Magnetic Properties of Uniaxial Ferromagnets

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Recently we have presented a Green-function method to investigate a ferromagnetic spin system with the single-ion uniaxial anisotropy and have obtained a set of coupled equations to determine magnetic quantities of the system such as spontaneous magnetization, paramagnetic susceptibility and the critical temperature as a function of temperature or the anisotropy constant.\,\textsuperscript{1,2} We have shown that these quantities obtained are reduced to the molecular-field (M.F.) results in the limit of large anisotropy and to the RPA results,\,\textsuperscript{3} more closely to Lines' results obtained by an improved decoupling procedure\,\textsuperscript{4} in the other limiting case of small anisotropy.

The aim of the present note is to ascertain such a characteristic feature of our results in numerical ways in comparison with results obtained from other theories. Numerical calculations are carried out for two simple systems ($S=1$) in simple-cubic lattice structure and 2-dimensional square lattice structure. Similar investigations for the former system have been examined by other authors.\,\textsuperscript{5,6}

Basic equations necessary for the present problem are summarized as follows:

\begin{align}
\langle S'\cdot S' \rangle &= 2\langle S' \rangle \Phi + (T + \langle S' \rangle) \Psi, \tag{1} \\
\langle (S')^2 \rangle &= \left\{ 1 + \Phi \right\} \langle S' \rangle + 2\Phi / (1 + 3\Phi), \tag{2} \\
\langle (S')^2 \rangle + \langle S' \cdot S' \rangle + \langle S' \rangle &= 2, \tag{3}
\end{align}

where

\begin{align}
\Phi &= \frac{1}{N} \\
\times \sum_{\mathbf{Q}} \left( \mathbf{Q}_+ - \mathbf{Q}_0 - D \right) f(\mathbf{Q}_+ - \mathbf{Q}_0 - D) f(\mathbf{Q}_-) \\
\Psi &= \frac{1}{N} \sum_{\mathbf{Q}} 2D f(\mathbf{Q}_+) - f(\mathbf{Q}_-). \tag{5}
\end{align}

In the above equations $f(x) = \left\{ \exp\left( x/k_B T \right) - 1 \right\}^{-1}$, and $\mathbf{Q}_0$ is given by Eq. (10), $\mathbf{Q}_+$ ($\mathbf{Q}_-$) by Eq. (26) in Ref. 1), respectively. From these equations one can obtain spin averages $\langle S' \rangle$ and $T' = \langle (S')^2 \rangle - 2$ simultaneously as a function of temperature, magnetic field $H_0$ and the anisotropy constant $D$. Spontaneous polarization $\langle S' \rangle_0$ which is obtained from Eqs. (1)\,\textendash\,(5) by putting $H_0=0$ and $T'$ in that case, are shown in Fig. 1 for two lattices with various values of $D$. In each case $\langle S' \rangle_0$ and $T'$ approach to the M.F. results for large values of $D$ and to RPA results in the limit of small $D$. For the 2-dimensional lattice the system with $D=0$ does not become ordered state even at $T$ =0, thus $\langle S' \rangle_0$ for this lattice disappears in the limit of small $D$. It should be noticed that temperature dependence of
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$\langle S^\prime \rangle_0$ is affected remarkably by the existence of the anisotropy and deviation of the present result from the RPA and M.F. result is seen in each lattice, especially in the square lattice. Equations to determine the critical temperature $T_c$ and paramagnetic susceptibility $\chi_0$ are obtained from Eqs. (1) $\sim$ (5) by expanding them with respect to $\langle S^\prime \rangle$, which are given by Eqs. (62) and (63) in Ref. 1). The critical temperature where $\langle S^\prime \rangle_0$ vanishes and the derivative of $\Gamma$ with respect to temperature changes discontinuously in Fig. 1 is also obtained by putting $1/\chi_0$ $\to$ 0 in these equations in the present approximation. $T_c$ and $1/\chi_0$ thus obtained are shown in Figs. 2 and 3 for various values of $D$. An characteristic feature of the present theory is again seen in these figures. In contrast to wide variation of $T_c$ and $1/\chi_0$ with respect to $D$ seen in the RPA results the present results are

![Fig. 1. $\langle S^\prime \rangle_0$ and $\Gamma$ for various values of the anisotropy constant $D/2J_z$. (a) simple-cubic lattice (z=6), (b) square lattice (z=4). The solid line with 0(RPA) represents the present and RPA results for $D=0$, and lines with $\infty$ (M.F.) the present and M.F. results for $D=\infty$, respectively.](image1)

![Fig. 2. The critical temperature as a function of the anisotropy constant $D/2J_z$. (a) simple-cubic lattice, (b) square lattice.](image2)

![Fig. 3. Paramagnetic susceptibility for various values of the anisotropy constant $D/2J_z$. (a) simple-cubic lattice, (b) square lattice. The solid line with 0(RPA) represents the present and RPA results for $D=0$, and those with $\infty$ (M.F.) the present and M.F. results for $D=\infty$, respectively.](image3)
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reduced to the M.F. results in the large limit of $D$. $k_B T_c$ for small $D$ is given by

\[ (4Jz/3W)(1 + (3/4)^{1/2}(A/W)(D/2Jz)^{1/2} + \cdots) \]

for the sc lattice and $(4\pi Jz/3)\log(Jz/D)$, the RPA result, for the square lattice, respectively. The RPA result for the former lattice is shown to have a factor $(2)^{1/2}$ instead of $(3/4)^{1/2}$ in the present result. The numerical calculations were carried out on the computer system NEAC 2200/500 at the Okayama University Computer Center and the HITAC 8800/8700 at the Computer Center, University of Tokyo.