Curie Temperature for Dilute Bond-Disordered Ferromagnet by the Use of Coherent Potential Approximation

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September 20, 1975

We report the Curie temperature $T_c$ for a bond-disordered anisotropic Heisenberg model for simple cubic lattice calculated by the simplest coherent potential approximation (CPA) and the random phase approximation (RPA). The Hamiltonian would be

$$\mathcal{H}_\alpha = \sum_{\langle i,m \rangle} \left[ -2I_{1m}(S_i^zS_{m}^z + S_i^\perp S_{m}^\perp) - 2J_{1m}S_i^\perp S_{m}^\perp \right],$$

(1)

where $I_{1m}$ and $J_{1m}$ are the exchange integrals which may take on either $I_A$ and $J_A$ or $I_B$ and $J_B$, respectively. Other notations are those which are usually used. Using the CPA explained in Ref. 1) for the bond-disordered Heisenberg model, we would obtain the self-consistent equations for the coherent exchange integrals $I$ and $J$, as follows:

$$\sum_{\alpha=A,B} \rho_\alpha \left[ J_\alpha (1-U_\alpha) + J_\alpha W_\alpha \right] = 0,$$

$$\sum_{\alpha=A,B} \rho_\alpha \left[ J_\alpha (1-U_\alpha) + J_\alpha W_\alpha \right] = 0,$$

(2)

$$U_\alpha = \frac{1}{N} \sum_{\mathbf{k}} \frac{J_\alpha - J_\alpha T_{\mathbf{k}}}{E - 12S(J - I_{\mathbf{T}_\mathbf{k}})}, \quad (\alpha=A,B)$$

$$W_\alpha = \frac{1}{N} \sum_{\mathbf{k}} \frac{J_\alpha - J_\alpha T_{\mathbf{k}}}{E - 12S(J - I_{\mathbf{T}_\mathbf{k}})},$$

$$\mathcal{J}_\alpha = 2S(J_\alpha - I_{\mathbf{T}_\mathbf{k}}), \quad \mathcal{J}_\alpha = 2S(J_\alpha - J),$$

$$\gamma_{\mathbf{k}} = \frac{1}{3} (\cos k_x + \cos k_y + \cos k_z),$$

where $\rho_A$ and $\rho_B$ are concentrations of A

![Fig. 1. Density of states of magnon for dilute (a) Ising and (b) Heisenberg ferromagnet of simple cubic lattice for various concentrations $\rho_A$ of $J_A$ bonds. Numerical numbers attached on the curves denote $\rho_A$. The $\delta$ functions are not shown in the figures.](https://academic.oup.com/ptp/article-abstract/54/6/1894/1848572/546/1848572/546)

![Fig. 2. $T_c$ versus $\rho_A$ for the dilute bond-disordered Ising and Heisenberg ferromagnet. The dots denote the values obtained by numerical calculations.](https://academic.oup.com/ptp/article-abstract/54/6/1894/1848572/546/1848572/546)
and B bonds, respectively. Hereafter we treat the dilute ferromagnet \((I_B=J_B=0)\).

In the Ising limit \((I_A=I=0)\), after obtaining \(J\) as a function of \(E\) from (2), we can calculate the density of states of magnon \(\rho(E)\), which is shown in Fig. 1(a). When \(p_A=I\), \(\rho(E)\) is the \(\delta\) function at \(E=6J_A\) as it should be. As \(p_A\) decreases, the height of the \(\delta\) function diminishes, while a band appears around \(E=5J_A\) which is the energy of localized mode for an impurity bond.

Rigorously, \(\rho(E)\) should consist of \(\delta\) functions at \(6J_A, 4J_A, 2J_A\) and 0, so that the appearance of the band would be attributed to the treatment by the CPA. When \(p_A=1/6\), the \(\delta\) function disappears and the band diverges at \(E=6J_A\).

\(\rho(E)\) for \(p_A<0.5\) is symmetric against that for \(p_A>0.5\) as seen in Fig. 1(a). Specially we note that \(\rho(E)\) diverges at \(E=0\) when \(p_A=1/6\). Using \(\rho(E)\) and the RPA, we obtain \(T_c\) analytically as follows:

\[
\frac{J_A}{2kT_c} = \int \frac{\rho(E)}{E} dE = \frac{5}{6(6p_A-1)}.
\]

As is shown in Fig. 2, \(T_c\) decreases linearly with \(p_A\) and the critical concentration is \(p_c=1/6=0.1667\). This value should be compared with those by the percolation theory \((p_c=0.24, 0.254)\), the Bethe approximation \((p_c=0.2)\), and the molecular field approximation \((p_c=0)\). Therefore considering from the standpoint of static statistical theory, it would be said that the CPA is between the molecular field approximation and the Bethe approximation.

Similar calculations can be carried out in the Heisenberg limit \((I_A=J_A, I=J)\). In order to calculate \(\rho(E)\) for \(p_A<1\), we have used the approximate formulae for the density of states given by Tonegawa\(^5\) for a pure system \((p_A=1)\), after obtaining \(J\) as a function of \(E\) from (2). The results are shown in Fig. 1(b). When \(p_A=1/3\), which is the critical concentration, \(\rho(E)\) diverges at \(E=0\). The \(T_c\) vs \(p_A\) curve calculated numerically, can be expressed well by \(kT_c/J_A=3p_A-1\) as shown in Fig. 2. This formula is identical to that given by Tahir-Kheli\(^6\) in the case of site model, which would be due to his ambiguous approximation.

When \(p_A\) is below \(p_c\), \(\rho(E)\) for both the Ising and the Heisenberg models has the \(\delta\) function at \(E=0\) and the band around \(E=J_A\) (Ising) or \(E=2J_A\) (Heisenberg), respectively. The coefficient of the \(\delta\) function is expressed by \(1-(p_A/p_c)\), and the area of the band is \(p_A/p_c\). The \(\delta\) function is the density of states due to spins surrounded by non-magnetic bonds, while the band is that due to spin pairs surrounded by non-magnetic bonds, because the excitation energy of the former is zero, while that of the latter is \(J_A\) (Ising) and \(2J_A\) (Heisenberg), respectively.