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Magnetic Resonance Either in Normal or Superconducting Species. Spin-Lattice Relaxation Time

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The spin-lattice relaxation time T_1 either in the superconducting and normal phases is investigated by the use of the Green's function method. The lattice, in this case, means the conduction electrons and the interaction is mainly due to the Fermi contact term. Electrons and nuclei are treated on the same footing, namely both are in the second quantized form. The coherent terms are summarized in a general fashion at the beginning.

In the BCS superconductor, the spin-lattice relaxation time (rate-constant) in considerably enhanced just below the critical temperature. This phenomenon has been observed and explained by Hebel and Slichter,[1] and it is one of the great triumphs of the BCS theory. However, in the recent observation of the high-temperature superconductor (HTS), or the copper oxide superconductor, this enhancement is lost. One of the probable origins of this is told that the pair working in this species is the d wave. Before the detailed analysis, it seems necessary to prepare the relaxation theory in the magnetic resonance useful not only for the normal state but also for the superconducting state.

Let us begin by reviewing the coherent factors in the theory of superconductivity from which the Slichter enhancement is explained.[2—4] The BCS ground state of the superconductor is written as

$$|0_{\mathrm{BCS}}>=\prod_k(u_k+v_kc^+_{k\uparrow}c^+_{-k\downarrow}|0>,$$

where c^+ and c are respectively the creation and annihilation operators for the true vacuum $|0>$, and u and v are the variation parameters. However, as is known,[2] c^+ and c are no longer the creation and annihilation operators for the BCS vacuum $|0_{\mathrm{BCS}}>$, but the operators for the quasi-particles introduced by the Bogoliubov transformation bear such roles.

$$\begin{pmatrix}\alpha_{k\uparrow}\\ \alpha^+_{-k\downarrow}\end{pmatrix}=\begin{pmatrix}u_k & v_k\\ -v_k & u_k\end{pmatrix}\begin{pmatrix}a_{k\uparrow}\\ a^+_{-k\downarrow}\end{pmatrix}.$$

When we describe various properties of the superconducting state in terms of the quasi-particle operators, the cross terms, u and v yield new effects. The coherent terms arise from these cross terms.

The external perturbation on the electron is written as

$$H'=\sum_{k\sigma,k'\sigma'}B_{k\sigma,k'\sigma'}c^+_{k\sigma}c_{k'\sigma'},\tag{1}$$

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where $B_{k\sigma,k'\sigma'}$ is the matrix element of the perturbing operator. When we rewrite $c^+_{k\sigma}$ and $c^+_{k\sigma}$ etc. by the Bogoliubov operators, various combinaitons of u and v arise. These are called the coherent factors.

The first condition for classification is the behavior under the time reversal: The time reversal to the above, $B_{-k'-\sigma',-k-\sigma}$ has the same absolute value but the phase is the same or the reverse. Combining this with the spin flip–flop, we can classify as follows:

1±. The spin flip–flop does not arise,

$$B_{k\sigma,k'\sigma}(c^+_{k\sigma}c_{k'\sigma}\pm c^+_{-k'-\sigma}c_{-k-\sigma}).$$

2±. The spin flip–flop does arise,

$$B_{k\sigma,k'-\sigma}(c^+_{k\sigma}c_{k'-\sigma}\pm c^+_{-k'\sigma}c_{-k-\sigma}).$$

The extended Nambu representation is introduced: for the ordinary states,

$$c^+_k=(c^+_{k\uparrow}\ c_{-k\downarrow}\ c_{-k\uparrow}\ c^+_{k\downarrow}),\qquad c_k=\begin{pmatrix}c_{k\uparrow}\\ c^+_{-k\downarrow}\\ c^+_{-k\uparrow}\\ c_{k\downarrow}\end{pmatrix},\tag{2}$$

and for the quasi-particles,

$$\gamma^+_k=(\gamma^+_{k\uparrow}\ \gamma_{-k\downarrow}\ \gamma_{-k\uparrow}\ \gamma^+_{k\downarrow}),\qquad \gamma_k=\begin{pmatrix}\gamma_{k\uparrow}\\ \gamma^+_{-k\downarrow}\\ \gamma^+_{-k\uparrow}\\ \gamma_{k\downarrow}\end{pmatrix}.\tag{3}$$

These are connected by the Bogoliubov transformation with each other as,

$$\gamma_k=U_k\boldsymbol{c}_k,\qquad \gamma^+_k=\boldsymbol{c}_kU^+_k,\tag{4}$$

where

$$U_k = \begin{pmatrix} \boldsymbol{u}_k & 0 \\ 0 & \boldsymbol{u}_k^+ \end{pmatrix}, \quad \text{with } \boldsymbol{u}_k = \begin{pmatrix} u_k & v_k \\ -v_k & u_k^+ \end{pmatrix}. \tag{5}$$

It is instructive to manipulate:
Case 1+.

$$\sum_\sigma (c^+_{k\sigma}c_{k'\sigma} + c^+_{-k'-\sigma}c_{-k-\sigma}) = \boldsymbol{c}_k^+\Sigma^3\boldsymbol{c}_{k'} = \gamma_k^+ U_k \Sigma^3 U^+_{k'}\gamma_{k'}, \tag{6}$$

where

$$\Sigma^3 = \begin{pmatrix} \sigma^3 & \\ & -\sigma^3 \end{pmatrix}. \tag{7}$$

This is the 4-4 matrix manipulation; however, it is enough to note the upper half of the result.

The upper half of Eq. 6

$$\begin{aligned} &= (c^+_{k\uparrow}\ c_{-k\downarrow}) \begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix} c_{k'\uparrow} \\ c^+_{-k'\downarrow}\end{pmatrix} \\ &= (\gamma^+_{k\uparrow}\ \gamma_{-k\downarrow})\begin{pmatrix}u&v\\-v&u\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix} \\ &\qquad \begin{pmatrix}u'&-v'\\v'&u'\end{pmatrix}\begin{pmatrix}\gamma_{k'\uparrow}\\ \gamma^+_{-k'\downarrow}\end{pmatrix}\\ &= (\gamma^+_{k\uparrow}\ \gamma_{-k\downarrow})\begin{pmatrix} uu'-vv' & -uv'-vu' \\ -vu'-uv' & vv'-uu'\end{pmatrix}\begin{pmatrix}\gamma_{k\uparrow}\\ \gamma^+_{-k'\downarrow}\end{pmatrix}, \end{aligned} \tag{8}$$

where u and v are abbreviations of u_k and v_k respectively, while u' and v' are those of $u_{k'}$ and $v_{k'}$. Similarly
Case 1−.

$$\sum_\sigma (c^+_{k\sigma}c_{k'\sigma} - c^+_{-k'-\sigma}c_{-k-\sigma}) = \boldsymbol{c}_k^+\mathbf{1}\boldsymbol{c}_{k'} = \gamma_k^+U_k\mathbf{1}U^+_{k'}\gamma_{k'}. \tag{9}$$

The upper half of the above is,

$$= (\gamma^+_{k\uparrow}\ \gamma_{-k\downarrow})\begin{pmatrix} uu'+vv' & -uv'+vu' \\ -vu'+uv' & vv'+uu'\end{pmatrix}\begin{pmatrix}\gamma_{k'\uparrow}\\ \gamma^+_{-k'\downarrow}\end{pmatrix}. \tag{10}$$

In the quasi-particle representation of Eqs. 8 and 10, the diagonal elements refer to the scattering terms, while the off-diagonal elements correspond to the pair creation of particle and hole. These matrix elements are called the coherent factors.

Let us turn to the case where the spin flip–flop is allowed.
Case 2+.

$$\begin{aligned}\sum_\sigma (c^+_{k\sigma}c_{k'-\sigma} + c^+_{-k'\sigma}c_{-k-\sigma}) &= \boldsymbol{c}_k^+\Sigma^J\boldsymbol{c}_{k'} \\ &= \gamma_k^+U_k\Sigma^J U^+_{k'}\gamma_{k'}. \end{aligned}\tag{11}$$

This relation connects the left half of γ_k^+ and the lower half of $\gamma_{k'}$, giving

$$= (\gamma^+_{k\uparrow}\ \gamma_{-k\downarrow})\begin{pmatrix} uu'+vv' & uv'-vu' \\ -vu'+uv' & -vv'-uu'\end{pmatrix}\begin{pmatrix}\gamma_{-k'\uparrow}\\ \gamma^+_{k'\downarrow}\end{pmatrix}. \tag{12}$$

Case 2−.

$$\begin{aligned}\sum_\sigma (c^+_{k\sigma}c_{k'-\sigma} - c^+_{-k'\sigma}c_{-k-\sigma}) &= \boldsymbol{c}_k^+\boldsymbol{J}\boldsymbol{c}_{k'} \\ &= \gamma_k^+U_k\boldsymbol{J}U^+_{k'}\gamma_{k'} \end{aligned}\tag{13}$$

This relation also connects the left half of γ_k^+ and the lower half of $\gamma_{k'}$, and we have

$$= (\gamma^+_{k\uparrow}\ \gamma_{-k\downarrow})\begin{pmatrix} uu'-vv' & uv'+vu' \\ -vu'-uv' & -vv'+uu'\end{pmatrix}\begin{pmatrix}\gamma_{-k'\uparrow}\\ \gamma^+_{k'\downarrow}\end{pmatrix}. \tag{14}$$

Note that, in this case, the scattering terms are off diagonal, and the creation and annihilation terms are diagonal. Here

$$\Sigma^J = \begin{pmatrix} & & & 1 \\ & & -1 & \\ & -1 & & \\ 1 & & & \end{pmatrix} \quad \boldsymbol{J} = \begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{pmatrix}. \tag{15}$$

By the use of relations[2,3)]

$$\begin{aligned} u_k^2 &= \frac{1}{2}\left(1+\frac{\epsilon_k}{E_k}\right), \quad v_k^2 = \frac{1}{2}\left(1-\frac{\epsilon_k}{E_k}\right), \\ E_k^2 &= \epsilon_k^2 + \Delta_k^2, \end{aligned}\tag{16}$$

where Δ_k is the gap-energy, the coherent factors are expressed substantially:

$$\begin{aligned} 1\pm.\ (uu' \mp vv')^2 &= \frac{1}{2}\left(1+\frac{\epsilon_k\epsilon_{k'}}{E_kE_{k'}} \mp \frac{\Delta_k\Delta_{k'}}{E_kE_{k'}}\right), \\ 2\pm.\ (uv' \mp vu')^2 &= \frac{1}{2}\left(1 \mp \frac{\Delta_k\Delta_{k'}}{E_kE_{k'}}\right). \end{aligned}\tag{17}$$

In the case 1+, we have the ultra-sonic attenuation, while the electro-magnetic interaction is in the case 2+ and the magnetic resonance is in the case 2−.

***T_1* in NMR.** The detailed analysis of the spin-lattice relaxation time T_1 in the nuclear magnetic resonance will be discussed in the next section. At this stage the results are given briefly.

$$T_1 \approx \sum_{kk'} |B_{kk'}|^2\,\frac{1}{2}\left(1+\frac{\Delta_k\Delta_{k'}}{E_kE_{k'}}\right) n_k(1-n_{k'})\,\delta\,(E_k - E_{k'} - \omega), \tag{18}$$

where ω is the applied radio frequency, and n_k is the Fermi function. The summation can be converted to the integration, and further using the relation of state densities,

$$N(E)\mathrm{d}E = N(\epsilon)\mathrm{d}\epsilon,$$

then one gets

$$\frac{N(E)}{N(\epsilon)} = \frac{d\epsilon}{dE} = \begin{cases} \dfrac{E}{(E^2-\Delta^2)^{1/2}} & (E>\Delta) \\ 0 & (E<\Delta) \end{cases}, \tag{19}$$

Equation 18 is written, for $\omega \ll \Delta$, as

$$\begin{aligned} T_1 \approx |B|^2N^2(0)\int_\Delta^\infty \frac{1}{2}\left(1+\frac{\Delta^2}{E(E+\omega)}\right) \\ \times\frac{E(E+\omega)k_BT(-\partial n/\partial E)dE}{(E^2-\Delta^2)^{1/2}[(E+\omega)^2-\Delta^2]^{1/2}}, \end{aligned}\tag{20}$$

where the coupling constant and the state density are replaced by their suitable averages. This integral is divergent.

Therefore T_1 of the superconductor is strongly enhanced just below the critical temperature, as stated previously.

General

The spin-lattice relaxation time of the nuclear spin I^z is given by the imaginary part of the magnetic susceptibility χ_{zz}, which is equal to $(\chi_{+-}+\chi_{-+})/2$ in the spatially homogeneous system. Here the $\pm$ correspond to $(I^x \pm iI^y)/2$ respectively. The ensemble average of the change, $\delta < I^+(t) >$ is given by the linear response theory as

$$\delta < I^+(t) >= i\int_{-\infty}^{t} \mathrm{d}t' \mathrm{Tr}\{\rho_{\mathrm{G}}[H^{\mathrm{ex}}(t'), I^+(t)]_-\}, \tag{21}$$

where ρ_{G} is the grand canonical statistical operator; however, the chemical potential is not given explicitly unless otherwise stated. The rotating magnetic field causing the magnetic transition is, assuming a single mode for simplicity,

$$H^{\mathrm{ex}}(t) = H_{\mathrm{R}}(I^+(t)\mathrm{e}^{i\omega t} + I^-(t)\mathrm{e}^{-i\omega t}), \tag{22}$$

where H_{R} and ω are, respectively, intensity and frequency of the radiation field. We assume that, in the later treatments, the spin-lattice relaxation arises from the interaction between nuclear and electron spins; in other words, the electron spins play the role of the lattice system:[2)]

$$H' = h\gamma g\beta_{\mathrm{B}} F(R,r)\boldsymbol{I}\cdot\boldsymbol{S}, \tag{23}$$

where $F(R,r)$ is a function of spatial coordinates of the nucleus R and that of the electron, r. The term γ is the gyromagnetic ratio of the nucleus, g is the g factor of the electron and β_{B} is the Bohr magneton of the electron.

Now the second-quantizations of the above are carried out.[5)] First of all, the ortho-normalized wave function describing the nuclear behaviour, $\xi_K(R)|M>$ is introduced as

$$\begin{aligned}(H_N + H_M)\xi_K(R)|M> &= (\epsilon_K + M\epsilon_{KI})\xi_K(R)|M> \\ &\equiv \epsilon_{KM}\xi_K(R)|M>, \end{aligned}\tag{24}$$

where H_{N} is the spatial part and H_M the Zeeman part. Then we have

$$\begin{aligned} I^\alpha &\to \sum_{KMK'M'} < \xi_K(R)M|I^\alpha|\xi_{K'}(R)M' > a^+_{KM}a_{K'M'} \\ &= \sum_{KMK'M'} < M|I^\alpha|M' > a^+_{KM}a_{K'M'}\delta_{KK'}. \end{aligned}\tag{25}$$

In the present case, $\xi_K(R)$ does nothing since H_N in Eq. 24 is a constant for $\xi_K(R)$. A similar equaition for the electrons is

$$\begin{aligned}(H_S + H_m)\phi_k(r)|m> &= (\epsilon_k + m\epsilon_{kS})\phi_k(r)|m> \\ &\equiv \epsilon_{km}\phi_k(r)|m>, \end{aligned}\tag{26}$$

so that

$$\begin{aligned} H' \to h\gamma g\beta_B &\sum_{\alpha MM'mm'}\sum_{KK'kk'} < M|I^\beta|M' >< m|S^\alpha|m' > \\ &\times < \xi_K(R)\phi_k(r)|F(R,r)|\xi_{K'}(R)\phi_{k'}(r) > a^+_{KM}a_{K'M'}c^+_{km}c_{k'm'}. \end{aligned}\tag{27}$$

If the nuclear motion is that of a harmonic oscillator, a^+_{KM} and a_{KM} are the creation and annihilation operator of the vibrational excitation. When the nuclei carry non-integer spins, these are considered to obey the fermi statistics, or to satisfy the anti-commutation relation:

$$[a^+_{KM}, a_{K'M'}]_+ = \delta_{KK'}\delta_{MM'}. \tag{28}$$

However as will be seen in the following, this selection of statistics not fatal for the theory. It is needless to say that operators for electrons satisfy the anti-commutation relations.

The change of I^+ in Eq. 21 is now written as (retain the I^- term in Eq. 22)

$$\begin{aligned} \delta < I^+(t) > &= i\gamma H_R \int_{-\infty}^{t} \mathrm{d}t'\mathrm{e}^{-i\omega t'} \\ &\quad \times Tr\{\rho_G \sum_{KM} < M-1|I^-|M >< M|I^+|M-1 > \\ &\quad \times [a^+_{K,M-1}(t')a_{K,M}(t'), a^+_{K,M}(t)a_{K,M-1}(t)]_-\} \\ &= -\gamma H_R \int_{-\infty}^{t} \mathrm{d}t'\mathrm{e}^{-i\omega t'} D_{K,M-1,M}(t'-t) \\ &= -\frac{1}{2}\gamma H_R \mathrm{e}^{-i\omega t}\int_{-\infty}^{\infty} \mathrm{d}s\mathrm{e}^{-i\omega s}\sum_{KM} D_{K,M-1,M}(s) \\ &= -\frac{1}{2}\gamma H_R \mathrm{e}^{-i\omega t}\sum_{KM} D_{K,M-1,M}(\omega). \end{aligned}\tag{29}$$

From this result, the magnetic susceptibility of the present system is

$$\chi_{+-}(\omega) = -\frac{\gamma}{2}\sum_{KM} D_{K,M-1,M}(\omega). \tag{30}$$

In the course of the derivation, the matrix elements of spin operators are put to be unity. Here $D_{K,M-1,M}(s)$ is a retarded Green's function,

$$D_{K,M-1,M}(s) = -i\theta(s)Tr\{\rho_G[a^+_{KM-1}(s)a_{KM}(s), a^+_{KM}a_{KM-1}]_-\}, \tag{31}$$

and $D_{K,M-1,M}(\omega)$ is its Fourier transform. Now our problem is to estimate this Green's function.

The retarded Green's function is easily obtained by the analytical continuation of the Matubara function (or the temperature Green's function with imaginary time τ) which is causal with respect to τ,

$$\mathscr{D}_{K,M-1,M}(\tau) = -Tr\{\rho_G Tr[a^+_{K,M-1}(\tau)a_{K,M}(\tau)a^+_{K,M}a_{K,M-1}]\}, \tag{32}$$

for which the Feynman diagram analysis is available.[5)]

Non-Interacting Case

The case without the spin-lattice interaction is trivial; however, it seems instructive for the later investigation. By the use of the simplified notation, $<\cdots>=Tr(\rho_{\mathrm{G}}\cdots)$, the Green's function in this case is written as

$$\begin{aligned}\mathscr{D}^0_{K,M-1,M}(\tau) &= - < Tr[a^+_{KM-1}(\tau)a_{K,M}(\tau)a^+_{KM}a_{KM-1}] >^0 \\ &= \mathscr{G}^0_{KM}(\tau)\mathscr{G}^0_{KM-1}(-\tau), \end{aligned}\tag{33}$$

where

$$\mathscr{G}^0_{KM} = - < T\tau[a_{KM}(\tau)a^+_{KM}] >. \tag{34}$$

The corresponding Fourier transform is

$$\mathscr{D}^0_{K,M-1,M}(\omega_n) = \frac{1}{\beta}\sum_{\nu_n}\mathscr{G}^0_{KM}(\nu_n)\mathscr{G}^0_{KM-1}(\nu_n - \omega_n), \tag{35}$$

where

$$\mathcal{G}^0_{KM}(\nu_n) = \frac{1}{i\nu_n - \epsilon_{KM}}. \tag{36}$$

Therefore

$$\begin{aligned}
&\mathcal{D}^0_{K,M-1,M}(\omega_n) \\
&= \frac{1}{\beta}\sum_{\nu_n} \frac{1}{i\nu_n - \epsilon_{KM}} \cdot \frac{1}{i\nu_n - i\omega_n - \epsilon_{KM-1}} \\
&= \frac{1}{\beta}\sum_{\nu_n}\left(\frac{1}{i\nu_n - \epsilon_{KM}} - \frac{1}{i\nu_n - i\omega_n - \epsilon_{KM-1}}\right)\frac{-1}{i\omega_n + \epsilon_{KM-1} - \epsilon_{KM}} \\
&= [n(\epsilon_{KM-1}) - n(\epsilon_{KM})]\frac{1}{i\omega_n - \epsilon_{KI}},
\end{aligned} \tag{37}$$

where the fact that ω_n is even is used. The retarded Green's function is obtained simply by replacing $i\omega_n$ by $\omega_n + i\eta$ (η is the positive infinitesimal). Thus we obtain

$$\delta < I^+(t) >= \mathrm{e}^{-i\omega t} H_R \sum_K (n(\epsilon_{K-}) - n(\epsilon_{K+}))\frac{1}{\omega - \epsilon_{KI} + i\eta}. \tag{38}$$

The magnetic susceptibility χ_{+-} thus becomes,

$$\chi_{+-}(\omega) = \gamma \sum_K \sum_K (n(\epsilon_{K-}) - n(\epsilon_{K+}))\frac{1}{\omega - \epsilon_{KI} + i\eta}, \tag{39}$$

of which the imaginary part is

$$\chi''_{+-}(\omega) = -\pi\gamma \sum_K (n(\epsilon_{K-}) - n(\epsilon_{K+}))\delta(\omega - \epsilon_{KI}). \tag{40}$$

Next, the procedure to estimate $\delta < I^-(t) >$ is entirely the same except for interchanging $\epsilon_{KM} \leftrightarrow \epsilon_{KM-1}$, so that the value of $\delta < I^-(t) >$ is the minus of that of $\delta < I^+(t) >$ with $\epsilon_{KM} \leftrightarrow -\epsilon_{KI}$. As has been said at the beginning,

$$\begin{aligned}
\chi''_{zz}(\omega) &= \frac{1}{2}(\chi''_{+-}(\omega) + \chi''_{-+}(\omega)) \\
&= \gamma \sum_K \sum_K [n(\epsilon_{K-}) - n(\epsilon_{K+})][\delta(\omega - \epsilon_{KI}) - \delta(\omega + \epsilon_{KI})].
\end{aligned} \tag{41}$$

The result consists of two parts: The first concerns with a statistical difference between the nuclear spin states, for which the Fermi statistics was assumed. Besides this, nuclei behave classically. Therefore the statistical terms of nuclei never change even in interacting cases. The non-interacting character is represented by the delta functions. In the real case, when the ω integration is performed, the very small quantity ϵ_{KI} is varied in the line width, so that both δ functions behave to give the same results, and χ''_{+-} and χ''_{-+} cancel out with each other. That is to say, the nuclear spin is in its equilibrium state.

Interacting Case; Normal

In the interacting system, $\mathcal{G}^0$ in Eq. 35 must be replaced by $\mathcal{G}$ including the interaction which, in the present case, is the spin-spin interaction between nuclei and electrons, has been given in Eq. 23:

$$\mathcal{D}_{KM-1,M}(\omega_n) = \frac{1}{\beta}\sum_{\nu_n} \mathcal{G}_{KM}(\nu_n)\mathcal{G}_{KM-1}(\nu_n - \omega_n), \tag{42}$$

where

$$\mathcal{G}_{KM}(\nu_n) = [(\mathcal{G}^0_{KM}(\nu_n))^{-1} - \Sigma_{KM}(\nu_n)]^{-1}. \tag{43}$$

The most important (divergent) self-energy part of this self-energy arises from the ring diagram in the Fig. 1. There

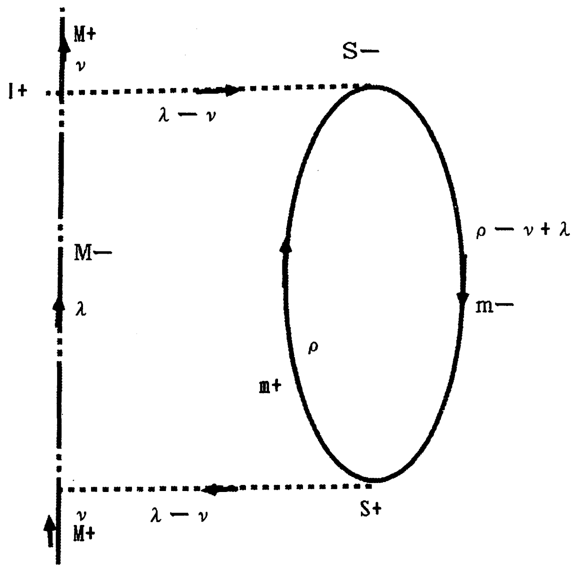

Fig. 1. Feynman diagram: the mechanism of spin-lattice relaxtion of nuclear spin due to the spin–spin interaction with electron.

the two-dot-interrupted line represents the propagator of the nuclear motion, the full line the electron propagator, and the dotted line the spin-spin interaction between electron and nucleus.

$$\begin{aligned}
\Sigma_{KM}(\nu_n) = &-\sum_{K'kk'}\sum_{\lambda_n\rho_n} | < M|I^+|M-1 >< m-1|S^-|m > |^2 \\
&\times < \chi_K(R)\phi_k(r)|F(R,r)|\phi_{k'}(r)\chi_{K'}(R) > |^2 \\
&\times \mathcal{G}^0_{K'M-1}(\lambda_n)\mathcal{S}^0_{km}(\rho_n)\mathcal{S}^0_{k'm-1}(\rho_n + \lambda_n - \nu_n),
\end{aligned} \tag{44}$$

where the minus sign is due to a fermion loop, and $\mathcal{S}$ is the electron propagator. The propagator part is calculated as follows:

$$\begin{aligned}
&\sum_{\lambda_n\rho_n} \mathcal{G}^0_{K'M-1}(\lambda_n)\mathcal{S}^0_{km}(\rho_n)\mathcal{S}^0_{k'm-1}(\rho_n + \lambda_n - \nu_n) \\
&= \sum_{\lambda_n\rho_n} \frac{1}{i\lambda_n - \epsilon_{K'M-1}} \cdot \frac{1}{i\rho_n - \epsilon_{km}} \cdot \frac{1}{i\rho_n + i\lambda_n - i\nu_n - \epsilon_{k'm-1}} \\
&= \sum_{\lambda_n} \frac{1}{i\lambda_n - \epsilon_{K'M-1}} \cdot \frac{1}{i\lambda_n - i\nu_n - \epsilon_{k'm-1} + \epsilon_{km}} \\
&\quad \times \sum_{\rho_n}\left(\frac{1}{i\rho_n - \epsilon_{km}} - \frac{1}{i\rho_n + i\lambda_n - i\nu_n - \epsilon_{k'm-1}}\right) \\
&= [n(\epsilon_{km}) - n(\epsilon_{k'm-1})] \\
&\quad \times \sum_{\lambda_n} \frac{1}{i\lambda_n - \epsilon_{K'M-1}} \cdot \frac{1}{i\lambda_n - i\nu_n - \epsilon_{k'm-1} + \epsilon_{km}} \\
&= [n(\epsilon_{km}) - n(\epsilon_{k'm-1})][n(\epsilon_{K'M-1}) - \overline{n}(\epsilon_{km} - \epsilon_{k'm-1})] \\
&\quad \times \frac{-1}{i\nu_n - \epsilon_{K'M-1} - \epsilon_{km} + \epsilon_{k'm-1}}.
\end{aligned} \tag{45}$$

Here $\overline{n}(\epsilon_{km} - \epsilon_{k'm-1})]$ is the bose function since $\lambda_n - \nu_n$ is even. Note that

$$\frac{1}{\beta}\sum_{\omega_n} \frac{1}{i\omega_n - \epsilon_k} = \mp \frac{1}{\mathrm{e}^{\beta\epsilon_k} \mp 1} \qquad \omega_n \text{ is even or odd.}$$

However, since we are at a low enough temperature such that $\epsilon_{km} - \epsilon_{k'm-1} \gg 1/\beta$, the classical limit is still employed, namely

$$\overline{n}(\epsilon_{km} - \epsilon_{k'm-1}) \simeq \mathrm{e}^{-\beta(\epsilon_{km} - \epsilon_{k'm-1})} \equiv n_\mathrm{B}(\epsilon_{km} - \epsilon_{k'm-1}), \tag{46}$$

where $n_{\rm B}$ is the Boltzmann function. Thus we obtain

$$\begin{aligned}\Sigma_{KM}(\nu_n) = \sum_{K'kk'} | < M|I^{+}|M-1 >< m-1|S^{-}|m > |^2 \\ \times < \xi_K(R)\phi_k(r)|F(R,r)|\xi_{k'}(r)\xi_{K'}(R) > |^2 \\ \times[n(\epsilon_{K'M-1}) - n_{\rm B}(\epsilon_{k+} - \epsilon_{k'-})][n(\epsilon_{km}) - n(\epsilon_{k'm-1})] \\ \times\frac{1}{i\nu_n - \epsilon_{K'M-1} + \epsilon_{k'm-1} - \epsilon_{km}}.\end{aligned} \tag{47}$$

Similarly, in order to get $\mathscr{G}_{KM-1}(\nu_n - \omega_n)$ which is another mate in the retarded Green's function, $\Sigma_{KM-1}(\nu_n - \omega_n)$ is evaluated as

$$\begin{aligned}\Sigma_{KM-1}(\nu_n - \omega_n) = \sum_{K'kk'} | < M-1|I^{-}|M >< m|S^{+}|m-1 > |^2 \\ \times < \chi_K(R)\phi_k(r)|F(R,r)|\phi_{k'}(R)\chi_{K'}(r) > |^2 \\ \times[n(\epsilon_{K'M}) - n_{\rm B}(\epsilon_{k+} - \epsilon_{k'-})][n(\epsilon_{km}) - n(\epsilon_{k'm-1})] \\ \times\frac{-1}{i\nu_n - i\omega_n - \epsilon_{K'M} + \epsilon_{km} - \epsilon_{k'm-1}}.\end{aligned} \tag{48}$$

Note that, in getting the retarded Green's function, ω_n is replaced by $\omega + i\eta$ in $\Sigma_{KM-1}(\nu_n - \omega_n)$, while $\Sigma_{KM}(\nu_n)$ does not need this step since it has no ω_n.

Hereafter in order to avoid the unnecessary complexity, it is restricted to the case that $I=1/2$ and $S=1/2$; further z components, $+1/2$ and $-1/2$, are indicated by + and − respectively.

Considering that, in the real problem, the electron staying in the k level sees the nucleus at its equilibrium position, and the interaction term $F(R,r)$ is dominated by the Fermi contact term, we can integrate our χ functions, yielding $\delta_{K',K}$. This implies the classical treatment of the nuclear spin as is usually done. Also we restrict ourselves to the case of $k=k'$ for electron; this term seems to contribute dominantly for the Fermi contact interaction. Then

$$\begin{aligned}\Sigma_{K+}(\nu_n) &= \sum_k |F_{kk}|^2 [n(\epsilon_{K-}) - n_B(\epsilon_{k+} - \epsilon_{k-})][n(\epsilon_{k+}) - n(\epsilon_{k-})] \\ &\quad\times\frac{-1}{i\nu_n - \epsilon_{K-} - \epsilon_{kS}} \\ &= -\sum_k \frac{K_k}{\nu_n - \epsilon_{K-} - \epsilon_{kS}} \\ &\simeq -\sum_k \frac{K_k}{\epsilon_{KI} - \epsilon_{kS}}.\end{aligned} \tag{49}$$

Here the final equality is obtained by putting $i\nu_n = \epsilon_{K+}$, and

$$\epsilon_{kS} = \epsilon_{k+} - \epsilon_{k-} \tag{50}$$

is the electron Zeeman energy and

$$\begin{aligned}F_{kk} &= < \phi_k(r)|F(R,r)|\phi_k(r) >, \\ K_k &= |F_k|^2 [n(\epsilon_{K-}) - n_B(\epsilon_{kS})]\cdot[n(\epsilon_{k+}) - n(\epsilon_{k'-})]\end{aligned} \tag{51}$$

Similarly

$$\Sigma_{K-}(\nu_n - \omega_n) = -\sum_k \frac{K_k}{i\nu_n - i\omega_n - \epsilon_{K+} + \epsilon_{kS}}. \tag{52}$$

If we here put $i\omega_n \to \omega + i\eta$,

$$\Sigma_{K-}(\nu_n - \omega_n) = \sum_k K_k \{P\frac{1}{\omega + \epsilon_{KI} - \epsilon_{kS}} - i\pi\delta(\omega + \epsilon_{KI} - \epsilon_{kS}\}, \tag{53}$$

where P stands for the principal part and in the final line, $i\nu_n$ is put equal to ϵ_{K-}.

Let us turn to estimating the retarded Green's function,

$$\begin{aligned}\mathscr{D}_{K,-+}(\omega) &= \mathscr{D}_{K-+}(i\omega_n)|_{i\omega_n \to \omega + i\eta} \\ &= \frac{1}{\beta}\sum_{\nu_n} \mathscr{G}_{K+}(\nu_n)\mathscr{G}_{K-}(\nu_n - \omega_n)\Big|_{i\omega_n \to \omega + i\eta} \\ &= \frac{1}{\beta}\sum_{\nu_n} \frac{1}{i\nu_n - \epsilon_{K+} - \Sigma_{K+}(\nu_n)} \\ &\quad\times\frac{1}{i\nu_n - i\omega_n - \epsilon_{K-} - \Sigma_{K-}(\nu_n - \omega_n)}\Big|_{i\omega_n \to \omega + i\eta} \\ &= \frac{1}{\beta}\sum_{\nu_n}\Big\{\frac{1}{i\nu_n - \epsilon_{K+} - \Sigma_{K+}(\nu_n)} \\ &\quad - \frac{1}{i\nu_n - i\omega_n - \epsilon_{K-} - \Sigma_{K-}(\nu_n - \omega_n)}\Big\} \\ &\quad\times\frac{-1}{i\omega_n + \epsilon_{K-} - \epsilon_{K+} + \Sigma_{K-}(\nu_n - \omega_n) - \Sigma_{K+}(\nu_n)}\Big|_{i\omega_n \to \omega + i\eta}\end{aligned} \tag{54}$$

Here considering that $\Sigma_{K+}(\nu_n)$ is a small, we may approximate as

$$\frac{1}{\beta}\sum_{\nu_n}\frac{1}{i\nu_n - \epsilon_{K+} - \Sigma_{K+}(\nu_n)} \simeq n(\epsilon_{K+}). \tag{55}$$

This term merely gives the particle density, so it is not so important for the present investigation. Thus, noticing that ω_n is even, and substituting Eqs. 49 and 55 into Eq. 54, we obtain

$$\begin{aligned}D_{K,-+}(\omega_n) &= (n(\epsilon_{K-}) - n(\epsilon_{K+})) \\ &\quad\Big/\Big\{\omega + i\eta + \epsilon_{KI} - \sum_{kk'}\frac{K_k}{\omega - i\eta - \epsilon_{KI} - \epsilon_{kS}} - \sum_k \frac{Kk}{\epsilon_{KI} + \epsilon_{kS}}\Big\} \\ &= (n(\epsilon_{K-}) - n(\epsilon_{K+})) \\ &\quad\Big/\Big\{\omega - \epsilon_{KI} + \sum_k K_k\Big[P\frac{1}{\omega + \epsilon_{KI} - \epsilon_{kS}} - \frac{1}{\epsilon_{KI} - \epsilon_{kS}} \\ &\qquad - i\pi\delta(\omega + \epsilon_{KI} - \epsilon_{kS})\Big]\Big\} \\ &= (n(\epsilon_{K-}) - n(\epsilon_{K+}))\frac{1}{\omega - \epsilon_{KI} + A - iB},\end{aligned} \tag{56}$$

where the first $i\eta$ in the second line is useless because the physical imaginary part has been obtained from $\Sigma_{K-}(\nu_n - \omega_n)$. Here

$$\begin{aligned}A &= \sum_k K_k\Big[P\frac{1}{\omega - \epsilon_{KI} - \epsilon_{kS}} - \frac{1}{\epsilon_{KI} - \epsilon_{kS}}\Big], \\ B &= \sum_k K_k \pi\delta(\omega - \epsilon_{KI} - \epsilon_{kS}), \\ &\equiv K_{k:{\rm res}}.\end{aligned} \tag{57}$$

In the final result, the k summation (integration) is carried out to obtain the value at the resonance point (k : res). Then the imaginary part of $D_{K,-+}(\omega)$ is

$${\rm Im}D_{K,-+}(\omega_n) = (n(\epsilon_{K-}) - n(\epsilon_{K+}))\frac{\pi B}{(\omega - \epsilon_{KI} - A)^2 + B^2}. \tag{58}$$

Thus we arrive at the imaginary part of the magnetic susceptibility, $\chi_{+-}(\omega)$,

$$\chi''_{+-}(\omega) = \gamma\sum_K (n(\epsilon_{K-}) - n(\epsilon_{K+}))\frac{\pi B}{(\omega - \epsilon_{KI} - A)^2 + B^2}. \tag{59}$$

The line shape obtained from this looks Lorenzian, but precisely observing the factor $n_{\rm B}(\epsilon_{kS})$ in K_k of B (see also Eq. 51) indicates the Gaussian shape at the center of the resonance curve.

Evaluating χ''_{-+} gives the result in which the interchange $n(\epsilon_{K+}\leftrightarrow n(\epsilon_{K-})$ arises. The final result is obtained from

$$\chi_{zz}(\omega)=\frac{1}{2}(\chi_{+-}(\omega)+\chi_{-+}(\omega)). \tag{60}$$

This requires a complicated manipulation which is not so fruitful from the physical view-point. The following approximation procedures are employed. In the real problem, the very small quantiy ϵ_{KI} is varied in the line width. When we carry out the ω integration, the peaks at the slightly different resonance points give almost the same contribution with different statistical weights. This almost cancelling scheme is given in such a way that

$$1/(a-x)-1/(a+x)\simeq 2x/a^2, \qquad a\gg x$$

Thus

$$\chi''_{zz}=\gamma\sum_K[n(\epsilon_{K-})-n(\epsilon_{K+})]\frac{4(\omega-A)\epsilon_{KI}}{(\omega-A)^2+B^2}\cdot\pi B. \tag{61}$$

Comparing this with the non-interacting case of Eq. 41, we note that the delta function in the latter salters to the line shape function which looks Lorenzian with a Gaussian envelope around the center.

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Green's Function. In this case, the electron propagators in the previous chapter are replaced by those in the superconducter. As has been done by BCS, let us assume the attractive, constant two-body potential g.

$$H_{\rm el}=\sum_{k\alpha\beta}\left\{\epsilon_{k\alpha}c^+_{k\alpha}c_{k\alpha}+\frac{1}{2}g(c^+_{k\alpha}c^+_{-k\beta})(c_{-k\beta}c_{k\alpha})\right\}, \tag{62}$$

where the electron is restricted to the Cooper pairs, and $\epsilon_{k\alpha}$ is the orbital energy, which also includes the Zeeman energy at the present case.

Now we use the extended Nambu representation of Eq. 2,

$$\boldsymbol{c}_k=\begin{pmatrix} c_{k\alpha}\\ c^+_{-k\beta}\\ c^+_{-k\alpha}\\ c_{k\beta}\end{pmatrix}, \qquad \boldsymbol{c}^+_k=(c^+_{k\alpha}\ c_{-k\beta}\ c_{-k\alpha}\ c^+_{k\beta}). \tag{63}$$

with the equal time commutator,

$$[\boldsymbol{c}_k,\boldsymbol{c}^+_{k'}]_+=\mathbf{1}\delta_{kk'}. \tag{64}$$

In these terms the Hamiltonian is rewritten as

$$H_{\rm el}=\sum_k\epsilon_k\boldsymbol{c}^+_k\Sigma^3\boldsymbol{c}_k+\frac{1}{2}g\sum_{kk'}\boldsymbol{c}^+_k\Sigma^+\boldsymbol{c}_k\cdot\boldsymbol{c}^+_{k'}\Sigma^-\boldsymbol{c}_{k'}, \tag{65}$$

where ϵ_k is the diagonal matrix of ϵ_γ:

$$\epsilon_k=\begin{pmatrix}\epsilon_{k\alpha}&&&\\&\epsilon_{-k\beta}&&\\&&\epsilon_{-k\alpha}&\\&&&\epsilon_{k\beta}\end{pmatrix}. \tag{66}$$

Let us define

$$\Sigma^3=\begin{pmatrix}\sigma^3&0\\0&-\sigma^3\end{pmatrix},\ \Sigma^+=\begin{pmatrix}\sigma^+&0\\0&-\sigma^-\end{pmatrix},\ \Sigma^-=\begin{pmatrix}\sigma^-&0\\0&-\sigma^+\end{pmatrix}, \tag{67}$$

with

$$\sigma^3=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\ \sigma^1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\ \sigma^2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},$$
$$\sigma^+=\frac{1}{2}(\sigma^1+i\sigma^2),\ \sigma^-=\frac{1}{2}(\sigma^1-i\sigma^2). \tag{68}$$

It is pointed out that Σ^+ selects the Cooper pair in the particle state, while Σ^- selects the pair in the hole state.

The above Hamiltonian is invariant under the scale transformation; then we have a current conservation; especially the charge conservation (Noether's theorem). If we have any quantity which does not commute this invariant charge, we can expect a phase transition (Goldstone's theorem).

The charge proportional to

$$\sum_{k\gamma}<c^+_{k\gamma}c_{k\gamma}>=\sum_{k>0}<\boldsymbol{c}^+_k\Sigma^3\boldsymbol{c}_k> \tag{69}$$

is invariant under the rotation about the Σ^3 axis in the space spaned by Σ^3, Σ^+, and Σ^-. Observing that

$$[\Sigma^+,\Sigma^3]=-2\Sigma^-, \quad [\Sigma^-,\Sigma^3]=2\Sigma^+ \tag{70}$$

suggests the phase transitions on the $\Sigma^+-\Sigma^-$ plane.

The phase transition cannot be achieved by the perturbational approach, but the effective Hamiltonian giving the phase transition should be included at the beginning, say the Hailtonian is modified such as

$$H^0=\sum_k\boldsymbol{c}^+_k(\epsilon_k+\rho\Sigma^++\eta\Sigma^-)\boldsymbol{c}_k,$$
$$H'=\frac{1}{2}g\sum_{kk'}\{(\boldsymbol{c}^+_k\Sigma^+\boldsymbol{c}_k)\cdot(\boldsymbol{c}^+_{k'}\Sigma^-\boldsymbol{c}_{k'})-\sum_k\boldsymbol{c}^+_k(\rho\Sigma^++\eta\Sigma^-)\boldsymbol{c}_k, \tag{71}$$

where ρ and η are the so-called gap enegies, which are assumed independent of k for simplicity. Note that the Hamiltonian, H^0 is symmetrically broken.

The temperature Green's function with the imaginary time τ is defined as

$$G^0_{kk'}(\tau)=-<T\tau|\boldsymbol{c}_k(\tau)\boldsymbol{c}^+_{k'}]>, \tag{72}$$

where $<\cdots>=Tr\{\rho_{\rm G}\cdots\}$. The equation of motion of $G^0_{kk'}$ is

$$\begin{aligned}\partial_\tau G^0_{kk'}(\tau)&=-\partial_\tau[\theta(\tau)<\boldsymbol{c}_k(\tau)\boldsymbol{c}^+_{k'}(0)>-\theta(-\tau)<\boldsymbol{c}^+_{k'}(0)\boldsymbol{c}_k(\tau)>]\\&=-\delta(\tau)<[\boldsymbol{c}_k(\tau),\boldsymbol{c}^+_{k'}(0)]_+>-<T\tau[\boldsymbol{c}_k(\tau),H^0]_-,\boldsymbol{c}^+_k(0)>\\&=-\delta_{kk'}+(\epsilon_k\Sigma^3+\rho\Sigma^++\eta\Sigma^-)G^0_{kk'}.\end{aligned} \tag{73}$$

In the coursce of the above derivation, the commutator in Eq. 64 was used.

We make the Fourier transform:

$$G^0_{kk'}(\tau)=\frac{1}{\beta}\sum_{\omega_n}{\rm e}^{-i\omega_n\tau}G^0_{kk'}(\omega_n), \tag{74}$$

Then the equation of motion becomes

$$(i\omega_n+\epsilon_k\Sigma^3+\rho\Sigma^++\eta\Sigma^-)G^0_{kk'}(\omega_n)=\delta_{kk'}. \tag{75}$$

Namely,

$$G^0_{kk'}(\omega_n) = \frac{1}{i\omega_n + \epsilon_k\Sigma^3 + \rho\Sigma^+ + \eta\Sigma^-} = \delta_{kk'}\left\{\frac{-i\omega_n + \epsilon_k\Sigma^3 + \rho\Sigma^+ + \eta\Sigma^-}{\omega_n^2 + E_k^2}\right\}, \quad (76)$$

where

$$E_k^2 = \epsilon_k^2 + \rho\eta. \quad (77)$$

Spin Dynamics. The matrix propagator is now obtained. First of all we examine the effects of the normal (the particle-hole type) part, which are diagonal parts in Eq. 76. For example,

$$G^0_{k\gamma}(\omega_n) = \left\{\frac{-i\omega_n + \epsilon_{k\gamma}}{\omega_n^2 + E_k^2}\right\}, \quad (78)$$

is a matrix element specified by Σ^3.

Investigations are going on as same as the previous section: The propagator product to be estimated is

$$\sum_{\lambda_n\rho_n} \mathscr{G}^0_{K-}(\lambda_n)\mathscr{S}^0_{k+}(\rho_n)\mathscr{S}^0_{k'-}(\rho_n + \lambda_n - \nu_n).$$

Here G^0_{K-} is the propagator for the nucleous indicated by the capital K, and two electron propagators are different in the Zeeman enegies, so that we can obtain the main contribution from the term of $k=k'$. Only the result corresponding to Eq. 45 is presented. Long and straightforward calculations yield a rather ordinary result:

$$\begin{aligned} = \frac{1}{4}\Bigg\{ & \frac{N^-}{-i\nu_n + E_{k-} - E_{k+} + \epsilon_{K-}}\left[1 + \frac{\epsilon_{k-}}{E_{k-}} + \frac{\epsilon_{k+}}{E_{k+}} + \frac{\epsilon_{k-}\epsilon_{k+}}{E_{k+}E_{k-}}\right] \\ & + \frac{N^+}{i\nu_n + E_{k-} + E_{k+} - \epsilon_{K-}}\left[-1 + \frac{\epsilon_{k-}}{E_{k-}} - \frac{\epsilon_{k+}}{E_{k+}} + \frac{\epsilon_{k-}\epsilon_{k+}}{E_{k+}E_{k-}}\right] \\ & + \frac{N^+}{-i\nu_n + E_{k-} + E_{k+} + \epsilon_{K-}}\left[1 + \frac{\epsilon_{k-}}{E_{k-}} - \frac{\epsilon_{k+}}{E_{k+}} - \frac{\epsilon_{k-}\epsilon_{k+}}{E_{k+}E_{k-}}\right] \\ & + \frac{N^-}{i\nu_n - E_{k-} + E_{k+} + \epsilon_{K-}}\left[-1 + \frac{\epsilon_{k-}}{E_{k-}} + \frac{\epsilon_{k+}}{E_{k+}} - \frac{\epsilon_{k-}\epsilon_{k+}}{E_{k+}E_{k-}}\right]\Bigg\}, \end{aligned} \quad (79)$$

where

$$N^{\mp} = [n(E_{k+}) - n(E_{k-})][n(\epsilon_{K-}) - n_{\mathrm{B}}(E_{k+} \mp E_{k-})]. \quad (80)$$

Looking at Eq. 79, we find that, among multipulicative factors $[\cdots]$, the first term amounts to about 4, while others nearly cancel out. Therefore we can retain only the first term, which is nothing but that obtained in the the normal case (see Eq. 45) by replacing ϵ_k by E_k. Then we shall arrive at the same result as Eq. 59, however with the above replacement.

$$\chi''_{+-}(\omega) = \gamma\sum_K (n(\epsilon_{K-1}) - n(\epsilon_{K+}))\frac{\pi B}{(\omega - \epsilon_{KI} - A)^2 + B^2}$$
$$\text{however} \quad A, B = A(E_k), B(E_k). \quad (81)$$

Now notations are getting more and more tedious. Let us review: The capital E is the quasi-particle energy. The ϵ is that of the normal electron. The capital K refers to the nuclei, while the small k refers to electrons.

We turn to taking the pair propagators into account. This is given, in the Fig. 1, by replacing the previous electron propagators by the pair propagators.

$$\Sigma_{K+}(\nu_n) = -\sum_{\lambda_n\rho_n}\sum_{kk'}|F_{kk'}|^2\mathscr{G}_{K-}(\lambda_n)\mathscr{F}^*_k(\rho_n)\mathscr{F}_{k'}(\rho_n + \lambda_n - \nu_n), \quad (82)$$

where the minus sign is due to a fermion loop, also $\mathscr{F}^*_k(\rho_n)$ which is the Fourier transform of $<T\tau(c^+_{-k-}(\tau)c^+_{k+})>$, is the 2-1 element of G^0_k, while $\mathscr{F}_k$ is the 1-2 element of G^0_k. To confirm the notation, for example $-k+$ means the negative k with the up spin. The above is precisely written by the use of Eq. 76,

$$= -\sum_{\lambda_n\rho_n}\sum_k |F_{k,-k}|^2\frac{1}{i\lambda_n - \epsilon_{K-}}\frac{\eta}{\rho_n^2 + E_k^2}\frac{\rho}{(\rho_n + \lambda_n - \nu_n)^2 + E_{k'}^2}.$$

In the present case, we must to consider the case where k is slightly different from k', since the off-diagonal propagators under investigation are not distinct in the Zeeman energy. The frequency sum is straightforward, giving

$$\begin{aligned} = -\sum_k |F_{k,k'}|^2 \frac{\rho\eta}{4E_kE_{k'}} \{ & [n(-E_k) - n(-E_{k'})][n(\epsilon_{K-}) - n_{\mathrm{B}}(E_k - E_{k'})] \\ & \times \frac{1}{-i\nu_n + E_{k'} - E_k + \epsilon_{K-}} \\ & + \{[n(-E_k) - n(E_{k'})][n(\epsilon_{K-}) - n_{\mathrm{B}}(E_k + E_{k'})] \\ & \times \frac{1}{i\nu_n + E_{k'} + E_k - \epsilon_{K-}} \\ & + \{[-n(E_k) + n(-E_{k'})][n(\epsilon_{K-}) - n_{\mathrm{B}}(-E_k - E_{k'})] \\ & \times \frac{1}{-i\nu_n + E_{k'} + E_k + \epsilon_K} \\ & + \Big\{[-n(E_k) + n(E_{k'})][n(\epsilon_{K-}) - n_{\mathrm{B}}(-E_k + E_{k'})] \\ & \times \frac{1}{-i\nu_n + E_{k'} - E_k + \epsilon_{K-}}\Big\}. \end{aligned} \quad (83)$$

Among these, the terms which satisfy the resonance condition, say, the first and last terms, are retained. The change of arguments in the first term, $(-E_k \rightarrow E_k)$ and $(-E_{k'} \rightarrow E_{k'})$ are allowed (the sum with repect to all the values of k and k' makes these interchanges no trouble), and finally $i\nu_n$ is approximately replaced by ϵ_{K+}. Thus we have

$$\Sigma_{K+}(\nu_n) = -\sum_{kk'}|F_{kk'}|^2\frac{\rho\eta}{2E_kE_{k'}}[n(E_k) - n(E_{k'})]n(\epsilon_{K-} - n_{\mathrm{B}}(E_{k'} - E_k)) \times \frac{1}{\epsilon_{KI} + E_k - E_{k'}}. \quad (84)$$

Next the term $\Sigma_{K+}(\nu_n - \omega_n)$ will be estimated to get $\mathscr{G}_{K-}(\nu_n - \omega_n)$ which is another mate in the retarded Green's function. Similarly

$$\Sigma_{K+}(\nu_n-\omega_n)=-\sum_{\lambda_n\rho_n}\sum_{kk'}|F_{kk'}|^2\left(\frac{1}{i\lambda_n-\epsilon_{k+}}\right)\times\left(\frac{\eta}{(\rho_n+\lambda_n-\nu_n+\omega_n)^2+E_{k'}^2}\right)\left(\frac{\rho}{\rho_n^2+E_k^2}\right).$$

After the frequency sum,

$$\begin{aligned}=&-\sum_{kk'}|F_{kk'}|^2\frac{\rho\eta}{4E_kE_{k'}}\{[n(-E_{k'})-n(-E_k)][n(\epsilon_{K+})-n_{\mathrm{B}}(E_k-E_{k'})]\\&\times\frac{1}{i\nu_n-i\omega_n-E_{k'}+E_k-\epsilon_{K+}}\\&+\{[n(-E_{k'})-n(E_k)][n(\epsilon_{K+})-n_{\mathrm{B}}(E_k+E_{k'})]\\&\times\frac{1}{-i\nu_n+i\omega_n+E_{k'}+E_k-\epsilon_{K+}}\\&+\{[-n(E_{k'})+n(-E_k)][n(\epsilon_{K+})-n_{\mathrm{B}}(-E_k-E_{k'})]\\&\times\frac{1}{i\nu_n-i\omega_n+E_{k'}+E_k+\epsilon_{K+}}\\&+\left\{[-n(E_{k'})+n(E_k)][n(\epsilon_{K+})-n_{\mathrm{B}}(E_k-E_{k'})]\right.\\&\left.\times\frac{1}{-i\nu_n+i\omega_n+E_{k'}-E_k+\epsilon_{K+}}\right\}.\end{aligned}\tag{85}$$

The first and last terms which are met with the resonance condition are retained; then we have

$$\begin{aligned}\Sigma_{K-}(\nu_n-\omega_n)=&-\sum_{kk'}|F_{kk'}|^2\frac{\rho\eta}{2E_kE_{k'}}(n(E_{k'})-n(E_k))\\&(n(\epsilon_{K+})-n_{\mathrm{B}}(E_k-E_{k'}))\times\frac{1}{i\omega_n+E_{k'}-E_k+\epsilon_{KI}}\\\to&-\sum_{kk'}|F_{kk'}|^2\frac{\rho\eta}{2E_kE_{k'}}(n(E_k)-n(E_{k'}))(n(\epsilon_{K+})-n_{\mathrm{B}}(E_k-E_{k'}))\\&\times\left\{P\frac{1}{\omega-E_{k'}+E_k+\epsilon_{KI}}-i\pi\delta(\omega-E_{k'}+E_k+\epsilon_{KI})\right\},\end{aligned}\tag{86}$$

where the last result is for the later investigation.

We are now at the final step to estimate the retarded Green's function $D_{K,-+}(\omega)$ taking into account the superconducting effect. To orient ourselves, we follow, for the time being, the same equations as are seen in Eq. 54.

$$\begin{aligned}\mathscr{D}_{K,-+}(\omega)&=D_{K-+}(i\omega_n)|_{i\omega_n\to\omega+i\eta}\\&=\frac{1}{\beta}\sum_{\nu_n}\mathscr{G}_{K+}(\nu_n)\mathscr{G}_{K-}(\nu_n-\omega_n)|_{i\omega_n\to\omega+i\eta}\\&=\frac{1}{\beta}\sum_{\nu_n}\frac{1}{i\nu_n-\epsilon_{K+}-\Sigma_{K+}(\nu_n)}\\&\quad\times\frac{1}{i\nu_n-i\omega_n-\epsilon_{K-}-\Sigma_{K-}(\nu_n-\omega_n)}\Bigg|_{i\omega_n\to\omega+i\eta}\\&=\frac{1}{\beta}\sum_{\nu_n}\left\{\frac{1}{i\nu_n-\epsilon_{K+}-\Sigma_{K+}(\nu_n)}\right.\\&\quad\left.-\frac{1}{i\nu_n-i\omega_n-\epsilon_{K-}-\Sigma_{K-}(\nu_n-\omega_n)}\right\}\\&\quad\times\frac{-1}{i\omega_n+\epsilon_{K-}-\epsilon_{K+}+\Sigma_{K-}(\nu_n-\omega_n)-\Sigma_{K+}(\nu_n)}\Bigg|_{i\omega_n\to\omega+i\eta}\end{aligned}\tag{87}$$

Here, as $\Sigma_{K+}(\nu_n)$ is a small correction term, approximately

$$\frac{1}{\beta}\sum_{\nu_n}\frac{1}{i\nu_n-\epsilon_{K+}-\Sigma_{K+}(\nu_n)}\simeq n(\epsilon_{K+}).\tag{88}$$

Thus, noticing that ω is even, and substituting Eqs. 85 and 86 into Eq. 87, we have

$$\begin{aligned}D_{K,-+}(\omega_n)=&(n(\epsilon_{K-})-n(\epsilon_{K+}))\\&\times1/\left\{\omega-\epsilon_{KI}+\sum_{kk'}|F_{kk'}|^2\frac{\rho\eta}{2E_kE_{k'}}(n(E_k)-n(E_{k'}))\right.\\&\times\left[P\frac{1}{\omega-E_{k'}+E_k+\epsilon_{KI}}\cdot(n(\epsilon_{K+})-n_{\mathrm{B}}(E_k-E_{k'}))\right.\\&+\frac{1}{E_k-+E_{k'}-\epsilon_{KI}}\cdot(n(\epsilon_{K-})-n_{\mathrm{B}}(E_{k'}-E_k))\\&\left.-i\pi\delta(\omega-E_{k'}+E_k+\epsilon_{KI})\right\}.\end{aligned}\tag{89}$$

This is rewritten as

$$D_{K,-+}(\omega_n)=(n(\epsilon_{K-})-n(\epsilon_{K+}))\frac{1}{\omega-\epsilon_{KI}+A'-i\pi B'},\tag{90}$$

where

$$\begin{aligned}A'=&\sum_{kk'}\frac{\rho\eta}{2E_kE_{k'}}|F_{kk'}|^2[n(E_k)-n(E_{k'})]\\&\times\left[P\frac{1}{\omega-E_{k'}+E_k+\epsilon_{KI}}\cdot(n(\epsilon_{K+})-n_{\mathrm{B}}(E_kE_{k'}))\right.\\&+\frac{1}{E_k-E_{k'}-\epsilon_{KI}}\cdot(n(\epsilon_{K-})-n_{\mathrm{B}}(E_{k'}-E_k)),\\B'=&\sum_{kk'}\frac{\rho\eta}{2E_kE_{k'}}|F_{kk'}|^2(n(E_k)-n(E_{k'}))(n(\epsilon_{K+})-n_{\mathrm{B}}(E_k-E_{k'}))\\&\times\delta(\omega-E_{k'}+E_k+\epsilon_{KI}).\end{aligned}\tag{91}$$

Thus we obtain the imaginary part of the magnetic susceptibility as

$$\chi''_{+-}(\omega)=\gamma\sum_K(n(\epsilon_{K-})-n(\epsilon_{K+}))\frac{\pi B'}{(\omega-\epsilon_{KI}+A')^2+B'^2}.\tag{92}$$

The partner, χ''_{-+} is obtained by the interchange $n(\epsilon_{K+})\leftrightarrow n(\epsilon_{K-})$ in the above. The final result is thus obtained from

$$\chi_{zz}(\omega)=\frac{1}{2}(\chi_{+-}(\omega)+\chi_{-+}(\omega)).\tag{93}$$

This requires a complicated manipulation. We are satisfied with a approximate procedure which has been carried out in the case of normal state (see above Eq. 61). Thus, we have

$$\chi''_{zz}=\gamma\sum_K[n(\epsilon_{K-})-n(\epsilon_{K+})]\frac{4(\omega+A')\epsilon_{KI}}{(\omega+A')^2+B'^2}\cdot\pi B'.\tag{94}$$

Combining the result in Eq. 81 and the above, we can obtain the final result in the superconducting phase. However in the former where, when dealing with electrons with $k+$ and $k'-$ which are distinct in the spin states, we can put $k=k'$. But in the latter we cannot. Comparing Eq. 91 with Eq. 57, leads

$$A'=\frac{\rho\eta}{2E_kE_{k'}}A,\quad B'=\frac{\rho\eta}{2E_kE_{k'}}B.\tag{95}$$

In obtaining this, we assumed $E_k-E_{k'}=\epsilon_{kS}$, which is the electron Zeeman energy. We thus obtain the coherent factor,

$$\frac{1}{2}\left(1+\frac{\rho\eta}{E_kE_{k'}}\right).\tag{96}$$

However it should be noted that, as is seen in the course of derivation, the present result is not exactly identical with that shown in the introduction.

Conclusion

If we review the present investigations from the view points of the line shape problem in the magnetic resonance, three cases can be clearly distingushed: In the non-interacting case, the line shape is written in terms of the delta function, in the interacting case of the normal phase, this is written by the Lorenz like function, and in the superconducting phase, this is further multiplied by the coherent factor. But the statistical factors referring to the nuclear states never change throughout.

From the view point of superconductivity, the present theory has almost nothing to give more than the current theories have done. However the theory is not merely to reproduce the experimental result, but to predict the mechanism hidden in the observations, in such a way that the manipulations tell step by step what is acting inside the matter. We might be satisfied with a little deeper understanding of superconductivity.

In the framework of the present investigation, the absence of the Slichter enhancement in the copperoxide superconductor may be attributed to anisotropy of the gap functions. Throuout this treatment, the gap functions are treated as if they were isotropic. This is not true when the electrons taking part in superconductivity are in the *d* orbitals. If we carry out a numerical estimation, the shape of *d* orbitals should be taken into account.

Scalapino[7)] has presented the sophisticated discussions on possibilities that the T_1 enhancement is lost, from the singular character of the *d*- and *s* gap functions.

If the spin-spin interaction of interest here is regarded as a source of the impurity scattering, the problem of the gapless superconductor might be considered, though we afraid that this mechanism will reduce the critical temperature.[8)]

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8) K. Maki, "Gapless Superconductors," in "Superconductivity," ed by R. D. Parks, Marcel Dekker, Inc., New York (1967). Here we find the four dimensional representation which is a little different from the present one.