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MAGNETIC PROPERTIES OF SOLID $^3$He WITH $^4$He IMPURITIES IN A HUBBARD-LIKE MODEL (*)

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Resume. — Les effets d'échange dans le $^3$He solide qui contient quelques atomes de $^4$He comme impuré sont étudiés à l'aide d'un Hamiltonien comme celui de Hubbard. Une transformation canonique a été faite pour trouver un Hamiltonien contenant des termes qui décrivent l'échange entre deux atomes de $^3$He et entre un atome de $^3$He et un atome de $^4$He. Pour tenter de savoir à quel degré les propriétés magnétiques du $^3$He solide pur restent les mêmes, un analogue du théorème de Lieb-Mattis concernant l'état le plus bas de l'Hamiltonien a été prouvé, mais seulement dans le cas unidimensionnel. Le modèle à trois bains avec un bain d'échange modifié a servi pour calculer la dépendance des temps de relaxation sur la concentration du $^3$He et la chaleur spécifique bain d'échange de $^3$He impur bcc.

Abstract. — A Hubbard-like Hamiltonian is used to study exchange-effects in solid $^3$He when a few $^4$He atoms are present as impurities. A canonical transformation has been performed to arrive at a Hamiltonian with terms that describe exchange between two $^3$He atoms, and a $^3$He atom and a $^4$He atom. In an attempt to see to what extent the magnetic properties of pure solid $^3$He remain unaltered, an analog of the Lieb-Mattis theorem concerning the ground state of the Hamiltonian has been proved, but only in the one-dimensional case. The three-bath model has been used to calculate the $^4$He concentration dependence of the relaxation times and the exchange-bath specific heat of impure bcc $^3$He.

I. Introduction. — There have been several experiments [1-5] in recent years which indicate that $^4$He impurities have a considerable effect on the magnetic properties of solid $^3$He. Relaxation time measurements [1] in impure solid $^3$He show that some of the parameters occurring in the three-bath model [6] are influenced by the $^4$He impurities: The measured ratio $R$ of the exchange-bath specific heat and the Zeeman bath specific heat increases linearly with $x$, the Zeeman-exchange relaxation time $\tau_{Z,EX}$, the transverse relaxation time $T_2$, and the exchange-lattice relaxation time $\tau_{EX,1}$ are all affected by the impurity atoms, some more strongly than the others [6]. We have used a Hubbard-like cell model [7] to study some of these $^4$He impurity-effects.

II. The Effective Exchange Hamiltonian. — Our model describes the hopping of helium atoms from site to site in the solid and explicitly takes into account the large energy $\phi(a')$ it would require to put two $^3$He atoms [a $^3$He atom a $^4$He atom] in the same cell. The model Hamiltonian can be written as

$$H = A \sum_{ij} t_{ij} c_i^\dagger c_j + A' \sum_{ij} t_{ij} a_i^\dagger a_j +$$

$$+ \phi \sum_{i} n_i n_i + \phi' \sum_{i} n_i \rho_i,$$

(1)

where $c_i^\dagger(a_i^\dagger)$ creates a $^3$He atom with spin $\sigma$ (a $^4$He atom) in the $i$th cell, and $n_i$ and $\rho_i$ are the $^3$He and $^4$He number operators for the $i$th cell. $t_{ij}$ and $t_{ij}'$ represent dimensionless hopping matrix elements. The number of $^4$He atoms in the lattice is assumed to be small, and the interactions between them are neglected.

The effective Hamiltonian correct to second order in $A$ and $A'$ may be found (both in the presence and in the absence of vacancies in the lattice) by using a canonical transformation method [8]. To discuss exchange in impure solid $^3$He, we shall need only the effective Hamiltonian when there is exactly one atom per site and no vacancies. This is given by [10]

$$\tilde{H} = \frac{1}{2} \sum_{ij} J_{ij} I_i I_j + \sum_{ij} J_{ij} n_i \rho_j + \frac{1}{2} \sum_{ij} J_{ij}^\dagger D_{i\rho}^+ D_{i\rho}^-,$$

(2)

where the spin operators $I_i$ are expressed in terms of the $^3$He creation and destruction operators in the usual way:

$$I_i^\dagger = c_i^\dagger c_i,$$

$$I_i = c_i^\dagger c_i,$$

$$I_i^\dagger = \frac{(n_i - n_i)}{2}.$$

Furthermore, $D_{i\rho}^\dagger = c_i^\dagger a_{\rho}$ and $D_{i\rho} = a_{\rho}^\dagger c_i$.

The exchange constants are given by the following:

$$J_{ij} = -\frac{A^2}{\phi} t_{ij}^2;$$

$$J_{ij}' = -\frac{A^2}{\phi'} t_{ij}^2 - \frac{A^2}{\phi} t_{ij}^2;$$

$$J_{ij}^\dagger = -\frac{4A^2}{\phi} t_{ij}^2.$$

(3)

III. Ordering of Energy Levels of the Effective Exchange Hamiltonian. — Lieb and Mattis [9] have proved the following theorem for a class of antiferromagnetic Hamiltonians: If $E(I)$ denotes the lowest energy value corresponding to total spin $I$, then $E(I) < E(I + 1)$ for all $I$. In particular, the ground state has the lowest possible value of $I$.

We have found that adaptations of the methods used by Lieb and Mattis succeed for $\tilde{H}$ given in (2) so long as we restrict ourselves to a linear chain of cells, but that due to the interplay between the fermion-fermion exchange term and the boson-fermion exchange term these methods and others that we divided ourselves failed in two and three dimensions.

Since we are unable to extend this statement to the case of a three-dimensional lattice, we must ask...
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whether the ground state of impure $^3$He is perhaps not antiferromagnetic. The presence of a boson in the lattice is somewhat similar to that of a vacancy in the lattice as far as spin-ordering properties are concerned. Nagaoka [11] has shown in three dimensions for a bcc lattice with $\phi \to \infty$, and with a vacancy present, the ground state is ferromagnetic, rather than antiferromagnetic. However, Nagaoka's proof is not conclusive for finite $\phi$ and therefore does not take into account both hopping and Heisenberg exchange. A complicated interplay of magnetic exchange interactions and order-disturbing hopping must occur in three dimensions in our model. At this time there is no rigorous answer to the question of the nature of the ordering of the ground state.

IV. Calculation of the Three-Bath Model Parameters for Impure Solid $^3$He. — In order to study the magnetic resonance properties in our model, we add Zeeman and dipole interaction terms to the Hamiltonian, i.e.,

$$H = \tilde{H} + H_z + H_d,$$  

(4)

where $\tilde{H}$ is given in (2), $H_z = \gamma B \sum_i I_i^z = \omega F$, and $H_d$ is the dipole-dipole interaction between the spins. We shall ignore lattice-dynamic effects. The first term on the right hand side of (2) will be called $H_{BF}$ and the third term $H_{BF}$. The second term is dropped since it is a constant in the space of states we are considering. In the pure system, $H_{BF}$ would be the part of the Hamiltonian associated with the exchange-energy bath. It may be shown that $H_{BF}$ commutes with $H_z$, but not with $H_{BF}$. Therefore, in modifying the three-bath model to describe relaxation mechanisms in impure $^3$He, we cannot assign a bath to the $H_{BF}$ part of the Hamiltonian, distinct from the usual exchange-bath [6] to form a «four-bath» model. However, since $H_{BF} + H_{BF}$ commutes with $H_z$, we are justified in modifying the exchange bath in the conventional three-bath model to correspond to $H_{BF} + H_{BF}$ or $H$ when $^4$He impurities are present. Having done so, we may find $R$, $T_{2,EX}$, and $T_2$, using the usual density matrix approach with the high temperature expansion of the traces [1, 12].

Our results are as follows: The ratio of the exchange specific heat to the Zeeman specific heat is given by

$$R(x) \approx R(0) \left\{ 1 + \frac{8}{3} \alpha^2 x \right\},$$  

(5)

where $x = \nu/N \ll 1$, $\nu$ is the number of $^4$He atoms, $N$ is the total number of sites, $x$ is the number of nearest neighbors to a site,

$$R(0) = \frac{3J^2 z}{8\omega^2} \quad \text{and} \quad \alpha = \frac{J'}{J}.$$ 

The following results are for impure bcc $^3$He and hold good when $x \ll 1$: The Zeeman-Exchange relaxation time $\tau_{Z,EX}$ is given by

$$\frac{1}{\tau_{Z,EX}(x)} = \frac{(2\pi)^{16} M_2(x)}{3 \omega_{0} (1 + \alpha^2 x)^{16}} \left[ \exp \left( \frac{-\omega^2}{2 \omega_{0}^2 (1 + \alpha^2 x)} \right) + 4 \exp \left( \frac{-2 \omega^2}{\omega_{0}^2 (1 + \alpha^2 x)} \right) \right].$$  

(6)

The adiabatic part of the transverse relaxation time is given by

$$T_2'(x) = \left( \frac{2}{\pi} \right)^{15} \frac{\omega_0 (1 + \alpha^2 x)^{15}}{M_2(x)}. \quad (7)$$

The full transverse relaxation time $T_2$ is given by

$$\frac{1}{T_2(x)} = \frac{(2\pi)^{16} M_2(x)}{3 \omega_0 (1 + \alpha^2 x)^{16}} \left[ \frac{3}{2} + \frac{5}{2} \exp \left( \frac{-\omega^2}{2 \omega_{0}^2 (1 + \alpha^2 x)} \right) + \exp \left( \frac{-2 \omega^2}{\omega_{0}^2 (1 + \alpha^2 x)} \right) \right]. \quad (8)$$

In all the expressions given above, $M_2(x) = (1 - x) M_2 \approx M_2$.

The quantities $M_2$ and $\omega_0$ are as defined in Reference (12). $\omega_0$ has the value [12] 2.38 J. We can also verify that

$$T_2(x) = \left[ T_2(x) \right]_{\omega(\beta) = 0} = \frac{10}{3} \left[ T_2(x) \right]_{\omega(\beta) = 0},$$

which is the Kubo-Tomita [13] relation. Further $[T_{2,EX}(\omega)]_{\omega = 0} = [T_2(x)]_{\omega = 0}$.

The experiment of Bernier and Landesman [3] (BL) was done using bcc $^3$He with $\xi \leq 10^{-3}$, molar volume $V = 20.06$ cm$^3$, and $\omega/2\pi = 2.19$ MHz. They found that

$$R(x) = R(0)(1 + 825 x). \quad (9)$$

$T_2(x)$ was found to be almost independent of $x$ in the range of $x$ used.

Comparing (9) with (5), we get

$$\alpha^2 = (J'/J)^2 \approx 309, \quad \text{or} \quad \frac{J'}{J} \approx 17.5. \quad (10)$$

With this value of $\alpha^2$, let us see how $T_2(x)$ should behave as $x$ varies. In the limiting cases $\omega = 0$ and $\omega/\beta \to \infty$, we find from (8) and (10) that

$$[T_2(x)/T_2(0)]_{\omega = 0} \text{ or } [\omega(\beta)]_{\omega = 0} \approx (1 + 309 x)^{1/2}.$$ 

Thus in these cases, as $x$ increases from 0 to $\sim 10^{-3}$, $T_2(x)$ shows a relative increase of $\sim 14\%$. For $[\omega(\beta)]^{2} \approx 5$, the value appropriate to the Bernier and Landesman experiment [3], we find from (8) that the relative increase in $T_2(x)$ is $\sim 6\%$ at most [12]. This is to be compared with the $\sim 83\%$ increase in $R(x)$ given by (9). The influence of $^4$He impurities on $R(x)$ is much stronger than that on $T_2(x)$ for the parameters used by BL. This is what was observed by them experimentally.

With the same values of the parameters as before, we find that $T_{2,EX}$ should decrease by $\sim 13\%$ as $x$ increases to $\sim 10^{-3}$ from zero. Since the experimental error in measuring $T_{2,EX}$ is $[1] \sim 10\%$, the dependence on $x$ is difficult to observe unless the experiments are further refined.

For a molar volume of 20.06 cm$^3$, the value of $J$ is about 0.97 MHz [2]. Therefore, from (10), $|J'| \approx 16.97$ MHz. Although this appears to be a large value for an exchange frequency compared to the value of $J$, it is not so large as to be unphysical. Exchange in pure $^3$He itself can occur at such a frequency, and
would correspond [1] to a molar volume of \( \sim 24 \text{ cm}^3 \), an accessible value for solid \(^3\text{He}\). We could then say that the system acts in some ways as if the lattice spacing around a \(^4\text{He}\) impurity atom increases by \( \sim 6\% \) over the original value in pure \(^3\text{He}\). This cannot be explained as being due to the usual volume strain, which predicts [1] a decrease in lattice spacing of \( \sim 1.7\% \). Ultimately, the full comparison with experimental results would require a careful analysis of the applicability of the cell model approach and the calculation of the parameters with realistic choices of wave functions.

**References**

[12] Richardson (R. C.), Landesman (A.), Hunt (E.) and Meyer (H.), *Phys. Rev.*, 1966, **146**, 244.