Spin ordering and coherent atomic motion in bcc solid ^{3}He

Nir Gov [a,1], Emil Polturak [b],

[a] *Department of Materials and Interfaces, The Weizmann Institute of Science, Rehovot 76100, Israel*
[b] *Physics Department, Technion-Israel Institute of Technology, Haifa 32000, Israel*

Abstract

We propose a new model to describe the nuclear magnetism of bcc ^{3}He. According to this model, in bcc ^{3}He there is correlated zero-point motion of the nuclei, which gives rise to electric and magnetic polarizations of the electronic cloud. Our model describes the resulting modification of the phonon spectra and predicts new localized modes, which have been observed during the past year. The polarization of the electronic cloud leads to hyperfine magnetic interactions with the nuclear spin. Magnetic ordering results from an indirect spin-spin interaction. The model predicts correctly both the u2d2 symmetry of the ordered phase and the volume dependence of the magnetic interaction. We further predict the excitation branches (spin waves) of the ordered phase.

Key words: Nuclear magnetism; Solid ^{3}He ; Hyperfine interactions ;

The spin-ordered phase of bcc ^{3}He presents a difficult challenge to accurate theoretical description [1]. The prevalent description is in terms of atomic exchange cycles involving several atoms (Multiple Spin Exchange (MSE) model). Successively higher order cycles produce competing ferro and antiferromagnetic interactions [2]. For qualitative description within this MSE model, one needs large exchange cycles, which become difficult to calculate and prove their convergence [1,3], i.e. the magnetic order one finds depends on the order of the largest exchange cycle included. This conceptual problem, despite the relative successes of the MSE picture, therefore raises the interest in another approach [4].

We propose that magnetic ordering of ^{3}He is a result of correlations in the zero point atomic motion, rather than through exchange of atoms. We show that the anharmonic zero-point motion produces an oscillating magnetic polarization of the electronic cloud which then has hyper-fine interaction with the nuclear spin in each atom. The nuclear spins interact with each other indirectly, through the electric dipolar interaction between the atoms. The present account is a brief summary of our work [4].

At "high" temperatures (T$\gg$1mK), the atomic motion in bcc ^{3}He can be treated in the same way as in ^{4}He [5]. We establish, using the experimental specific heat, sound velocity and NMR data, the likely occurrence in bcc ^{3}He of long-range correlations in the zero-point motion of the atoms along the major axes [4]. These correlations can be described [5] in terms of coherent electric dipole interactions, and lead to the following modifications of the excitations spectra: (1) The observed marked (factor of 2) softening of the transverse T$_1$(110) phonon and (2) the appearance of a new optic-like mode at energy $2E_0$ (where E_0 is the Brillouin zone-boundary energy of the T$_1$(110) phonon). The second effect predicted by this model was recently observed in ^{4}He [6].

The effect of the anharmonic zero-point motion along the major axes of bcc Helium, is to introduce corrections to the adiabatic (Born-Oppenheimer) description of the atoms. In particular, these corrections produce a mixing of the electronic s and p levels, so that the electronic wave function is: $|\psi\rangle \simeq |s\rangle + \lambda\,|p\rangle$, where $\lambda \sim 10^{-2}$ is the mixing parameter [5]. In this

---

[1] E-mail: nirgov@wisemail.weizmann.ac.il

state, the atom will acquire an oscillatory electric dipole moment: $|\mu| = e\langle\psi|x|\psi\rangle \simeq 2e\lambda\langle s|x|p\rangle$. This electric dipole is accompanied by a magnetic polarization of the electronic cloud. The lowest $|p\rangle$ level of the He atom has the electrons in a spin $S = 1$ state. The electronic spin is then aligned along the direction of electric polarization due to dipolar interaction between the spins of the two electrons, of size: $\sim$ 1.4K. In the solid, the $S = 1$ sublevels are broadened due to the finite overlap of the electrons associated with neighboring atoms, leading to a sharp reduction in the electronic spin polarization with decreasing molar volume [4].

The ^{3}He nuclear spin $I = 1/2$ has hyperfine interaction with the electronic magnetic moment, of the contact type: $E_{mag} = \left\langle -\frac{8\pi}{3}\mathbf{N}_e \cdot \mathbf{N}_n \delta(r)\right\rangle$, where $\mathbf{N}_n$ is the effective nuclear magnetic moment, and the maximum electronic magnetic moment is $\mathbf{N}_e \sim 2\lambda g\mu_B$. We find the maximum value of $E_{mag}/k_B \simeq 4.5$mK for V=24 cm^3/mole. This energy is much larger than the direct nuclear dipole-dipole interaction ($\sim 0.1\mu$K), i.e. of the order of the transition temperature of nuclear ordering in bcc ^{3}He.

Due to the on-site hyperfine interactions, the local oscillation frequency of the electric dipole changes by $\sim E_{mag}/\hbar$. The resulting modulation of the electric dipole array can be described using its natural excitations, i.e. T$_1$(110) phonons. Keeping the lowest order in the expansion, this is equivalent to stating that in addition to the coherently oscillating dipoles μ, there is now an independent small component of the dipole, μ_m. In terms of E_{mag} and E_0, the size of this component is given by: $\mu_m \simeq \sqrt{(E_{mag}/E_0)}\mu$. Numerically, μ_m is about 10^{-2} of the oscillating dipole μ. At each lattice site the component of the electric dipole moment μ_m follows the nuclear spin. Since $\langle\mu\cdot\mu_m\rangle = 0$, the contribution of μ_m to the dipolar energy comes from their interaction with each other

$$E^m_{dip} = -\sum_{i\neq 0}\mu_{\mathbf{m},\mathbf{0}}\cdot\mu_{\mathbf{m},\mathbf{i}}\left[\frac{3\cos^2\left(\hat{\mu}_{\mathbf{m}}\cdot\hat{\mathbf{r}_{0i}}\right)-1}{|\mathbf{r}_{0i}|^3}\right] \qquad (1)$$

For this dipolar interaction to be non-zero, the μ_m's on different sites should be phase correlated, i.e. long-range nuclear spin order.

We therefore naturally obtain that the u2d2 configuration of the nuclear spins which has the lowest dipolar energy (1), is the one found experimentally [7]. Note that in our model, the symmetry of the ordered phase is independent of any quantitative parameters. This is in contrast to the MSE theory where this symmetry is determined by a competition between many parameters [1,2].

We then treat the indirect spin-spin interaction along the lines described in our treatment of the phonon modes [5]. The reduction in the ground-state energy of the u2d2 phase, compared to the paramagnetic phase at T=0, is calculated to be $\sim 50\mu$K per atom (V$\simeq$ 24cm^3/mole). We also calculated the velocities of the spin waves along various directions of the crystal: $6.0 - 10.0$ cm/sec, similar to those extracted from melting pressure measurements [8], where a value of 8.4 ± 0.4cm/sec was found.

From these values we calculate the free energy and arrive at the specific heat, transition temperature T_c, entropy discontinuity at T_c and the temperature dependence of the NMR frequency shift Ω_0. All these quantities compare very well with the available data [4].

To conclude, our model enables us to describe both the phonon spectra and the nuclear magnetic ordering of bcc ^{3}He using a single parameter, the dipolar energy E_0 (or equivalently, the mixing coefficient λ). In addition, the model predicts the correct symmetry of spin ordering both in the u2d2 and in the HFP and the volume dependence of the magnetic interactions. The predicted symmetries are independent of the strength of the effective spin-spin interaction.

Acknowledgements

We thank Tony Leggett, Gordon Baym, Assa Auerbach and Ady Mann. for many useful discussions and suggestions. This work was supported by the Israel Science Foundation, the Technion VPR fund for the Promotion of Research, the Fulbright Foreign Scholarship grant, NSF grant no. DMR-99-86199 and NSF grant no. PHY-98-00978.

References

[1] M. Cross and D. Fisher, *Rev. Mod. Phys.* **57** (1985) 881

[2] M. Roger, J.H. Hetherington and J.M. Delrieu, *Rev. Mod. Phys.* **55** (1983) 1; D.D. Osheroff and H. Godfrin, *Phys. Rev. B* **38** (1988) 4492.

[3] D.M. Ceperley and G. Jacucci, *Phys. Rev. Lett.* **58** (1987) 1648; B. Cowan and M. Fardis, *Low Temp. Phys.* **23** (1997) 448; J. DuBois and P. Kumar, *J. Low Temp. Phys.* **98** (1995) 37.

[4] N. Gov and E. Polturak, *J. Low Temp. Phys.* **121** (2000) 683; N. Gov and E. Polturak, *J. Low Temp. Phys.* **128** (2002).

[5] N. Gov and E. Polturak, *Phys. Rev. B* **60** (1999) 1019; N. Gov, *Phys. Rev. B* **62** (2000) 910.

[6] T. Markovich, E. Polturak, J. Bossy, and E. Farhi, *Phys. Rev. Lett.* **88** (2002) 195301; E. Polturak, presentation in this conference.

[7] D.D. Osheroff, M.C. Cross and D.S. Fisher, *Phys. Rev. Lett.* **44** (1980) 792.

[8] D.D. Osheroff and C. Yu, *Phys. Lett.* **77A** (1980) 458.