

Abstract Submitted
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Paramagnetic iron spin dynamics simulations¹ XIUPING TAO, D. P. LANDAU, Center for Simulation Physics, University of Georgia, Athens, GA 30602, T. C. SCHULTHESS, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, G. M. STOCKS, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — The contradiction^{2,3,4} about paramagnetic BCC iron spin dynamics is investigated using a classical Heisenberg model with four shells of interacting neighbors and exchange parameters derived from electronic structure calculations. For $T \geq T_c$ (up to at least $1.2T_c$), the spin dynamics simulated dynamic structure factor $S(\vec{q}, E)$ ⁵, with \vec{q} fixed, has two symmetric peaks and a third peak at zero energy. Fitting results show that the symmetric peaks are due to spin-waves. The dispersion curves soften in energy with increasing temperatures and generally lie lower than those of the experiments², but both sets have the same qualitative features and suggest that spin wave excitations persist above T_c .

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²J. W. Lynn, Phys. Rev. B **11**, 2624 (1975).

³G. Shirane, O. Steinsvoll, Y. J. Uemura and J. Wicksted, J. Appl. Phys. **55**, 1887 (1984).

⁴H. A. Mook and J. W. Lynn, J. Appl. Phys. **57**, 3006 (1985).

⁵Shan-Ho Tsai, Alex Bunker and D. P. Landau, Phys. Rev. B **61**, 333 (2000).

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