \alpha_2 \cdot \xi_{\text{AF}}^2, \quad (2.3)$$

where Θ , α_0 , α_1 and α_2 are constants. Since $\chi_Q\omega_{\text{sf}} \propto \xi_{\text{AF}}^0$ in Eq.(2.3), the dynamical exponent z is 2. Just above the superconducting transition temperature T_c [7], $\xi_{\text{AF}} \sim 2a$ in optimally-doped YBCO, whereas it exceeds $100a$ in slightly under-doped NCCO. (a is the unit-cell length; we put $a = 1$ hereafter.) The relationship $\omega_{\text{sf}} \gtrsim T$ ($\omega_{\text{sf}} \lesssim T$) is satisfied in the over-doped (under-doped) YBCO. Using this phenomenological model, T_c is well reproduced by solving the strong-coupling Eliashberg equation [3].

Theoretically, the relationships in Eqs.(2.2) and (2.3) are explained by the SCR theory, due to both self-energy correction and vertex correction to the dynamical susceptibility, referred to as the “mode-mode coupling effect” [8]. These

relationships are also reproduced by the FLEX approximation [9–15], in which only the mode-mode coupling effect due to the self-energy correction is considered: In the FLEX approximation, $\chi_{\mathbf{q}}^s(0)$ in the mean-field approximation (or RPA) is strongly suppressed by the imaginary part of the self-energy. In pure 2D systems, T_N is suppressed to zero by the self-energy, so the Mermin-Wagner theorem is satisfied in the FLEX approximation [16, 17]. Similar results are obtained by the SCR and FLEX approximation.

2.2 Model Hamiltonian and FLEX Approximation

Here, we introduce the effective Hamiltonian of strongly correlated metals. It is given by the kinetic term and the interaction term. The kinetic term is frequently represented by the tight-binding model, given by the set of hopping integrals between different Wannier functions. The interaction term is usually approximated as the local Coulomb interaction, considering the screening effect. In many transition metal oxides or heavy fermions, Fermi surfaces are composed of more than one d - or f -orbitals. In the case of cuprate HTSCs, however, orbital degrees of freedom are absent. The corresponding single-orbital Hubbard model is given as

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}^0 c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + U \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}'-\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow}, \quad (2.4)$$

where U is the Coulomb interaction, and $\epsilon_{\mathbf{k}}^0$ is the spectrum of the conduction electron. In a square lattice, $\epsilon_{\mathbf{k}}^0$ is given by

$$\epsilon_{\mathbf{k}}^0 = 2t_0(\cos k_x + \cos k_y) + 4t_1 \cos k_x \cos k_y + 2t_2(\cos 2k_x + \cos 2k_y), \quad (2.5)$$

where $c_{\mathbf{k}\sigma}^\dagger$ is the creation operator of an electron with momentum $\mathbf{k}$ and spin σ . We represent the electron filling by n , and $n = 1$ corresponds to the half-filling. n is smaller (larger) than unity in YBCO and LSCO (NCCO). To fit the band structures given by the local density approximation (LDA) for YBCO [18], NCCO [19], and LSCO [20, 21] and by the angle resolved photoemission (ARPES) experiments for YBCO [22], NCCO [23, 24] and LSCO [25], we select the following set of parameters [26, 27].

(I) YBCO (hole-doping) and NCCO (electron-doping):

$$t_0 = -1, \quad t_1 = 1/6, \quad \text{and} \quad t_2 = -1/5. \quad (2.6)$$

(II) LSCO (hole-doping):

$$t_0 = -1, \quad t_1 = 1/10, \quad \text{and} \quad t_2 = -1/10. \quad (2.7)$$

The Fermi surfaces for YBCO and NCCO without interaction are shown in Fig. 2.1a. The deformation of the Fermi surface in the presence of U has been discussed in Ref. [27]. Note that the Fermi surface in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ (BSCCO) is similar to that in YBCO [28]. Since $|t_0| \sim 4000$ K in HTSCs, $T = 0.1$ in the present study corresponds to 400 K.

In the RPA, the dynamical spin and charge susceptibilities are given by

$$\chi_{\mathbf{q}}^{s(c),\text{RPA}}(i\omega_l) = \chi_{\mathbf{q}}^{00} \cdot \left\{ 1 - (+)U\chi_{\mathbf{q}}^{00}(i\omega_l) \right\}^{-1}, \quad (2.8)$$

$$\chi_{\mathbf{q}}^{00}(i\omega_l) = -T \sum_{\mathbf{k},n} G_{\mathbf{q}+\mathbf{k}}^0(i\omega_l + i\epsilon_n) G_{\mathbf{k}}^0(i\epsilon_n), \quad (2.9)$$

where $G_{\mathbf{k}}^0(i\epsilon_n) = (i\epsilon_n + \mu - \epsilon_{\mathbf{k}}^0)^{-1}$ is the non-interaction Green function.

Using the complex integration, Eq. (2.9) is given as

$$\chi_{\mathbf{q}}^{00}(i\omega_l) = \sum_{\mathbf{k}} \int_C \frac{d\epsilon}{2\pi i} f(\epsilon) \frac{1}{(\epsilon - i\omega_l + \epsilon_{\mathbf{k}+\mathbf{q}})(\epsilon - \epsilon_{\mathbf{k}})}, \quad (2.10)$$

where $f(\epsilon) = (1 + e^{\beta\epsilon})^{-1}$, which has poles at $\epsilon = i(2n + 1)\pi T$ on the imaginary axis, and the corresponding residue is $-T$. The complex integration path C is shown in Fig. 2.2a. By changing the integration path to Fig. 2.2b, we have only to pick up two residues at $\epsilon = \epsilon_{\mathbf{k}}$ and $\epsilon = -i\omega_l + \epsilon_{\mathbf{k}+\mathbf{q}}$:

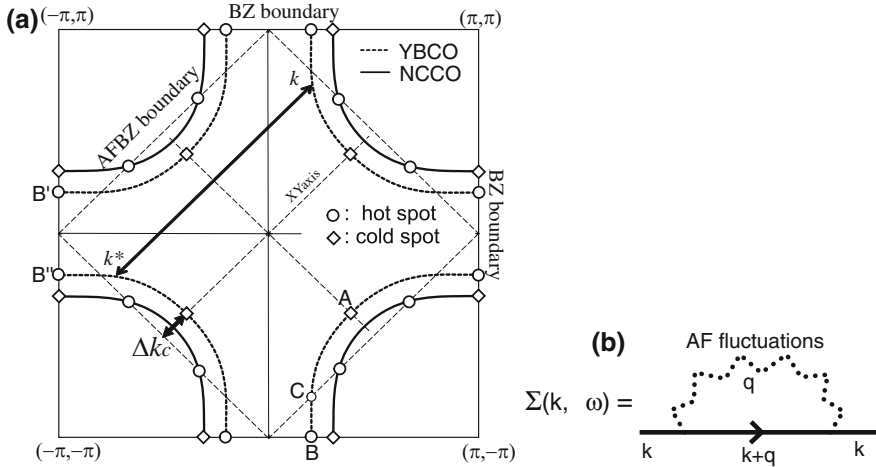
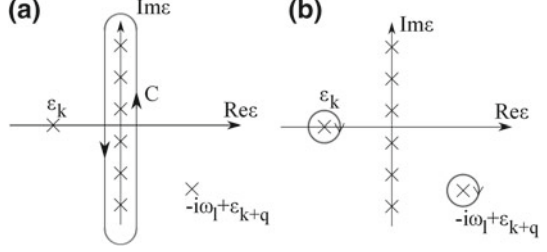


Fig. 2.1 **a** The Fermi surfaces for YBCO ($n < 1$) and NCCO ($n > 1$). The location of the hot spots and the cold spots are shown. In the FLEX approximation, the hot spot in YBCO shifts to point B, by reflecting the large DOS at $(\pi, 0)$. **b** Diagrammatic representation of the self-energy in the one-loop (FLEX) approximation

Fig. 2.2 **a** The complex integration path C in the complex ϵ plane. **b** A modified complex integration path C'



$$\begin{aligned}
 \chi_{\mathbf{q}}^{00}(i\omega_l) &= \sum_{\mathbf{k}} \left\{ \frac{-f(\epsilon_{\mathbf{k}})}{i\omega_l + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}} + \frac{-f(-i\omega_l + \epsilon_{\mathbf{k}+\mathbf{q}})}{-i\omega_l - \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}+\mathbf{q}}} \right\} \\
 &= \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}+\mathbf{q}}) - f(\epsilon_{\mathbf{k}})}{i\omega_l + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}}
 \end{aligned} \quad (2.11)$$

It is easy to verify that $\chi_{\mathbf{q}}^{00}(i\omega_l)$ is a real function. However, it becomes a complex function after the analytic continuation $i\omega_l (l > 0) \rightarrow \omega + i\delta$ or $i\omega_l (l < 0) \rightarrow \omega - i\delta$.

By expanding $\chi_{\mathbf{q}}^{00}(i\omega_l) \approx \chi_{\mathbf{Q}}^{00}(0) - b(\mathbf{q} - \mathbf{Q})^2 + c|\omega_l|$, we obtain $\chi_{\mathbf{q}}^{s(c), \text{RPA}}(i\omega_l) \approx \chi_{\mathbf{Q}}^{00}(0)[1 - U\chi_{\mathbf{Q}}^{00}(0) + Ub(\mathbf{q} - \mathbf{Q})^2 - Uc|\omega_l|]^{-1}$. After the analytic continuation $i\omega_l (l > 0) \rightarrow \omega_l + i\delta$, we obtain the MMP model in Eq. (2.1) with $\xi_{\text{AF}}^2 = Ub/(1 - \alpha_{\text{St}})$, $\omega_{\text{sf}} = (1 - \alpha_{\text{St}})/Uc$, and $\chi_Q = \chi_{\mathbf{Q}}^{00}(0)/(1 - \alpha_{\text{St}})$, where $\alpha_{\text{St}} = U\chi_{\mathbf{Q}}^{00}(0)$ is the Stoner factor. α_{St} is close to unity near AF-QCP.

In the FLEX approximation [9], the Green functions in Eq. (2.9) are replaced with the Green functions with self-energy:

$$G_{\mathbf{k}}(i\epsilon_n) = (i\epsilon_n + \mu - \epsilon_{\mathbf{k}}^0 - \Sigma_{\mathbf{k}}(i\epsilon_n))^{-1}, \quad (2.12)$$

The FLEX is classified as a conserving approximation whose framework was constructed by Baym and Kadanoff [29] and by Baym [30]. For this reason, we can calculate the CVC without ambiguity, by following the Ward identity $\Gamma^I = \delta\Sigma/\delta G$. Here, the Green function and the self-energy are given by

$$\Sigma_{\mathbf{k}}(i\epsilon_n) = T \sum_{\mathbf{q}, l} G_{\mathbf{k}-\mathbf{q}}(i\epsilon_n - i\omega_l) \cdot V_{\mathbf{q}}(i\omega_l), \quad (2.13)$$

$$V_{\mathbf{q}}(i\omega_l) = U^2 \left(\frac{3}{2} \chi_{\mathbf{q}}^s(i\omega_l) + \frac{1}{2} \chi_{\mathbf{q}}^c(i\omega_l) - \chi_{\mathbf{q}}^0(i\omega_l) \right) + U, \quad (2.14)$$

$$\chi_{\mathbf{q}}^{s(c)}(i\omega_l) = \chi_{\mathbf{q}}^0 \cdot \left\{ 1 - (+)U\chi_{\mathbf{q}}^0(i\omega_l) \right\}^{-1}, \quad (2.15)$$

$$\chi_{\mathbf{q}}^0(i\omega_l) = -T \sum_{\mathbf{k}, n} G_{\mathbf{q}+\mathbf{k}}(i\omega_l + i\epsilon_n) G_{\mathbf{k}}(i\epsilon_n), \quad (2.16)$$

where $\epsilon_n = (2n + 1)\pi T$ and $\omega_l = 2l\pi T$, respectively. The self-energy in Eq. (2.13) is schematically shown by Fig. 2.1b. $\chi_{\mathbf{q}}^{s(c)}(i\omega_l)$ is the spin (charge) susceptibility, and $\chi_{\mathbf{q}}^0(i\omega_l)$ is the irreducible susceptibility. We solve the Eqs. (2.13)–(2.16) self-consistently, choosing μ so as to satisfy $n = T \sum_{\mathbf{k}, n} G_{\mathbf{k}}(i\epsilon_n) \cdot e^{i\epsilon_n \cdot 0+}$.

The FLEX approximation is suitable for the analysis of nearly AF Fermi liquids. Many authors have applied this approximation to the square-lattice Hubbard model [9–12]. Although it is an approximation, the obtained results are in good agreement with the results obtained from the quantum Monte Carlo simulations for a moderate U [9]. The FLEX approximation has also been applied to the ladder compound $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ [13], organic κ -(BEDT-TTF) compounds [31–35], and various extended Hubbard models [36].

Note that the FLEX approximation can not reproduce the pseudo-gap behaviors below $T^* \sim 200\text{K}$ in slightly under-doped systems. In Chap. 6, we improve this approximation by taking both spin and SC fluctuations into account (FLEX+ T -matrix approximation), and reproduce experimental pseudo-gap behaviors.

Figure 2.3 shows $\chi_{\mathbf{q}}^s(\omega = 0)$ given by the FLEX approximation, both for YBCO ($n = 0.85$; optimum doping) at $T = 0.02$ and for NCCO ($n = 1.20$, slightly over-doping) at $T = 0.04$, respectively [27]. In optimum YBCO, the Stoner factor $U\chi_{\mathbf{Q}}^0(0) \sim 0.98$ at $T = 0.02$, and the AF correlation length ξ_{AF} is approximately $2\sim 3a$ (a denotes the lattice spacing). On the other hand, ξ_{AF} in NCCO ($n = 1.20$) exceeds $10a$ at $T = 0.02$. (The broadness of $\chi(\mathbf{q})$ in YBCO originates from the closeness of the Fermi surface to the van-Hove singular point at $(\pi, 0)$.) We stress that, in both cases, $\chi_{\mathbf{q}}^s(\omega = 0)$ becomes incommensurate in the RPA, inconsistently with neutron experiments. Therefore, the self-energy correction given by the FLEX approximation is important to reproduce appropriate dynamical spin susceptibilities.

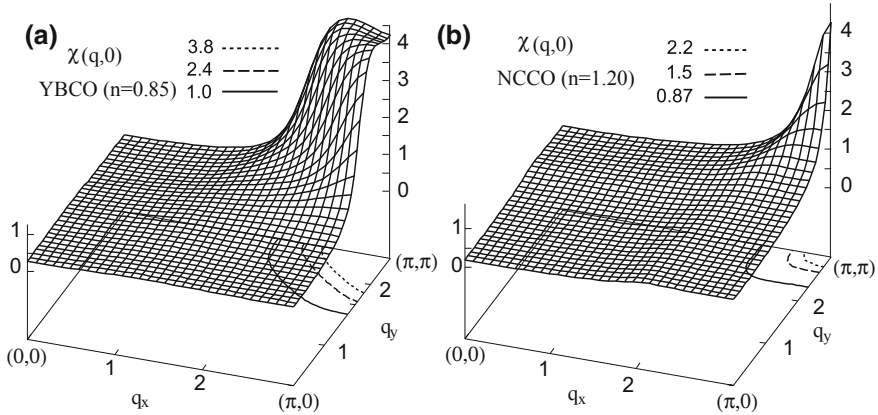


Fig. 2.3 $\chi(\mathbf{q}, \omega = 0)$ for **a** YBCO ($n = 0.85$) at $T = 0.02$ and **b** for NCCO ($n = 1.20$) at $T = 0.04$, given by the FLEX approximation. In YBCO, $\xi_{\text{AF}} = 2a\sim 3a$, whereas ξ_{AF} for NCCO exceeds $\sim 10a$ at $T = 0.02$. a is the lattice spacing [27]

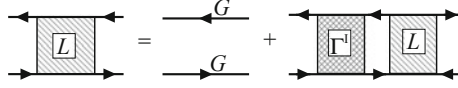


Fig. 2.4 Bethe-Salpeter equation for two-particle Green function $L(k, k')$. $\Gamma^I(k, k')$ is the irreducible four point vertex with respect to the particle-hole channel $G_{k''+q}G_{k''}$

We also stress that the NMR results are quantitatively reproducible in the FLEX approximation.¹

In the FLEX approximation, the Mermin-Wagner theorem is satisfied as proved in Appendix A of Ref. [16, 17]. Hence, the critical region ($U\chi_Q^0(0) \gtrsim 0.99$) is stable in 2D systems since the SDW order ($U\chi_Q^0(0) = 1$) is prevented by the Mermin-Wagner theorem. That is, $U_{\text{cr}} = \infty$ in 2D systems.

In the next stage, we derive the two-particle Green function $L(k, k')$, by which transport coefficients are represented in the linear response theory. According to the microscopic Fermi liquid theory [37, 38], $L(k, k')$ can be obtained by the solution of the following Bethe-Salpeter equation:

$$\begin{aligned} L(k, k'; q) &= -G_{k+q}G_k\delta_{k,k'}/T - G_{k+q}G_k\Gamma(k, k'; q)G_{k'+q}G_{k'} \\ &= -G_{k+q}G_k\delta_{k,k'}/T \\ &\quad - T \sum_{k''} G_{k+q}G_k\Gamma^I(k, k''; q)G_{k''+q}G_{k''}L(k'', k'; q), \end{aligned} \quad (2.17)$$

which is expressed by Fig. 2.4. Here $k = (\mathbf{k}, i\epsilon_n)$, $\Gamma(k, k'; q)$ is the full four-point vertex, and $\Gamma^I(k, k'; q)$ is the irreducible four-point vertex. In the conserving approximation (like the FLEX approximation), it is given by the Fourier transformation of the Ward identity in real space; $\hat{\Gamma}^I = \delta\hat{\Sigma}/\delta\hat{G}$. Then, transport coefficient obtained by $L(k, k')$ automatically satisfies conservation laws, proved in Refs. [29, 30]. This is a great advantage of the conserving approximation for the study of transport phenomena. In the FLEX approximation, irreducible four-point vertex is given in Eq.(5.1) in Sect. 5.1.

2.3 Hot/Cold-Spot Structure and T -Linear Resistivity in Nearly AF Metals

One of the important aspects in nearly AF Fermi liquids is the “hot/cold-spot structure” of the quasiparticle damping rate, $\gamma_{\mathbf{k}} = \text{Im}\Sigma_{\mathbf{k}}(-i\delta)$ [3, 5, 9, 39–41]. That is, $\gamma_{\mathbf{k}}$ becomes anisotropic in the presence of AF fluctuations. Note that $\tau_{\mathbf{k}} = \hbar/2\gamma_{\mathbf{k}}$,

¹ I calculated the $1/T_1T$ of Cu nuclei for $n = 0.85$ using the FLEX approximation. I used Eq.(2.12) in Ref. [4] by correcting misprints, assuming that $A_{\perp} = B = 3.3 \times 10^{-7}$ eV. The obtained $1/T_1T$ under $\mathbf{H} \perp \hat{c}$ is 1–2(m/s) at ~ 200 K, which is consistent with experiments.

and we put $\hbar = 1$ in the textbook. The portions of the Fermi surface at which $\gamma_{\mathbf{k}}$ takes the maximum and minimum values are referred to as *hot spots* and *cold spots*, respectively [5, 41]. According to the spin fluctuation theory, the hot spots usually exist around the crossing points with the AF Brillouin zone (AFBZ)-boundary, whereas the cold spot is at the points where the distance from the AFBZ-boundary is the largest. Their positions are shown in Fig. 2.1a. The electronic states around the cold spots play the major role for various transport phenomena. Note that the hot spot in YBCO shifts to the Brillouin zone boundary (point B), by reflecting the large DOS at $(\pi, 0)$.

Figure 2.5 shows the $\mathbf{k}$ -dependence of $\gamma_{\mathbf{k}}$ on the Fermi surface given by the FLEX approximation [27]. In YBCO, the hot spot moves to the BZ-boundary [point B] in Fig. 2.1a, by reflecting the large DOS at the van-Hove singularity point $(\pi, 0)$. Therefore, the spectral weight at the Fermi energy, $\rho_{\mathbf{k}}(\omega) = \gamma_{\mathbf{k}}/((\omega + \mu - \epsilon_{\mathbf{k}})^2 + \gamma_{\mathbf{k}}^2)$ at $\omega = 0$, is strongly reduced around $(\pi, 0)$ due to large γ_{hot} , consistently with the ARPES experiments [42]. In NCCO, in contrast, the hot and cold spots are located at point C and B, respectively. The location of the cold spot in NCCO was first predicted by the FLEX approximation in Ref. [27] in 1999, and it was later confirmed by ARPES [23, 24]. According to the spin fluctuation theories [5], $\gamma_{\text{hot}} \propto \sqrt{T}$, and $\gamma_{\text{cold}} \propto T$ except that $\xi_{\text{AF}} \gg (\Delta k_c)^{-1}$; Δk_c is shown in Fig. 2.1a.

The critical value of U for a spin density wave (SDW) transition in the RPA (i.e., the mean-field approximation) is $U_{\text{cr}}^{\text{RTA}} \sim 2.3$ in LSCO ($n = 0.9$). In YBCO and NCCO, $U_{\text{cr}}^{\text{RTA}} \sim 3.5$ for both YBCO ($n = 0.9$) and NCCO ($n = 1.1$), since the nesting is not good due to the large next-nearest and third-nearest hopping integrals (t_1 and t_2). In YBCO, the dimensionless coupling constant $UN(0)$ is large, since the van-Hove singular point is close to the Fermi level. Here, $N(0)$ is the DOS at the Fermi level. Therefore, $\text{Im}\Sigma_{\mathbf{k}}(0)$ takes a large value, which significantly reduces the interacting DOS at $(\pi, 0)$ as well as $\chi_{\mathbf{q}}^s(0)$ at $\mathbf{q} = (\pi, \pi)$ [27]. This effect is smaller in NCCO since the saddle point is far below the Fermi level. For this reason, ξ_{AF} for NCCO is much larger than that for YBCO in the FLEX approximation, consistently with experiments.

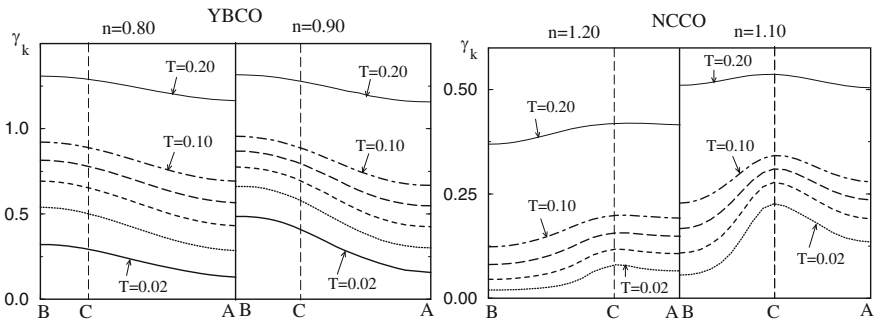


Fig. 2.5 The $\mathbf{k}$ -dependence of $\gamma_{\mathbf{k}}$ on the Fermi surface at various temperatures given by the FLEX approximation. The cold spot in YBCO (NCCO) is point A (B)

The real-frequency Green function is given by the analytic continuation of $G_{\mathbf{k}}(i\epsilon_n)$ in Eq. (2.12). In a Fermi liquid, the advanced (retarded) Green function $G_{\mathbf{k}}^{A(R)}(\epsilon) = G_{\mathbf{k}}(\epsilon - (+)i\delta)$ for $\epsilon \sim 0$ and $|\mathbf{k}| \sim k_F$ is represented as

$$G_{\mathbf{k}}^{A(R)}(\epsilon) = z_{\mathbf{k}}/(\epsilon - E_{\mathbf{k}}^* - (+)i\gamma_{\mathbf{k}}^*), \quad (2.18)$$

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}}^0 + \Sigma_{\mathbf{k}}(0) - \mu, \quad E_{\mathbf{k}}^* = z_{\mathbf{k}} E_{\mathbf{k}}, \quad (2.19)$$

$$\gamma_{\mathbf{k}} = \text{Im} \Sigma_{\mathbf{k}}^A(0), \quad \gamma_{\mathbf{k}}^* = z_{\mathbf{k}} \gamma_{\mathbf{k}}, \quad (2.20)$$

where $z_{\mathbf{k}}$ is the renormalization factor $z_{\mathbf{k}} = 1/(1 - \partial \text{Re} \Sigma_{\mathbf{k}}(\epsilon)/\partial \epsilon)_{\epsilon=0}$ and $E_{\mathbf{k}}^*$ is the renormalized quasi-particle spectrum, which is the solution of $\text{Re} G_{\mathbf{k}}^{-1}(E_{\mathbf{k}}^*) = 0$. The quasiparticle spectrum is given by

$$\rho_{\mathbf{k}}(\epsilon) = \frac{1}{\pi} \text{Im} G_{\mathbf{k}}^A(\epsilon). \quad (2.21)$$

The DOS is expressed as $N(\epsilon) = \sum_{\mathbf{k}} \rho_{\mathbf{k}}(\epsilon)$. In the case of $z_{\mathbf{k}} \gamma_{\mathbf{k}} \ll \mu$,

$$\rho_{\mathbf{k}}(\epsilon) = z_{\mathbf{k}} \delta(\epsilon - E_{\mathbf{k}}^*) \quad (2.22)$$

for $\epsilon \approx 0$.

In the FLEX approximation, $\gamma_{\mathbf{k}}$ is given by the analytic continuation of Eq. (2.13):

$$\gamma_{\mathbf{k}} = \frac{1}{2} \sum_{\mathbf{q}} \int d\epsilon \left[\text{cth} \frac{\epsilon}{2T} - \text{th} \frac{\epsilon}{2T} \right] \text{Im} V_{\mathbf{q}}(\epsilon + i\delta) \rho_{\mathbf{k}+\mathbf{q}}(\epsilon) \quad (2.23)$$

where $V_{\mathbf{q}}(\omega + i\delta)$ is given by the analytic continuation of Eq. (2.14). Using the spin fluctuation model in Eq. (2.1), $\text{Im} V_{\mathbf{q}}(0)$ in Eq. (2.23) is replaced with $(3U^2/2) \text{Im} \chi_{\mathbf{q}}^s(\omega) = (3U^2/2) \omega \chi_Q \omega_{\text{sf}} / (\omega_{\mathbf{q}}^2 + \omega^2)$, where $\omega_{\mathbf{q}} = \omega_{\text{sf}} + \omega_{\text{sf}} \xi_{\text{AF}}^2(\mathbf{q} - \mathbf{Q})^2$. According to Refs. [5, 27], Eq. (2.23) is approximately transformed to

$$\gamma_{\mathbf{k}} \approx \frac{3U^2}{4\pi} \int_{\text{FS}} \frac{dk'_{\parallel}}{v_{\mathbf{k}'}} \chi_Q \omega_{\text{sf}} \frac{(\pi T)^2}{4\omega_{\mathbf{k}-\mathbf{k}'}(\omega_{\mathbf{k}-\mathbf{k}'} + \pi T/2)}, \quad (2.24)$$

so $\gamma_{\mathbf{k}}$ at the hot spot in 2D systems is given by [5]:

$$\gamma_{\text{hot}} \propto T \xi_{\text{AF}} \quad \text{for } \pi T/2\omega_{\text{sf}} \gg 1 \quad (2.25)$$

$$\gamma_{\text{hot}} \propto T^2 \xi_{\text{AF}}^3 \quad \text{for } \pi T/2\omega_{\text{sf}} \ll 1. \quad (2.26)$$

Since $\xi_{\text{AF}}^2 \propto T^{-1}$, $\gamma_{\text{hot}} \propto \sqrt{T}$ for any value of ω_{sf}/T : This result is recognized in the numerical study in Fig. 2.5. Also, γ_{cold} in 2D systems is obtained as [5]:

$$\gamma_{\text{cold}} \propto T \quad \text{for } \pi T/2\omega_{\text{sf}} \sim (\xi_{\text{AF}}\Delta k_c)^2, \quad (2.27)$$

$$\gamma_{\text{cold}} \propto T^2 \quad \text{for } \pi T/2\omega_{\text{sf}} \ll (\xi_{\text{AF}}\Delta k_c)^2. \quad (2.28)$$

According to Eqs. (2.2) and (2.3), $\pi T/2\omega_{\text{sf}}$ is constant if $\Theta \approx 0$, and it is of order unity in optimally-doped HTSCs. Therefore, $\gamma_{\text{cold}} \propto T$ when $\xi_{\text{AF}}\Delta k_c \sim O(1)$, and $\gamma_{\text{cold}} \propto T^2$ when $\xi_{\text{AF}}\Delta k_c \gg 1$: Δk_c represents the “deviation from the nesting condition at the cold spot” shown in Fig. 2.1. Note that the measure part of the Fermi surface becomes cold when $\xi_{\text{AF}}\Delta k_c \gg 1$.

Now, we consider the T -dependence of resistivity by dropping the CVC. In the SCR theory [39], the resistivity is derived from the Born approximation $\rho \propto \langle \gamma_{\mathbf{k}} \rangle_{\text{FS}} \equiv \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \rho_{\mathbf{k}}(0)$. In the case of $\omega_{\text{sf}} \gg T$, Eq. (2.24) is simplified as

$$\gamma_{\mathbf{k}} \approx \sum_{\mathbf{q}} \frac{(\pi T)^2}{2} \text{Im} \dot{V}_{\mathbf{q}}(0) \rho_{\mathbf{k}+\mathbf{q}}(0), \quad (2.29)$$

where $\dot{V}_{\mathbf{q}}(0) = dV_{\mathbf{q}}(\omega + i\delta)/d\omega|_{\omega=0}$. Using Eqs. (2.1) and (2.29), the resistivity is given as [39, 43]

$$\begin{aligned} \rho_{\text{SCR}} &\propto \langle \gamma_{\mathbf{k}} \rangle_{\text{FS}} \\ &\propto T^2 \sum_{\mathbf{q}} \text{Im} \dot{V}_{\mathbf{q}}(0) \sum_{\mathbf{k}} \rho_{\mathbf{k}}(0) \rho_{\mathbf{k}+\mathbf{q}}(0) \\ &\propto T^2 \xi_{\text{AF}}^{4-d}, \end{aligned} \quad (2.30)$$

where d is the dimension of the system. In deriving Eq. (2.30), we utilized the fact that the $\mathbf{q}$ -dependence of $\text{Im} \dot{V}_{\mathbf{q}}(0) = (\pi/2) \sum_{\mathbf{k}} \rho_{\mathbf{k}}(0) \rho_{\mathbf{k}+\mathbf{q}}(0)$ is moderate. Since $\xi_{\text{AF}} \propto \sqrt{\chi Q} \propto T^{-0.5}$ near the AF-QCP [39], ρ_{SCR} is proportional to $T^{d/2}$ ($d = 2, 3$). Note that the Fermi liquid behavior $\rho_{\text{SCR}} \propto T^2$ is recovered when $\xi_{\text{AF}} = \text{constant}$ away from the AF-QCP, like in over-doped systems at low temperatures.

However, Eq. (2.30) would be appropriate only when $\gamma_{\mathbf{k}}$ is moderately anisotropic [41, 44]: According to the linear response theory, the correct resistivity is give by

$$\rho \propto 1 / \langle \gamma_{\mathbf{k}}^{-1} v_{\mathbf{k}x}^2 \rangle_{\text{FS}} \sim \gamma_{\text{cold}}. \quad (2.31)$$

According to Eqs. (2.27) and (2.28), T -linear behavior of ρ would be realized for $\xi_{\text{AF}}\Delta k_c \sim O(1)$ (moderately anisotropic $\gamma_{\mathbf{k}}$ case). This would be the case of optimally doped or slightly under-doped YBCO and LSCO. On the other hand, $\rho \propto T^2$ for $\xi_{\text{AF}}\Delta k_c \gg 1$ (highly anisotropic $\gamma_{\mathbf{k}}$ case), since the dominant part of the Fermi surface becomes the cold spot.

In Sect. 5.2, we will calculate the resistivity using the FLEX approximation including the CVC. The obtained ρ follows an approximate T -linear behavior in under-doped LSCO and NCCO, and it shows a T^2 -like behavior in the over-doped NCCO. As for the resistivity, the CVC is quantitatively important.

In real systems with finite randomness, impurity scattering rate γ_{imp} , which gives the residual resistivity, dominates the elastic scattering rate $\gamma_{\mathbf{k}}$ at sufficiently low temperatures. In this case, the “ T^2 -resistivity in the close vicinity of the AF-QCP” is not observed: In fact, for $\gamma_{\text{imp}} \gg \gamma_{\mathbf{k}}$, Eq. (2.31) is given by

$$\rho \propto 1/(\langle \gamma_{\mathbf{k}} + \gamma_{\text{imp}} \rangle_{\text{FS}})^{-1} \propto \gamma_{\text{imp}} + \langle \gamma_{\mathbf{k}} \rangle_{\text{FS}}. \quad (2.32)$$

Therefore, according to Eq. (2.30), $\rho = \rho_0 + aT^{d/2}$ ($d = 2, 3$) holds near the AF-QCP in the presence of impurities. In most cases, $a > 0$ is assured even if the CVC is taken into account. ($a = 0$ is realized only in a special case where the Fermi surface is completely isotropic and the Umklapp process is absent; see Sect. 3.2.)

2.4 Validity of the Spin Fluctuation Theories

In Sect. 2.2, we explained that the FLEX approximation explains characteristic electronic properties in optimally-doped HTSC. For example, it can reproduce experimental behavior of the dynamical spin susceptibility $\chi_{\mathbf{q}}^s(\omega)$, which is given in Eq. (2.1). Experimentally, AF correlation starts to increase below $T_0 \sim 600$ K. Using the obtained $\chi_{\mathbf{q}}^s(\omega)$, both the damping rate $\gamma_{\mathbf{k}}$ and CVC are appropriately calculated. For example, the hot/cold spot structure of $\gamma_{\mathbf{k}}$ (Fig. 2.1a) is reproduced well for both hole-doped and electron-doped systems, and the anomalous transport are well reproduced. These facts assure the validity of the FLEX approximation.

Now, we discuss the “weak pseudo-gap behavior” below T_0 : Below T_0 , the AF fluctuations suppress the DOS [45–48], Knight shift [49–51] and uniform susceptibility [52, 53]. The weak pseudo-gap in the DOS is shallow and wide in energy. The obtained weak pseudo-gap behaviors in the FLEX approximation are too moderate, after the self-consistent determination of the self-energy and Green function. In fact, a large weak pseudo-gap in the DOS is reproduced at the first iteration stage of the FLEX. Similar tendency is reported in the GW approximation: This is a first principle calculation for the self-energy, which is given by the convolution of the Green function G and the screened interaction W within the RPA. Although the descriptions of the bandwidth reduction and satellite structure in the quasiparticle spectrum are satisfactory in a partially self-consistent GW method, they are smeared out in the fully self-consistent GW due to strong feedback effect [54–56]. Mathematically, this too strong feedback effect should be canceled by the vertex correction in the self-energy.

Therefore, to produce a weak pseudo-gap, it is better to apply the (i) fully self-consistent calculation with vertex corrections or (ii) partially (or no) self-consistent calculation. Along the lines of method (i), Schmalian and Pines calculated the self-energy with all the vertex corrections in the $(\mathbf{k}, \mathbf{k} + \mathbf{Q})$ model by applying a high-temperature approximation [57, 58]. Using a similar technique, the pseudo-gap due to strong SC fluctuations had been calculated [59]. It is noteworthy that the

fourth-order-perturbation theory with respect to U well reproduces the weak pseudo-gap since the vertex corrections for the self-energy are considered [60]. This method also reproduces the difference of T_c between YBCO and LSCO [61, 62], and the p -wave SC state in Sr_2RuO_4 [63, 64].

Along the lines of method (ii), Vilk and Tremblay proposed a two-particle self-consistent (TPSC) method [65], where full self-consistency is not imposed on the self-energy. Therein, the renormalized spin susceptibility is given by the RPA, by using the effective Coulomb interaction $U_{\text{eff}} (< U)$ that is determined so as to satisfy the sum rule for the susceptibility. This philosophy has been applied to extend the dynamical mean field theory (DMFT) by including self-energy correction due to spin fluctuations [66, 67]. These theories can explain the weak pseudo-gap in the DOS. However, they are not suitable for the study of the transport phenomena since the conservation laws are not satisfied. To calculate the transport phenomena with satisfying the conservation laws, the FLEX approximation is very useful.

References

1. T. Moriya, Y. Takahashi, K. Ueda, J. Phys. Soc. Jpn. **59**, 2905 (1990)
2. K. Ueda, T. Moriya, Y. Takahashi, J. Phys. Chem. Solids **53**, 1515 (1992)
3. P. Monthoux, D. Pines, Phys. Rev. B **47**, 6069 (1993)
4. A.J. Millis, H. Monien, D. Pines, Phys. Rev. B **42**, 167 (1990)
5. B.P. Stojkovic, D. Pines, Phys. Rev. B **55**, 8576 (1997)
6. V. Barzykin, D. Pines, Phys. Rev. B **52**, 13585 (1995)
7. E.M. Motoyama, G. Yu, I.M. Vishik, O.P. Vajk, P.K. Mang, M. Greven, Nature **445**, 186 (2007)
8. T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer, Berlin, 1985)
9. N.E. Bickers, S.R. White, Phys. Rev. B **43**, 8044 (1991)
10. T. Dahm, L. Tewordt, Phys. Rev. B **52**, 1297 (1995)
11. T. Takimoto, T. Moriya, J. Phys. Soc. Jpn. **67**, 3570 (1994)
12. S. Koikegami, S. Fujimoto, K. Yamada, J. Phys. Soc. Jpn. **66**, 1438 (1997)
13. H. Kontani, K. Ueda, Phys. Rev. Lett. **80**, 5619 (1998)
14. S. Wermbter, Phys. Rev. B **55**, R10149 (1997)
15. D. Manske, I. Eremin, K.H. Bennemann, Phys. Rev. B **67**, 134520 (2003)
16. H. Kontani, M. Ohno, Phys. Rev. B **74**, 014406 (2006)
17. H. Kontani, M. Ohno, J. Magn. Magn. Mater. **310**, 483 (2007)
18. J. Yu, S. Massidda, A.J. Freeman, D.D. Koelling, Phys. Lett. A **122**, 203 (2012)
19. S. Massidda, N. Hamada, J. Yu, A.J. Freeman, Phys. C **157**, 571 (1989)
20. A.J. Freeman, J. Yu, Phys. B **150**, 50 (1988)
21. J.-H. Xu, T.J. Watson-Yang, J. Yu, A.J. Freeman, Phys. Lett. A **120**, 489 (1987)
22. J.C. Campuzano, G. Jennings, M. Faiz, L. Beaulaigue, B.W. Veal, J.Z. Liu, A.P. Paulikas, K. Vandervoort, H. Claus, R.S. List, A.J. Arko, R.J. Bartlett, Phys. Rev. Lett. **64**, 2308 (1990)
23. N.P. Armitage, D.H. Lu, C. Kim, A. Damascelli, K.M. Shen, F. Ronning, D.L. Feng, P. Bogdanov, Z.-X. Shen, Phys. Rev. Lett. **87**, 147003 (2001)
24. N.P. Armitage, F. Ronning, D.H. Lu, C. Kim, A. Damascelli, K.M. Shen, D.L. Feng, H. Eisaki, Z.-X. Shen, P.K. Mang, N. Kaneko, M. Greven, Y. Onose, Y. Taguchi, Y. Tokura, Phys. Rev. Lett. **88**, 257001 (2002)
25. A. Ino, C. Kim, M. Nakamura, T. Yoshida, T. Mizokawa, A. Fujimori, Z.-X. Shen, T. Kakeshita, H. Eisaki, S. Uchida, Phys. Rev. B **65**, 094504 (2002)
26. T. Tanamoto, H. Kohno, H. Fukuyama, J. Phys. Soc. Jpn. **61**, 1886 (1992)

27. H. Kontani, K. Kanki, K. Ueda, Phys. Rev. B **59**, 14723 (1999)
28. M. Lindroos, S. Sahrakorpi, V. Arpiainen, R.S. Markiewicz, A. Bansil, J. Phys. Chem. Solids **67**, 244 (2006)
29. G. Baym, L.P. Kadanoff, Phys. Rev. **124**, 287 (1961)
30. G. Baym, Phys. Rev. **127**, 1391 (1962)
31. H. Kino, H. Kontani, J. Phys. Soc. Jpn. **67**, 3691 (1998)
32. H. Kondo, T. Moriya, J. Phys. Soc. Jpn. **67**, 3695 (1998)
33. J. Schmalian, Phys. Rev. Lett. **81**, 4232 (1998)
34. H. Kino, H. Kontani, T. Miyazaki, J. Phys. Soc. Jpn. **73**, 25 (2004)
35. H. Kino, H. Kontani, T. Miyazaki, J. Phys. Soc. Jpn. **75**, 104702 (2006)
36. S. Onari, R. Arita, K. Kuroki, H. Aoki, Phys. Rev. B **68**, 024525 (2003)
37. P. Nozières, *Theory of Interaction Fermion Systems* (Benjamin, New York, 1964)
38. A.A. Abrikosov, L.P. Gor'kov, I.E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975)
39. T. Moriya, K. Ueda, Adv. Phys. **49**, 555 (2000)
40. K. Yamada, *Electron Correlation in Metals* (Cambridge University Press, Cambridge, 2004)
41. R. Hlubina, T.M. Rice, Phys. Rev. B **51**, 9253–9260 (1995)
42. A. Damascelli, Z. Hussain, Z.-X. Shen, Rev. Mod. Phys. **75**, 473 (2003)
43. H. Kohno, K. Yamada, Prog. Theor. Phys. **85**, 13 (1991)
44. A. Rosch, Phys. Rev. Lett. **82**, 4280 (1999)
45. Ch. Renner, B. Revaz, J.-Y. Genoud, K. Kadowaki, Ø. Fischer, Phys. Rev. Lett. **80**, 149 (1998)
46. N. Miyakawa, P. Guptasarma, J.F. Zasadzinski, D.G. Hinks, K.E. Gray, Phys. Rev. Lett. **80**, 157 (1998)
47. R.M. Distasupil, M. Oda, N. Momono, M. Ido, J. Phys. Soc. Jpn. **71**, 1535 (2002)
48. T. Sato, T. Yokoya, Y. Naitoh, T. Takahashi, K. Yamada, Y. Endoh, Phys. Rev. Lett. **83**, 2254 (1999)
49. M. Takigawa, A.P. Reyes, P.C. Hammel, J.D. Thompson, R.H. Heffner, Z. Fisk, K.C. Ott, Phys. Rev. B **43**, 247–1991 (1991)
50. H. Alloul, T. Ohno, P. Mendels, Phys. Rev. Lett. **63**, 1700 (1989)
51. K. Ishida, Y. Kitaoka, G-q Zheng, J. Phys. Soc. Jpn. **60**, 3516 (1991)
52. D.C. Johnston, Phys. Rev. Lett. **62**, 957 (1989)
53. M. Oda, H. Matsuki, M. Ido, Solid State Commun. **74**, 1321 (1990)
54. B. Holm, F. Aryasetiawan, Phys. Rev. B **56**, 12825 (1997)
55. B. Holm, U. von Barth, Phys. Rev. B **57**, 2108 (1998)
56. P. Garcia-Gonzalez, R.W. Godby, Phys. Rev. B **63**, 075112 (2001)
57. J. Schmalian, D. Pines, B. Stojkovi, Phys. Rev. B **60**, 667 (1999)
58. J. Schmalian, D. Pines, B. Stojkovi, Phys. Rev. Lett. **80**, 3839 (1998)
59. S. Fujimoto, J. Phys. Soc. Jpn. **71**, 1230 (2002)
60. H. Ikeda, S. Shinkai, K. Yamada, submitted to J. Phys. Soc. Jpn. (2007)
61. S. Shinkai, H. Ikeda, K. Yamada, J. Phys. Soc. Jpn. **74**, 2592 (2005)
62. S. Shinkai, H. Ikeda, K. Yamada, J. Phys. Soc. Jpn. **75**, 104712 (2006)
63. T. Nomura, K. Yamada, J. Phys. Soc. Jpn. **69**, 3678 (2000)
64. T. Nomura, K. Yamada, J. Phys. Soc. Jpn. **71**, 1993 (2002)
65. M. Vilk, A.-M.S. Tremblay, J. Phys. I France **7**, 1309 (1997)
66. H. Kusunose, J. Phys. Soc. Jpn. **75**, 054713 (2006)
67. T. Saso, J. Phys. Soc. Jpn. **68**, 3941 (1999)

Transport Phenomena in Strongly Correlated Fermi
Liquids

Kontani, H.

2013, XI, 173 p. 64 illus., Hardcover

ISBN: 978-3-642-35364-2