Theme of the Workshop on Itinerant-Electron Magnetism, and Spin Fluctuations

Kazuyoshi Yoshimura\textsuperscript{1,2,3,4}

\textsuperscript{1}Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan
\textsuperscript{2}Research Center for Low Temperature and Material Sciences, Kyoto University, Kyoto 606-8501, Japan
\textsuperscript{3}International Research Unit of Integrated Complex System Science, Kyoto University, Kyoto 606-8501, Japan
\textsuperscript{4}International Research Unit of Advanced Future Studies, Kyoto University, Kyoto 606-8502, Japan

E-mail: yoshimura.kazuyoshi.8e@kyoto-u.ac.jp, kyhv@kuchem.kyoto-u.ac.jp

Abstract: The international workshop on itinerant-electron magnetism (IWIE) was held during September 25-27, 2015 in the seminar house of Graduate School of Science, Kyoto University, Kyoto, Japan. Here, I explain the theme of this workshop, and stress the development of itinerant-electron magnetism in several decades. The workshop was also organized in commemoration of Professor Yoshinori Takahashi’s retirement from University of Hyogo, Japan. Here, I also explain some of his works contributing to the development of itinerant magnetism.

1. Itinerant-Electron Magnetism and Spin Fluctuations

In these several decades, a lot of important theoretical and experimental approaches have been conducted for understanding the itinerant-electron magnetism [1-20, and references in them]. Among them epoch-making was the great success of the spin-fluctuation theory for weak itinerant ferromagnets and antiferromagnets by Toru Moriya and his coworkers based on the self-consistent renormalization (SCR) of spin fluctuations to magnetic free energy since 1973 (the SCR theory) [6, 8-11], exceeding the Stoner mean field theory [1] and the dynamical mean field theory, called the random phase approximation (RPA) theory with no mode-mode coupling of spin fluctuations [5]. Afterwards, the spin fluctuation theory has been developed toward the unified theory between the weakly itinerant regime [6] and the localized moment regime [4] in metallic magnets by a phenomenological method by T. Moriya and Yoshinori Takahashi (1978) [8]. Furthermore, the SCR theory was successfully extended to explain the characteristic magnetic behaviors of heavy-fermion systems [17]. Then, the SCR theory has been developed and rearranged in a quantitative way by
Takahashi and Moriya in 1985 (Quantitative Aspect of Spin Fluctuations) [12], by which we can compare the experiments and the SCR theory quantitatively by means of a set of (several numbers of) spin-fluctuation parameters [12, 15, 16, 18-20].

2. SCR Theory of Spin Fluctuations

In the SCR theory of spin fluctuations for itinerant-electron magnetic systems [6, 8-14, 19, 20], the definitions of spin fluctuations, $\langle S^2 \rangle = \langle S^2 \rangle_T + \langle S^2 \rangle_{Z.P.}$, which are magnetic excitations and band fluctuations in itinerant-electron magnetic systems, are

$$
\left\{
\begin{aligned}
\langle S^2 \rangle_T &= \frac{6}{N_0} \sum_q \int_0^{\omega_0} \frac{d\omega}{\pi} n(\omega) \text{Im} \chi(q, \omega) \\
\langle S^2 \rangle_{Z.P.} &= \frac{3}{N_0} \sum_q \int_0^{\omega_0} \frac{d\omega}{\pi} \text{Im} \chi(q, \omega)
\end{aligned}
\right.,
$$

where $\langle S^2 \rangle_T$ is the thermal spin fluctuations, $\langle S^2 \rangle_{Z.P.}$ is the zero-point spin fluctuations, $q$ is the wave vector of the spin fluctuation, $\omega$ is the frequency of the spin fluctuation, $N_0$ is the number of magnetic atoms in the system, and $\text{Im} \chi(q, \omega)$ is the imaginary part of the dynamical magnetic susceptibility as a function of $q$ and $\omega$. Furthermore, $n(\omega)$ is the bosonic factor. The difference of $\langle S^2 \rangle_T$ from $\langle S^2 \rangle_{Z.P.}$ is only the presence of $n(\omega)$ [13, 19, 20]. The SCR theory of spin fluctuations, which is the mode-mode coupling theory between different wave $q$-vectors of spin fluctuations, has explained many experimental magnetic properties of the itinerant ferromagnets and antiferromagnets, for example, the low ferromagnetic transition temperature, called the Curie temperature $T_C$, and the low antiferromagnetic transition temperature, called Néel temperature $T_N$, in itinerant-electron systems and the dynamical measurements of spin dynamics in itinerant magnets [6, 8-20]. The Curie-Weiss law in $\chi$ above $T_C$ was successfully explained by the $T$-linear increase of $\langle S^2 \rangle_T$ in the SCR theory [6, 9-12, 14].

In the SCR theory of spin fluctuations, $\text{Im} \chi(q, \omega)$ is usually written by the following double Lorentzian formula as [9-14, 19, 20]

$$
\left\{
\begin{aligned}
\text{Im} \chi(q, \omega) &= \frac{\chi(0,0)}{1 + q^2 / \kappa^2} \cdot \frac{\omega \Gamma_q}{\omega^2 + \Gamma_q^2} \\
\Gamma_q &= \Gamma_0 \omega_0 \left(\kappa^2 + q^2\right), \quad \kappa^2 = \frac{1}{2A} \frac{N_0}{\chi}
\end{aligned}
\right.,
$$

where $\kappa$ and $\Gamma_q$ represent the $q$ (momentum)- and $\omega$ (energy)-widths of the spin fluctuation spectrum, and $\kappa^2$ corresponds to the inverse susceptibility, $1/\chi$. In the SCR theory, $\kappa$ and $\Gamma_q$ are important spin-fluctuation quantities for expressing magnetic quantities. Furthermore, $\Gamma_0$ and $A$ are the parameters representing $\omega$ -width and $q$-damping width of the double Lorentzian form. Here, by utilizing a set of spin fluctuation parameters, $p$, $F$, $T_0$ and $T_A$, magnetic quantities, such as $T_C$, and
the temperature dependence of the magnetic susceptibility above $T_C$, can be expressed quantitatively by the SCR theory [9-16, 18-20], where $p_s$ is the spontaneous Bohr magneton number, $\bar{F}_f$, which can be obtained experimentally from the Allott-plot ($M^2$ vs $H/M$ plot ($M$ being magnetization and $H$ being magnetic field)), is the coefficient of the $M^4$-term in Landau expansion of magnetic free energy, and $T_0$ and $T_A$ are the characteristic temperatures corresponding to the $q$- and $\omega$- widths of the spin fluctuation spectrum deduced from $\Gamma_0$ and $\bar{A}$ as

$$\begin{cases}
T_0 = \Gamma_0 q_B^2 / 2\pi \\
T_A = \bar{A} q_B^2
\end{cases},$$

(3)

where $q_B$ is the wave vector $q$ at the Brillouin zone boundary. For example, the SCR theory gives $T_C$ through the following SCR relation among spin-fluctuation parameters as

$$p_s^2 / 4 = 15 c T_0 (T_C / T_0)^{4/3},$$

(4)

where $c$ is the constant being 0.3353... [12].

3. Takahashi’s Theory of Spin Fluctuations

After providing quantitative evidence for the SCR theory in 1985 [12], Takahashi has developed the spin-fluctuation theory [13] in different approaches with some assumptions: total spin-fluctuation amplitude conservation (TAC) and global consistency (GC) for a few decades (1986 ~ present) [13, 19, 20], which lead us to the new unified picture of metallic magnetism with a wide variety of itinerant-electron magnets based upon the spin-fluctuation approaches [19, 20].

First, he assumed that the following TAC equation (5) is valid even in explaining magnetic properties at finite temperatures [13]. Therefore, total spin fluctuations, namely, the total square amplitude of the local spin fluctuation, are constant and conserved even in the itinerant system as [13, 19, 20]

$$\left< S_{bc}^2 \right> = \left< S_{bc}^2 \right>_T + \left< S_{bc}^2 \right>_{Z.P.} = \text{const.}$$

(5)

Equation (5) is naturally satisfied in the localized moment system. Takahashi assumed the eq. (5) is valid even in an itinerant system, although that is not intuitive in the itinerant system. By using the relation deduced from the eq. (5), the magnetic properties at finite temperatures can be reproduced and explained [13, 15, 16, 18-23]. This allows the new unification of the itinerant-electron magnetism [13, 19, 20] from the Pauli paramagnetic weak limit [6] to the localized-moment limit, even in the metallic state [4], leading the unified relation between $p_s/p_{\text{eff}}$ (paramagnetic Bohr magneton number obtained from the Curie constant above $T_C$) and $T_C/T_0$ independent of magnetic materials as

$$p_{\text{eff}} / p_s = 1.4 \times \left( T_C / T_0 \right)^{2/3},$$

(6)

which gives the new universal picture (the universal $p_{\text{eff}}/p_s$ vs $T_C/T_0$ plot) among various ferromagnetic materials [13, 19, 20, 22] instead of phenomenological Rhodes-Wohlfarth plot ($p_{\text{eff}}/p_s$ vs $T_C$ plot), which was discussed based on the mean field theory [7].

Next, Takahashi has assumed the global consistency (GC) at $T_C$ [13]. In the Stoner and
SCR theories assumed the Landau expansion up to the $M^4$-term is important in magnetic free energy, there occurred the discontinuity at $T_C$ in these theories. He has assumed that the $M^6$-term is important at $T_C$, resulting in the continuity in $M$ at $T_C$ (GC) [13, 19, 20]. By this assumption he obtained the following relation at $T_C$ as

$$\left( \frac{M}{M_s} \right)^4 = 2\left[ 3\pi \left( 2 + \sqrt{5} \right) \right] \frac{N_0 \mu_B^2 \chi^2}{T_A P_s^2} \frac{T_C^2}{M} H.$$  (7)

which leads to the validity of $M^4$ vs $H/M$ plot instead of $M^2$ vs $H/M$ plot at $T_C$, where $M_s$ is the spontaneous magnetization and $\mu_B$ is the Bohr magneton. Furthermore, consequently from eq. (7) we can obtain the value of $T_A$ from the $M^4$ vs $H/M$ plot experimentally. These results from Takahashi’s theory of spin fluctuations have been proved quantitatively by several experiments [19-23].

4. Exotic Superconductivity and Spin Fluctuations

Since the novel superconductors have been discovered in the strongly correlated electron systems, such as heavy-fermion compounds and intermetallics [24], the organic systems [25], the high-$T_c$ cuprates [26, 27], and Fe pnictides [28, 29], the correlations and interplays between the itinerant magnetism and the novel superconductivity, called exotic superconductivity, have been important, and the itinerant-electron characteristics have recently become one of the most difficult and important problems in the solid state sciences [30-33]. The formalism of the BCS mean field theory [34-36] should be valid even in high-$T_c$ cuprate and iron pnictides superconductors, as well as other strongly correlated electron superconductors, such as heavy-fermion superconductors and organic superconductors, although the mediation mechanism of Cooper pairs may be different from that of BCS theory [30-33]. In high-$T_c$ cuprates, microscopic experiments have shown that the magnetic excitations were crucial [37], leading to the possible mechanism involving magnetic interaction-mediated Cooper pairs [30-33]. In the spin-fluctuation theory, the superconducting transition temperatures $T_c$ are found to be universally scaled by the characteristic temperature corresponding to the energy width of spin fluctuations, $T_0$, in exotic superconductors [32].

5. International Workshop on Itinerant-Electron Magnetism (IWIEM)

In this workshop on itinerant-electron magnetism, we had a plan to bring together an international group of leading theoreticians and experimental scientists on magnetism to discuss advanced topics in condensed matter physics, especially related to spin fluctuations in itinerant-electron magnetism including exotic superconductivity with magnetic origins, and to shape the future development of this field. We also planned to invite young scientists as well as graduate students. We hoped that such young scientists had chances to talk with invited speakers and organizers on their own interests.

Finally, this workshop was organized for a celebration of and in commemoration of Professor Yoshinori Takahashi’s retirement from University of Hyogo, Japan.

6. Invited Presentations of IWIEM

The invited talks (speakers and titles) in this workshop were as follows:

**Rafik Ballou**, Institute Néel, CNRS & University Joseph Fourier, Grenoble, France, “The Spin Liquid Phase Conundrum in the Metallic Magnet YMn$_2$.”
Nicholas Curro, Department of Physics, University of California, Davis, California, USA, “NMR Studies of Inhomogeneous Glassy Behavior driven by Nematic Fluctuations in Iron Arsenide Superconductors”

Minghu Fang, Department of Physics, Zhejiang University, Hangzhou, China, “Superconductivity and Itinerant Electron Magnetism in TiCo$_{2-x}$Ni$_x$S$e_2$ System”

Asaya Fujita, Green Magnetic Material Research Center, AIST Chubu, Nagoya, Japan, “Entropics: science and engineering of caloric phenomena related to itinerant-electron magnetism and spin fluctuations”

Swee K. Goh, Department of Physics, The Chinese University of Hong Kong, Hong Kong, China, “Structural Quantum Criticality in Superconducting (Ca$_x$Sr$_{1-x})_3$Rh$_4$Sn$_{13}$”

Jürgen Haase, Faculty of Physics and Earth Sciences, University of Leipzig, Leipzig, Germany, “Uniform Spin Susceptibility and a New Phase Diagram from NMR of Cuprate Superconductors”

Zenji Hiroi, The Institute for Solid State Physics, The University of Tokyo, Chiba, Japan, “Revisiting the Metal-Insulator Transition of VO$_2$: Molecular Orbital Crystallization”

Kenji Ishida, Department of Physics, Graduate School of Science, Kyoto University, Japan, “Nuclear Magnetic Resonance Studies on Ferromagnetic Superconductor UCoGe”

Masayuki Itoh, Department of Physics, Graduate School of Science, Nagoya University, Nagoya, Japan, “Heavy-Fermion Behavior and Metal-Insulator Transition in Vanadium Oxides Investigated by NMR”

Ryosuke Kadono, Muon Science Laboratory, Institute of Materials Structure Science, KEK, Ibaraki, Japan, “Quasi-One-Dimensional Spin Dynamics at Low Energies in d-electron Heavy-Fermionlike Metals”

Shinsaku Kambe, Advanced Science Research Center, Japan Atomic Energy Agency, Ibaraki, Japan, “Distributed Twofold Ordering in URu$_2$Si$_2$”

Toru Sakai, Graduate School of Material Science, University of Hyogo, Hyogo, Japan, Japan Atomic Energy Agency, SPring-8, Sayo, Hyogo, Japan, “Quantum Spin Liquid in the Kagome-Lattice Antiferromagnet and Related Systems”

Noriaki Sato, Department of Physics, Graduate School of Science, Nagoya University, Japan, “Quantum Critical Behavior in Magnetic Quasicrystals and Approximant Crystals”

Yoshinori Takahashi, Graduate School of Material Science, University of Hyogo, Japan, “Theoretical Development in Itinerant Electron Ferromagnetism”

Masashi Takigawa, The Institute for Solid State Physics, The University of Tokyo, Chiba, Japan, “NMR Investigations on Novel Fluctuations in f Electrons”

Takeshi Waki, Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University, Japan, “Itinerant Electron Magnetism in Cr-based MAX Phase Compounds”

Hiroyuki Nakamura, Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University, Japan, “Closing Address”

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References
[1] Stoner E C “Collective Electron Ferromagnetism” 1938 Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 165 372–414; “Collective Electron Ferromagnetism II. Energy and Specific Heat” 1939 ibid. 169 339–371
[2] Mott N F “The Basis of the Electron Theory of Metals, with Special Reference to the Transition Metals” 1949 Proc. Phys. Soc. (London) A62 416-422; “Metal-Insulator Transition” 1968 Rev. Mod. Phys. 40 677–683
[3] Hubbard J H, “Electron Correlations in Narrow Energy Bands” 1963 Proc. Roy. Soc. A276 238-257; 1964 ibid. A277 237-259; 1964 ibid. A281 401-419
[4] Anderson P W “New Approach to the Theory of Superexchange Interactions” 1959 Phys. Rev. 115 2-13; “Localized Magnetic States in Metals” 1961 ibid. 124 41-53
[5] Murata K K and Doniach S “Theory of Magnetic Fluctuations in Itinerant Ferromagnets” 1972 Phys. Rev. Lett. 29 285–288
[6] Moriya T and Kawabata A “Effect of Spin Fluctuations on Itinerant Electron Ferromagnetism I & II” 1973 J. Phys. Soc. Jpn. 34 639-651; 1973 ibid. 35 669-676
[7] Wohlfarth E L “Magnetic Properties of Crystalline and Amorphous Alloys: A Systematic Discussion Based on the Rhodes-Wohlfarth Plot” 1978 J. Magn. & Magn. Mater. 7 113-120
[8] Moriya T and Takahashi Y “Spin Fluctuation Theory of Itinerant Electron Ferromagnetism – A Unified Picture” 1978 J. Phys. Soc. Jpn. 45 397-408
[9] Moriya T “Recent Progress in the Theory of Itinerant Electron Magnetism” 1979 J. Magn. & Magn. Mater. 14 1-46
[10] Moriya T “Electron correlation and magnetism in narrow-band systems” 1981 (Springer-Verlag)
[11] Moriya T “Spin Fluctuations in Itinerant Electron Magnetism” 1985 (Springer-Verlag, Springer Series in Solid-State Sciences 56, Berlin Heidelberg NewYork Tokyo)
[12] Takahashi Y and Moriya T “Quantitative Aspects of the Theory of Weak Itinerant Ferromagnetism” 1985 J. Phys. Soc. Jpn. 54 1592-1598
[13] Takahashi Y “On the Origin of the Curie-Weiss Law of the Magnetic Susceptibility in Itinerant Electron Ferromagnetism” 1986 J. Phys. Soc. Jpn. 55 3553-3573
[14] Moriya T “A unified picture of magnetism” in “Metallic Magnetism” 1987 (ed. H. Capellmann, Springer-Verlag, Berlin)
[15] Yoshimura K, Takigawa M, Takahashi Y, Yasuoka H and Nakamura Y “NMR Study of Weakly Itinerant Ferromagnetic Y(Co$_{1-x}$Al$_x$)$_2$” 1987 J. Phys. Soc. Jpn. 56 1138-1155
[16] Yoshimura K, Mekata M, Takigawa M, Takahashi Y and Yasuoka H “Spin Fluctuations in Y(Co$_{1-x}$Al$_x$)$_2$: A Transition System from Nearly to Weakly Itinerant Ferromagnetism” 1988 Phys. Rev. B 37 3593-3602
[17] Moriya T and Takimoto T “Anomalous Properties around Magnetic Instability in Heavy Electron Systems”1995 J. Phys. Soc. Jpn. 64 960-969
[18] Yoshimura K, Imai T, Kiyama T, Thurber K R, Hunt A W and Kosuge K “$^{17}$O NMR Observation of Universal Behavior of Ferromagnetic Spin Fluctuation in the Itinerant Magnetic System Sr$_{1-x}$Ca$_x$RuO$_3$” 1999 Phys. Rev. Lett. 83 4397-4400
[19] Takahashi Y and Yoshimura K “Itinerant Electron Magnets and Spin Fluctuations” 2012 (1st ed., Uchida Rokakuho, ISBN4-621-07307-9)
[20] Takahashi Y “Spin Fluctuation Theory of Itinerant Electron Magnetism” 2013 (Springer-Verlag,
[21] Ohta H and Yoshimura K “Anomalous Magnetization in the Layered Itinerant Ferromagnet LaCoAsO” 2009 Phys. Rev. B 79 184407/1-5

[22] Yang J, Chen B, Wang H, Mao Q, Imai M and Yoshimura K “Magnetic Properties in layered AC0.5S0.5 (A=K, Rb, Cs) with the ThCr2Si2-type structure” 2013 Phys. Rev. B 88 064406/1-9

[23] Imai M, Michioka C, Ohta H, Matsuo A, Kindo K, Ueda H, and Yoshimura K “Anomalous itinerant-electron metamagnetic transition in the layered Sr1-xCaxCu2P2 system” 2014 Phys. Rev. B 90 014407/1-6

[24] Steglich F, Aarts J, Bredl C D, Lieke W, Meschede D, Franz W, Schäfer H “Superconductivity in the Presence of Strong Pauli Paramagnetism: CeCu2Si2” 1979, Phys. Rev. Lett. 43 1892–1896

[25] Lebed A G (Ed.) “The Physics of Organic Superconductors and Conductors” 2008 (Springer-Verlag, Springer Series in Materials Science, Vol. 110, Berlin Heidelberg New York)

[26] Bednorz J G and Müller K A “Possible high Tc superconductivity in the Ba–La–Cu–O system” 1986 Zeitschrift für Physik B Condensed Matter 64 189-193

[27] Wu M K, Ashburn J R, Torng C J, Hor P H, Meng R L, Gao L, Huang Z J, Wang Y Q, Chu C W “Superconductivity at 93 K in a New Mixed-Phase Y-Ba-Cu-O Compound System at Ambient Pressure” 1987 Phys. Rev. Lett. 58 908–910

[28] Kamihara Y, Hiramatsu H, Hirano M, Kawamura R, Yanagi H, Kamiya T, Hosono H “Iron-Based Layered Superconductor: LaOFeP” 2006 J. Am. Chem. Soc. 128 10012–10013

[29] Kamihara Y, Watanabe T, Hirano M, Hosono H “Iron-Based Layered Superconductor La[O1-xFx]FeAs (x = 0.05–0.12) with Tc = 26 K” 2008 J. Am. Chem. Soc. 130 3296–3297

[30] Anderson P W “Twenty-five Years of High-Temperature Superconductivity – A Personal Review” 2013 Journal of Physics: Conference Series 449 012001/1-10; “Resonating Valence Bonds: A New Kind of Insulator?” 1973 Mat. Res. Bull. 8 153-160

[31] Nagaosa N and Lee P A “Normal-state properties of the uniform resonating-valence-bond state” 1990 Phys. Rev. Lett. 64 2450-2453; Lee P A and Nagaosa N “Gauge theory of the normal state of high-Tc superconductors” 1992 Phys. Rev. B 46 5621-5639

[32] Moriya T “Antiferromagnetic spin fluctuation and superconductivity” 2006 Proc. Jpn. Acad. Ser. B 82 1-16; Moriya T and Ueda K “Antiferromagnetic spin fluctuation and superconductivity” 2003 Rep. Prog. Phys. 66 1299–1341; Moriya T, Takahashi Y and Ueda K “Antiferromagnetic spin fluctuations and superconductivity in high-Tc oxides” 1992 J. Magn. & Magn. Mater. 104-107 456-460; Moriya T, Takahashi Y and Ueda K “Antiferromagnetic spin fluctuations and superconductivity –A Possible Model for High Tc Oxides” 1990 J. Phys. Soc. Jpn. 59 2905-2915

[33] Pines D “Finding New Superconductors: The Spin-Fluctuation Gateway to High Tc and Possible Room Temperature Superconductivity” 2013 J. Phys. Chem. B 117 13145–13153

[34] Bardeen J, Cooper L and Schrieffer J R “Theory of superconductivity” 1957 Phys. Rev. 108 1175-1204

[35] Gorkov L P “Microscopic Derivation of the Ginzburg-Landau Equations in the Theory of Superconductivity” 1959 Sov. Phys. JETP 9 1364-1367

[36] Bogoliubov N N 1958 Nuovo Cimento 7 794; “A New Method in the Theory of Superconductivity. I, II, III” 1958 Sov. Phys. JETP 34 41-55

[37] Imai T, Slichter C P, Yoshimura K and Kosuge K “Low Frequency Spin Dynamics in Undoped and Sr-Doped La2CuO4” 1993 Phys. Rev. Lett. 70 1002-1005; Imai T, Slichter C P, Yoshimura K,
Kato M and Kosuge K “Spin-Spin Correlation in the Quantum Critical Regime of La$_2$CuO$_4$” 1993

Phys. Rev. Lett. 71 1254-1257