Cu hyperfine coupling constants of HgBa$_2$CaCu$_2$O$_{6+\delta}$

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Abstract. We estimated the ratios of $^{63}$Cu hyperfine coupling constants in the double-layer high-$T_c$ superconductor HgBa$_2$CaCu$_2$O$_{6+\delta}$ from the anisotropies in Cu nuclear spin-lattice relaxation rates and spin Knight shifts to study the nature of the ultraslow fluctuations causing the $T_2$ anomaly in the Cu nuclear spin-echo decay. The ultraslow fluctuations may come from uniform magnetic fluctuations spread around the wave vector $q = 0$, otherwise the electric origins.

1. Introduction
Spin polarized neutron scattering experiments indicate the emergence of an intra-unit-cell (IUC) $q = 0$ magnetic moments in the pseudogap states of the high-$T_c$ cuprate superconductors, while no NMR and $\mu$SR experiment indicates any static ordering of local magnetic moments [1]. The IUC moments are associated with the loop current ordered state [2]. Recently discovered ultraslow fluctuations in the pseudogap states of HgBa$_2$CaCu$_2$O$_{6+\delta}$ (Hg1212) via $^{63}$Cu nuclear spin-echo decay experiments [3] might reconcile an issue on the IUC moments. No wipeout effect on NMR spectra is characteristic of the ultraslow fluctuations of Hg1212, in contrast to the spin-charge stripe orderings [4, 5].

Knowledge of the hyperfine coupling constants helps us to clarify the nature of the local field fluctuations in NMR measurements [6]. In this paper, we report the estimation of the $^{63}$Cu hyperfine coupling constants in the double-CuO$_2$-layer high-$T_c$ superconductors Hg1212 from the anisotropies in $^{63}$Cu nuclear spin-lattice relaxation rates and spin Knight shifts [7], and discuss the nature of the ultraslow fluctuations [3].

2. Estimations of $^{63}$Cu hyperfine coupling constants
The $^{63}$Cu hyperfine coupling parameters ($A_{cc}^{bf}$ and $A_{ab}^{bf}$) consist of the anisotropic on-site $A_{cc}$ (the $c$ axis component) and $A_{ab}$ (the $ab$ plane component) due to the 3$d$ electrons and the isotropic supertransferred component $B$($>0$) [6]. The ratios of the individual components in the three coupling constants can be estimated from the anisotropy data [7] of the $^{63}$Cu Knight shifts ($^{63}K_{cc}$ and $^{63}K_{ab}$) and the $^{63}$Cu nuclear spin-lattice relaxation rates [(1/$T_1$)$_{cc}$ and (1/$T_1$)$_{ab}$] via the antiferromagnetic dynamical spin susceptibility [6, 8, 9, 10, 11].
of cc or ab of $^{63}K$ and $1/T_1$ indicate the direction of a static magnetic field applied along the c axis or in the $ab$ plane. The procedure to estimate the coupling constant ratios is shown below.

2.1. $^{63}$Cu Knight shifts
The $^{63}$Cu Knight shifts $^{63}K_{cc,ab}$ at a magnetic field along the c axis or in the $ab$ plane are the sum of the spin shift $K_{spin}$ and the orbital shift $K_{orb}$ as $^{63}K_{cc,ab} = K_{spin}^{cc,ab} + K_{orb}^{cc,ab}$. The spin shift is $K_{spin}^{cc,ab}(T) = A_{cc,ab}^{hf} \chi_{cc;ab}^{spin}(T)$ with the hyperfine coupling parameters $A_{cc,ab}^{hf}$ and the uniform spin susceptibility $\chi_{cc;ab}^{spin}(T)$. For a temperature-dependent isotropic spin susceptibility $\chi_s^{cc} = \chi_s^{ab}$, the ratio $\Delta K_{spin}^{cc} / \Delta K_{spin}^{ab} = (dK_{spin}^{cc} / dT) / (dK_{spin}^{ab} / dT)$ is equal to the ratio $A_{cc,ab}^{hf} / A_{ab}^{hf}$.

Figure 1 shows $^{63}K_{cc}$ plotted against $^{63}K_{ab}$ with temperature as an implicit parameter for Hg1212 from underdoped to overdoped, which are adopted from [7]. The solid straight lines are the least-squares fitting results. The dashed straight line for overdoped Hg1212 is a visual guide with assuming the same slope as the optimally doped Hg1212. The straight lines show nearly parallel shift. Since the orbital shifts of $K_{orb} = 1.14-1.16$ % and $K_{orb} = 0.19-0.20$ % are estimated below $T_c$, then the parallel shift indicates a constant spin component above $T_c$. Similar parallel shift is found in the single crystal NMR for HgBa$_2$CuO$_{4+\delta}$ [12].

An easy plane magnetic anisotropy causes such a constant spin component in the paramagnetic spin susceptibility [13]. The anisotropic superexchange interaction in the $S = 1/2$ XXZ Heisenberg Hamiltonian yields the easy plane anisotropy in the paramagnetic state [14, 15]. The optimally hole doping makes the anisotropy weak [13, 16]. Although the multicomponents in the spin susceptibility are suggested from the anisotropic spin Knight shifts [12, 17], we believe that the doped superconductors with a single spin component can show a finite anisotropy and that the constant spin component does not impede a single spin component analysis to estimate the Cu hyperfine coupling constants.

The $^{63}$Cu hyperfine coupling parameters $A_{cc}^{hf}$ and $A_{ab}^{hf}$ are expressed by $A_{cc}$, $A_{ab}$, and $B$ as $A_{cc}^{hf} = A_{cc} + 4B$ and $A_{ab}^{hf} = A_{ab} + 4B$ [6, 8, 18]. Then, the anisotropy ratio $r_u$ of the
temperature-dependent $K_s^{cc}$ and $K_s^{ab}$ is given by

$$r_u = \frac{\Delta K_s^{cc}}{\Delta K_s^{ab}} = \frac{A_{cc} + 4B}{A_{ab} + 4B}. \quad (1)$$

Figure 1 shows $r_u = 0.31$ for the underdoped and $0.34$ for the optimally doped samples. The value of $r_u = 0.34$ is assumed for the overdoped sample.

2.2. $^{63}$Cu nuclear spin-lattice relaxation rate

Figure 2 shows the ratio of $^{63}(1/T_1)_{ab}/^{63}(1/T_1)_{cc}$ plotted against temperature for Hg1212 from underdoped to overdoped (adopted from Ref. [7]). The anisotropy ratio $r_{AF}$ of $(1/T_1)_{ab}$ and $(1/T_1)_{cc}$ is given by

$$r_{AF} = \frac{(1/T_1)_{ab}}{(1/T_1)_{cc}} \approx \frac{1}{2} \left( 1 + \left( \frac{A_{cc} - 4B}{A_{ab} - 4B} \right)^2 \right), \quad (2)$$

for the leading term of the enhanced antiferromagnetic susceptibility [11]. For convenience, we introduce an alternative parameter of $r_A = \sqrt{2r_{AF} - 1}$. We adopted the values of $r_{AF}$ ($r_A$) = 2.3 (1.90), 2.0 (1.73), and 1.8 (1.61) from underdoped to overdoped (figure 2) to estimate the coupling constant ratios.

2.3. $^{63}$Cu hyperfine coupling constant ratios

From the constraints of $A_{cc} < 0$ [18] and $A_{ab}/4B < 1$ on (1) and (2), we obtain the expressions of the ratios of the $^{63}$Cu hyperfine coupling constants,

$$\frac{A_{cc}}{4B} \approx -\frac{r_A + r_u - 2r_{AF}r_u}{r_A - r_u}, \quad (3)$$

$$\frac{A_{ab}}{4B} \approx \frac{r_A + r_u - 2}{r_A - r_u}, \quad (4)$$

and then

$$\frac{A_{ab}}{A_{cc}} \approx -\frac{r_A + r_u - 2}{r_A + r_u - 2r_{AF}r_u}. \quad (5)$$

Thus, (3)-(5) with a set of $r_u$ and $r_A$ enable us to estimate the ratios of the $^{63}$Cu hyperfine coupling constants.

Table 1 shows the estimated ratios of $A_{cc}/4B$, $A_{ab}/4B$ and $A_{ab}/A_{cc}$ for Hg1212 from (3)-(5) with the experimental $r_u$ and $r_{AF}$ in figures 1 and 2. The on-site coupling ratio $A_{ab}/A_{cc}$ depends on the hole concentration in Hg1212.

Table 1. Anisotropies ($r_u$ and $r_{AF}$) of $^{63}K_s$ and $^{63}T_1$, and the ratios of $^{63}$Cu hyperfine coupling constants ($A_{cc}$, $A_{ab}$, $B$) for underdoped (un), optimally doped (op) and overdoped (ov) Hg1212. $T_c$ is in kelvin. The value of $r_u$ for overdoped Hg1212 is assumed after the optimally doped value in figure 1.

| $T_c$ | $r_u$ | $r_{AF}$ | $A_{cc}/4B$ | $A_{ab}/4B$ | $A_{ab}/A_{cc}$ |
|------|------|---------|-------------|-------------|----------------|
| un   | 103  | 0.31    | 2.3         | -0.65       | +0.13          | -0.20          |
| op   | 127  | 0.34    | 2.0         | -0.64       | +0.05          | -0.078         |
| ov   | 93   | 0.34    | 1.8         | -0.67       | -0.04          | +0.058         |
The 3d\((x^2 - y^2)\) orbital electron of Cu\(^{2+}\) in the tetragonal crystal field produces the on-site hyperfine fields. The ratio \(A_{ab}/A_{cc}\) is expressed as

\[
\frac{A_{ab}}{A_{cc}} \approx -\frac{-\kappa + \frac{2}{7} - \frac{11}{7} \gamma}{-\kappa - \frac{4}{7} - \frac{62}{7} \gamma},
\]

where \(\kappa(> 0)\) is the core polarization parameter, \(\frac{2}{7}\) and \(-\frac{4}{7}\) are the spin-dipole field coefficients, and \(\gamma(< 0)\) is the spin-orbit coupling parameter [9, 19, 20]. The empirical values of \(\kappa = 0.25\) and 0.325 were estimated for Cu\(^{2+}\) ions in the dilute copper salts [20]. The first-principles cluster calculations give \(\kappa = 0.265\) (un), 0.315 (op) and 0.387 (ov), assuming \(\gamma = 0.044\) [9, 19].

2.4. \(^{63}\)Cu hyperfine coupling constants of HgBa\(_2\)CuO\(_{4+\delta}\) and Hg1212

Let us show the \(^{63}\)Cu hyperfine coupling constants of the optimally doped single-CuO\(_2\)-layer superconductor HgBa\(_2\)CuO\(_{4+\delta}\) (\(T_c = 98\) K). From the uniform spin susceptibility \(\chi_s = 1.47 \times 10^{-4}\) emu/mole-f.u. [23] and the in-plane \(^{63}\)Cu \(K_{spin}^{ab} = 0.48\%\) [24], we estimated the in-plane \(^{63}\)Cu hyperfine coupling parameter \(A_{ab}^{hf} = A_{ab} + 4B = (N_A \mu_B/\chi_s)K_{spin}^{ab} = 182\) kOe/\(\mu_B\) for HgBa\(_2\)CuO\(_{4+\delta}\) (\(N_A\) is Avogadro’s number and \(\mu_B\) is the Bohr magneton). Substituting \(r_u = 0.53\) and \(r_{AF} = 1.8\) [24] into (3)-(5) and using \(A_{ab} + 4B = 182\) kOe/\(\mu_B\), we obtained the values

\[
A_{cc} = -65, \quad A_{ab} = 21, \quad \text{and} \quad B = 40 \text{ kOe/}\mu_B
\]

for the optimally doped HgBa\(_2\)CuO\(_{4+\delta}\).

By adopting \(A_{ab} + 4B = 182\) kOe/\(\mu_B\) for Hg1212 after HgBa\(_2\)CuO\(_{4+\delta}\), we estimated the individual components of \(A_{cc}, A_{ab}, \text{and} B\) (Table 2). Figure 3 shows \(A_{cc}, A_{ab}, \text{and} B\) (Table 2) plotted against the hole concentration \(P_{sh}\) [7] for Hg1212. In Table 2 and figure 3, with increase in the hole concentration, the absolute value of the negative \(A_{cc}\) increases, \(A_{ab}\) shows a sign change, and the \(B\) term slightly increases.

The reported \(B\) term is in the range from 36 to 155 kOe/\(\mu_B\) in the other cuprate superconductors [10, 25, 26, 27, 28], assuming \textit{a priori} the fixed values of \(A_{cc} = -170\) and \(A_{ab} = 37\) kOe/\(\mu_B\) [25, 27, 28]. The cation-cation supertransferred hyperfine field \(B\) between 3d and 4s orbitals depends on the strength of the \(p-d\) covalent bond parameter [29]. The doping dependent \(B\) term in Table 2 indicates the development of the covalency with the hole concentration in Hg1212.

Table 2. \(^{63}\)Cu hyperfine coupling constants in units of kOe/\(\mu_B\) for underdoped (un), optimally doped (op) and overdoped (ov) Hg1212, assuming \(A_{ab} + 4B = 182\) kOe/\(\mu_B\).

|        | \(A_{cc}\) | \(A_{ab}\) | \(B\) |
|--------|---------|---------|-----|
| un     | -105    | +21     | 40  |
| op     | -111    | +8.7    | 43  |
| ov     | -127    | -7.4    | 47  |
3. Local field fluctuations in $^{63}\text{Cu}$ nuclear spin-echo decay rate $1/T_{2L}$

3.1. $^{63}\text{Cu}$ nuclear spin-echo decay rate $1/T_{2L}$

Figures 4(a)–4(c) show the $^{63}\text{Cu}$ nuclear spin-echo decay rates $(1/T_{2L})_{cc,ab}$’s for Hg1212 from underdoped (a), optimally doped (b) and overdoped (c) [3]. The notations conform to those in [3]. The enhancements in $(1/T_{2L})_{cc,ab}$ at 220–240 K indicate the ultraslow fluctuations [3]. The peak temperature of $(1/T_{2L})_{cc}$ is nearly independent of the doping level, but the enhancement is suppressed by overdoping.

Figure 4(d) shows the anisotropy ratio of the local field fluctuations $\Delta J_{cc}/\Delta J_{ab} = [(1/T_{2L})_{cc} - (1/T_{2L})_{ab}]/[(1/T_{2L})_{ab} - (1/T_{2L})_{cc}]$ derived from $1/T_{2L}$ and $1/T_{1}$ (Redfield’s $1/T_{2L}$) [3]. $\Delta J_{\gamma\gamma}$ ($\gamma = cc$ and $ab$) expresses the additional fluctuations causing the enhancement in $1/T_{2L}$. One should note that $\Delta J_{cc}/\Delta J_{ab} < 1$ is characteristic of the ultraslow fluctuations.

Figure 4(e) shows the phase diagram of Hg1212, where the superconducting transition temperature $T_c$, the pseudo spin-gap temperature defined by the maximum temperature of $1/T_{2L}$, the pseudo spin-gap temperature defined by the peak temperature of $1/T_{2L}$ [7] (open triangles) against hole concentration $P_{sh}$. The dotted curve with a shaded region is a visual guide for the onset temperature $T^*$ of decrease in $^{63}\text{Cu}$ Knight shift [7]. Nearly AF stands for the Curie-Weiss law in Cu $1/T_1T$ [7].
1/${T_1}T$, $T_p$ defined by the peak temperature of $(1/T_{2L})_{cc}$, and the onset temperature $T^*$ of the decrease in the Cu Knight shift are plotted against the hole concentration $P_{sh}$ in Cu$^{2+}$P$_{sh}$ [3, 7]. With hole doping, $T^*$ decreases, while $T_p$ is nearly independent of the hole concentration $P_{sh}$. The ultraslow fluctuations emerge in the underdoped regime and diminish in the overdoped regime.

3.2. Local field fluctuations

Local field fluctuations of $J_{ab}$ ($B \perp c$ axis) and $J_{cc}$ ($B || c$ axis) causing the nuclear spin relaxations of $T_1$ and $T_2$ are defined by

$$J_{\gamma \gamma} = \sum_q F_{\gamma \gamma}(q) S(q, \nu_n),$$

(7)

$$F_{\gamma \gamma}(q) \equiv (4B)^2 f_{\gamma \gamma}(q) = [A_{\gamma \gamma} + 2B(\cos(q_x) + \cos(q_y))]^2,$$

(8)

where $\gamma = ab$ and $cc$, and $\nu_n$ is an NMR frequency [3]. The electron spin-spin correlation function $S(q, \nu)$ (a frequency $\nu$) is related to the dynamical spin susceptibility $\chi''(q, \nu)$ through the fluctuation-dissipation theorem. $F_{\gamma \gamma}(q)$ is called the form factor of the wave vector $q$ dependent hyperfine coupling constant, whose filtering effects in the $q$ space play a significant role in the anisotropy and the site differentiation on NMR [8, 9, 10]. $\Delta J_{\gamma \gamma}$ expresses the additional fluctuations to $J_{\gamma \gamma}$ [3].

Figure 5 shows the $q$ dependence of $f_{ab, cc}(q)$ for Hg1212 along the diagonal $q = (q, q)$ in the first Brillouin zone, using the estimated coupling constant ratios in Table 1. Since $f_{cc}(\pi, \pi) > f_{ab}(\pi, \pi$, the antiferromagnetic spin fluctuation $\chi'(q)$ localized around $q = [\pi, \pi]$ leads to the anisotropy $J_{cc}/J_{ab} \approx 3$ in contrast to the experimental ratio $\Delta J_{cc}/\Delta J_{ab} < 1$ in figure 4(d) [3]. $\Delta J_{\gamma \gamma}$ expresses the development of the ultraslow fluctuations [3]. Thus, the antiferromagnetic fluctuations are excluded from the ultraslow fluctuations.

Let us assume a toy model of $\chi'(q, \nu_n) = \chi_0^d \Theta(q_c - |q_x|) \Theta(q_c - |q_y|)$ ($\Theta(x)$ is the Heaviside step function). $q_c$ is a cut-off wave number. $\chi'(q) \propto S(q, \nu_n)$ takes a constant value $\chi_0^d$ over

![Figure 5. $^{63}$Cu hyperfine coupling form factors $f_{cc}(q)$ and $f_{ab}(q)$ as functions of $q$ in the wave vector $q = (q, q)$ $[(0, 0) \rightarrow (\pi, \pi)]$. Inset shows the diagonal in the first Brillouin zone.](image1)

![Figure 6. $\Delta J_{cc}/\Delta J_{ab}$ as a function of the cut-off $q_c$ in a toy model upon a static spin susceptibility $\chi'(q) = \chi_0^d \Theta(|q_x| < q_c)$ and 0 ($|q_x| > q_c$). Experimental constraint leads to $q_c < 2.3$.](image2)
\[ |q_{x,y}| < q_c. \] For this toy model, the ratio \( \Delta J_{cc}/\Delta J_{ab} \) is calculated as

\[
\frac{\Delta J_{cc}}{\Delta J_{ab}} = \frac{\sum_{|q_{x,y}|<q_c} f_{cc}(q)}{\sum_{|q_{x,y}|<q_c} f_{ab}(q)}.
\] (9)

Figure 6 shows the numerical \( \Delta J_{cc}/\Delta J_{ab} \) as a function of \( q_c \). The experimental \( \Delta J_{cc}/\Delta J_{ab} < 0.9 \) in figure 4(d) imposes on the function in figure 6 and then leads to \( q_c < 2.3 \). The magnetic ultraslow fluctuations must be confined within \( q_c < 2.3 \). If the magnetic ultraslow fluctuations have the easy plane anisotropy, the upper limit of the cut-off value \( q_c \) will be smaller than 2.3. Thus, we obtained a model constraint on the magnetic ultraslow fluctuations, using the anisotropic hyperfine coupling constants.

Although the step function \( \chi(q) \) with \( q_c < 2.3 \) is not localized at \( q = 0 \), it is parallel to the IUC \( q = 0 \) magnetic moments observed by the spin polarized neutron scattering method [1]. The ultraslow fluctuations may be associated with the IUC \( q = 0 \) magnetic moments. However, if the enhancement in \( 1/T_2L \) is due to quadrupole fluctuations, one should explore the alternative fluctuations of charge or lattice for the electric ultraslow fluctuations.

4. Conclusions
The systematic hole doping dependences of the \(^{63}\text{Cu} \) hyperfine coupling constants (\( A_{cc}, A_{ab} \) and \( B \)) were found for Hg1212 from underdoped to overdoped. A model constraint on the magnetic ultraslow fluctuations in Hg1212 was derived from the anisotropy ratios of the \(^{63}\text{Cu} \) hyperfine coupling constants. The model expresses the magnetic fluctuations spread around \( q = 0 \). Possible electric ultraslow fluctuations causing the \( T_2 \) anomaly remain to be explored.

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