Nearest-neighbor exchange in solid ^{3}He

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The effect of including nearest-neighbor exchange into the spin Hamiltonian proposed for solid ^{3}He is studied using the full diagonalization of a 16-quantum-spin cluster.

Stipdonk and Hetherington[1] have recently attempted to fit the experimental data on the nuclear magnetic properties of solid ^{3}He at low temperatures by adding nearest-neighbor two-spin exchange to a phenomenological Hamiltonian[2] involving three-spin ring exchange and planar four-spin exchange. They determine parameters by analyzing the high-temperature data in terms of a high-temperature series, and calculate properties of the low-temperature ordered phases using classical mean field theory. The main purpose of adding two-spin exchange is to bring down the theoretical estimate for the magnetic field at which a transition occurs between the low-field antiferromagnetic phase (thought to be the $u2d2$ phase) and a high-field ferromagnetic phase (canted normal antiferromagnet)[2] at zero temperature, to give better agreement with experiment.[3] This is achieved at the expense of introducing a second antiferromagnetic phase between the $u2d2$ phase and the paramagnetic phase in the predicted phase diagram. The experimental evidence seems to be against such a phase diagram, but sufficient uncertainty exists that the hypothesis may not be entirely ruled out on these grounds.

It is known that quantum corrections to the classical description of the three-spin–four-spin exchange Hamiltonian are typically very large. Evidence for this comes from spin wave calculations[2] and the diagonalization of the quantum Hamiltonian for a small system.[4] Here we present the results extending our diagonalization of the 16-spin ($2\times2\times2$ cube plus body centers, with periodic boundary conditions) quantum system to include two-spin exchange. (For a discussion of the method and the limitations of this approach, see Ref. 4.) The Hamiltonian we use is

$$H = J\sum_{\langle ij\rangle}^{\mathrm{NN}}(P_{ij}-\tfrac{1}{2}) - J_t\sum_{\langle ijk\rangle}^{T}(P_{ijk}+P_{ijk}^{-1}-\tfrac{1}{2}) + K_P\sum_{\langle ijkl\rangle}^{P}(P_{ijkl}+P_{ijkl}^{-1}-\tfrac{1}{4}) \ , \quad (1)$$

where $P_{ijk\ldots}$ is the cyclic permutation operator acting on the spin coordinates at sites $i,j,k\ldots$. The pair exchange term with weight J runs over all nearest-neighbor pairs; the triple exchange term with weight $-J_t$ runs over all triangles in the

TABLE I. Values of J,J_t,K_P consistent with $\Theta_w=-1.8$ mK and $e_2=6.8$ (mK)^2.

J (mK)	J_t (mK)	K_P (mK)
0	0.144	0.387
0.1	0.148	0.374
0.2	0.152	0.359
0.3	0.154	0.342
0.4	0.155	0.322
0.5	0.156	0.322
0.6	0.155	0.276
0.7	0.152	0.248
0.8	0.147	0.217
0.9	0.140	0.181
1.0	0.130	0.137

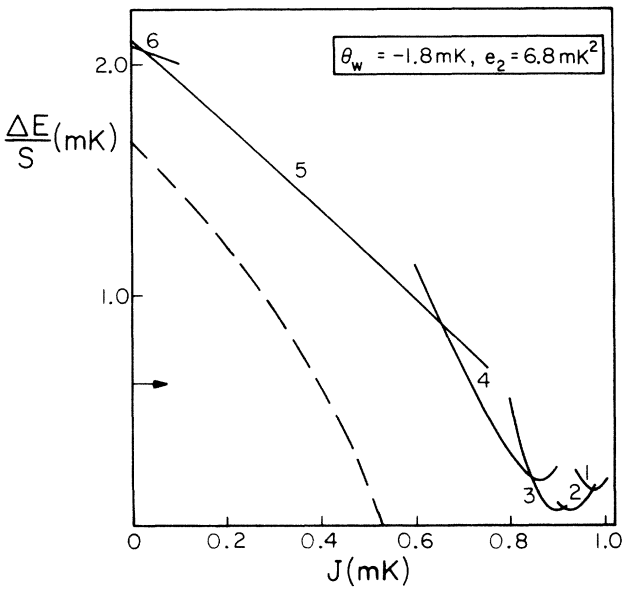

FIG. 1. Plot of the transition field $H_1(S)=\Delta E(S)/S$ at $T=0$ K to a state with given spin S, from the ground state in zero field (always $S=0$ for these parameters), as a function of the two-spin coupling J. For each value of J, values of the three-spin coupling J_t and the four-spin coupling K_P are chosen to fit high-temperature data as discussed in the text. Solid line: 16-spin-quantum calculation with values of S as marked. Dashed line: classical estimate. (In the latter we have neglected perturbations in either phase due to the magnetic field: The inclusion of a finite susceptibility would give only small corrections.) For solid ^{3}He the predicted transition field is $H_1=(6.4\Delta E/S)$ kG with ΔE in mK. The arrow on the ordinate shows the experimental transition field $H_1=4$ kG.

lattice consisting of two nearest neighbors and one next-nearest neighbor; the four-spin exchange term is restricted to run over only planar rings of four nearest neighbors. Our parameters J,J_t,K_P are the same as those of Stipdonk and Hetherington,[1] except for an overall sign change.

To present our results we plot the transition field $H_1(S)$ at zero temperature between the singlet ground state and the lowest-energy state with a specified nonzero spin (magnetization) S, against the value of the nearest-neighbor exchange J. $H_1(S)$ is given by $\Delta E(S)/S$, where $\Delta E(S) = E(S) - E_0$ is the difference in the energy $E(S)$ of the lowest-energy state of spin S and the singlet ground state energy, E_0. For each J, the values of J_t and K_P were chosen to fit the high-temperature series coefficients e_2 and Θ_w defined from the specific heat for N particles:

$$C = \tfrac{1}{4}N(e_2/T^2 - e_3/T^3 + \cdots) , \tag{2}$$

and the susceptibility χ:

$$\chi^{-1} = 4N^{-1}(T - \Theta_w + B/T + \cdots) . \tag{3}$$

At melting pressure $e_2 \simeq 6.80$ (mK)^2; the value of Θ_w is rather uncertain: For comparison purposes we follow Stipdonk and Hetherington in using $\Theta_w = -1.8$ mK. The values of J_t and K_P for a sequence of J are shown in Table I. Our results for $H_1(S)$ vs J are shown in Fig. 1. Two conclusions are suggested. The first is that a significantly larger nearest-neighbor exchange rate is needed to bring the transition field down to the experimentally observed value of about 4 kG: For this value we would predict a value of $J = 0.72$ mK (with $J_t = 0.15$ mK, $K_P = 0.24$ mK) compared with the classical prediction of $J = 0.38$ mK (with $J_t = 0.155$ mK and $K_P = 0.33$ mK). This is to be compared with the relatively small correction ($\sim 20\%$) for the prediction of the transition field at $J = 0$. Our large value of J alone, neglecting the small K_P and J_t, leads to a prediction (including quantum fluctuations) for the transition between the paramagnetic and normal antiferromagnetic phases at 2.0 mK, well above the observed transition to the $u2d2$ phase. The second conclusion, which is also evident from the classical results, is that the small H_1 is achieved by a rather delicate tuning of the value of J to approach the transition value at which the "normal antiferromagnetic phase" takes over as the low-field phase from the $u2d2$ phase.[2] If this is indeed the case, the field H_1 might be expected to be particularly sensitive to the application of pressure.

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