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NMR frequency in superfluid phases of ^{3}He

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All unitary solutions of the weak-coupling gap equation for $l=1$ pairing are exhibited, and their rotational degeneracies highlighted. The role of the Zeeman and dipolar energies in resolving these degeneracies is examined. These interactions are used to calculate the NMR frequency, and the assumptions used by Anderson and Leggett in earlier calculations are clarified. In particular, "classical" equations are given which are equivalent to Leggett's quantum-mechanical analysis.

The recently observed anomalies[1-7] in the thermodynamic and transport properties of liquid ^{3}He at temperatures around 2 mK have attracted considerable attention. Theoretical explanations have centered around the concept that transitions are taking place into superfluid phases with condensation of quasiparticles into spin-triplet (odd-l) pairs. To account for the observed shifts of the NMR frequency[2] in the superfluid phases Leggett has presented an argument[8] based on sum rules and the hypothesis that the shifted line saturates the spectral weight. These arguments alone are unable to predict successfully all aspects of the experimental observations. An intuitive heuristic approach has been used by Anderson[9] to yield results at some variance with Leggett's conclusions.[8] In a second paper[10] Leggett has calculated the NMR frequency from a microscopic basis, with results differing in some respects from those both of Anderson[9] and Leggett's[8] earlier work. In the present paper we also approach the NMR-frequency problem from the viewpoint of the microscopic theory. We clarify the assumptions found necessary by Anderson and Leggett to obtain a shifted line in agreement with existing observations. Moreover, "classical" equations are presented which are equivalent to Leggett's analysis.

The theoretical model which we adopt is that of Balian and Werthamer,[11] in which we presume pairing of quasiparticles into an $l=1$, $s=1$ state. We also assume weak coupling, in the sense that we do not accommodate retarded or frequency-dependent interactions. In the Balian-Werthamer (BW) formalism[11] a 2×2 gap matrix in spin space, $\Delta^{\vec{k}}$, is defined [BW(19)] which for p-wave solutions may be written as [BW(48)]

$$\Delta^{\vec{k}} = \hat{k}\cdot\overleftrightarrow{\mathrm{d}}\cdot\vec{\sigma}\sigma_2\,, \tag{1}$$

in terms of a complex tensor $\overleftrightarrow{\mathrm{d}}$. Restricting attention to the unitary class of gap matrices [BW(22)], we have proved that the gap equation (BW25) for $l=1$ has four and only four degenerate manifolds of solutions. This extends to all temperatures—the result derived by others[12] for the temperature region just below T_C. The four manifolds are characterized in Table I, together with the associated quasiparticle energy $E_{\vec{k}}$ and susceptibility tensor $\overleftrightarrow{\chi}$.

The parameter families $\hat{\xi}_i^L$ and $\hat{\xi}_i^S$ are each an independent set of orthonormal basis vectors, which serve to define the degeneracy within each manifold. The $\hat{\xi}_i^L$ and the $\hat{\xi}_i^S$ are associated with the orbital and the spin-angular momenta of the pairs, respectively. Thus the susceptibility tensor is defined with respect to the $\hat{\xi}_i^S$ alone, while the quasiparticle energies are given in terms just of the $\hat{\xi}_i^L$.

BW have proved that, in the absence of any spin-dependent quasiparticle interactions, the isotropic state is the variational state of absolute lowest free energy for all $T<T_C$. The fact that more than one superfluid state is actually observed seems to indicate that the BW assumptions must be modified in some way. Anderson and Brinkman[14] have pointed out that the strong spin fluctuations in the normal ^{3}He liquid, particularly at pressures near the solidification line, reduce the free energy of states with anisotropic susceptibility relative to the isotropic state. They conclude that the axial state is the energetically favored one for spin fluctuations met within liquid ^{3}He. A spin-dependent effective pair potential is easily incorporated into the BW formalism by replacing (BW1) and (BW26) by[15]

$$\mathcal{V} = -\frac{3}{2}\sum_{\vec{k}\vec{k}'}\hat{k}\cdot\hat{k}'\sum_{1234}\left(V_1\delta_{2,3}\delta_{1,4}+\vec{\sigma}_{23}\cdot\overleftrightarrow{\mathrm{I}}_1\cdot\vec{\sigma}_{14}\right)\times a^\dagger_{-\vec{k}1}a^\dagger_{\vec{k}2}a_{\vec{k}'3}a_{-\vec{k}'4}\,. \tag{2}$$

Each of the four manifolds of Table I is still a solution to the gap equation generalized to include an exchange interaction, provided that the tensor $\overleftrightarrow{\mathrm{I}}_1$ has the same symmetry as the $\overleftrightarrow{\chi}$ of that manifold. Conclusions similar to those of Anderson and

Brinkman can then be drawn. We confine further attention only to the isotropic and the axial states.

A shift of the NMR frequency from the Larmor value $\omega_0 = \gamma H$ is possible only if there are spin-nonconserving terms in the Hamiltonian. It has been suggested[8,9,16] that the dipole-dipole interaction $\mathcal{H}_d$ among the ^{3}He nuclei is responsible for the NMR shift. To examine the effect of $\mathcal{H}_d$ we first calculate the first-order change in free energy which it induces in the paired phases. We find

$$\langle\mathcal{H}_d\rangle = V_d^{(i)}\left(-1 + \sum_{i,j=1}^{3} \tfrac{1}{2}(\hat{\xi}_i^S \cdot \hat{\xi}_i^L \hat{\xi}_j^S \cdot \hat{\xi}_j^L + \hat{\xi}_i^S \cdot \hat{\xi}_j^L \hat{\xi}_j^S \cdot \hat{\xi}_i^L)\right) \quad \text{(isotropic)}, \quad (3)$$

$$\langle\mathcal{H}_d\rangle = V_d^{(a)}[\tfrac{1}{3} - (\hat{\xi}^S \cdot \hat{\xi}^L)^2] \quad \text{(axial)}, \quad (4)$$

where $V_d^{(i,a)}$ are positive coefficients of order $(\hbar^2\gamma^2/R^3)(\Delta^2/\epsilon_F^2)$, for which we do not give specific expressions here. The dipolar interaction lifts the degeneracy in the manifolds associated with arbitrary relative rotations of spin and momentum spaces. In the presence of an applied static magnetic field $\vec{H}$, that portion of the free energy which depends on the directions of the $\hat{\xi}^S$, the $\hat{\xi}^L$, and the total induced spin polarization $\vec{S}$ may be written as

$$\delta F = \tfrac{1}{2}\vec{S}\cdot\overleftrightarrow{\chi}^{-1}\cdot\vec{S} + \langle\mathcal{H}\rangle . \quad (5)$$

Reference to Eq. (4) and Table I for $\overleftrightarrow{\chi}$ shows that δF is minimized in the axial state when $\hat{\xi}^S$ and $\hat{\xi}^L$ are parallel and $\hat{\xi}^S$ is perpendicular to $\vec{S}$. For the isotropic state, on the other hand, there is no preferred orientation for $\hat{\xi}^S$ relative to the applied field.[17]

To investigate the situation during an NMR observation, in which $\vec{S}$ deviates from its equilibrium value, we turn to the quantum-mechanical equation of motion for the spin operator $\vec{S}$,

$$\begin{aligned}\dot{\vec{S}} &= i[\vec{S}, \mathcal{H}] \\ &= \gamma\vec{S}\times\vec{H} + i[\vec{S}, \mathcal{H}_d] . \end{aligned} \quad (6)$$

Taking expectation values of both sides in the molecular field states of Table I, an evaluation similar to that for $\langle\mathcal{H}_d\rangle$ leads to

$$\dot{\vec{S}} = \gamma\vec{S}\times\vec{H} + V_d^{(i)} \sum_{i,j} (\hat{\xi}_i^L \cdot \hat{\xi}_i^S \hat{\xi}_j^L \times \hat{\xi}_j^S + \hat{\xi}_i^L \cdot \hat{\xi}_j^S \hat{\xi}_j^L \times \hat{\xi}_i^S) \quad \text{(isotropic)}, \quad (7)$$

$$\dot{\vec{S}} = \gamma\vec{S}\times\vec{H} - 2V_d^{(a)}\hat{\xi}^L \cdot \hat{\xi}^S \hat{\xi}^L \times \hat{\xi}^S \quad \text{(axial)}. \quad (8)$$

Our assumption in this procedure is that the deviation from equilibrium does not admix differing stationary manifolds, but the degeneracy of each manifold is recognized by allowing the $\hat{\xi}^S$ and $\hat{\xi}^L$ parameters to become time dependent. For the isotropic state, Anderson averages the $\hat{\xi}_i^S$ over all orientations. This leads to a vanishing of the second term in Eq. (7), so that the precession frequency of $\vec{S}$ is unshifted from its Larmor value. This is not based on a solid foundation, since in a situation of broken symmetry the direction of $\hat{\xi}_i^S$'s are specified even for the isotropic state. The remaining problem from Anderson's point of view is to find the dynamical behavior of $\hat{\xi}^S$ and $\hat{\xi}^L$ in the axial state.

One way to obtain results consistent with the observed NMR frequencies is to make the same assumptions as Anderson,[9] namely, that

$$\frac{d}{dt}\hat{\xi}^L = 0 \quad (9)$$

and

$$\frac{\partial\,\delta F}{\partial\,\hat{\xi}^S} = 0 . \quad (10)$$

Presumably Eq. (9) is true because interaction of the surface with orbital currents locks $\hat{\xi}^L$ to an optimum position and any motion relative to it involves energies of the order of the gap energy, which are too large compared to those involved in an NMR experiment. Equation (10) is more mysterious, and we are not able to add further justification as to why $\hat{\xi}^S$ adiabatically follows the in-

TABLE I. Four manifolds of unitary solutions to the weak-coupling $l = 1$ gap equation, with the resulting quasiparticle energies and spin susceptibilities. The quantity Y is the angular average of the Yosida function, defined by (BW51).

	$\vec{d}$	E_k^2	$\overleftrightarrow{\chi}/\chi_n$
Polar (Ref. 12)	$\Delta\hat{\xi}^L\hat{\xi}^S$	$\epsilon_k^2 + \vert\Delta\vert^2(\hat{k}\cdot\hat{\xi}^L)^2$	$Y\hat{\xi}^S\hat{\xi}^S + (\overleftrightarrow{1} - \hat{\xi}^S\hat{\xi}^S)$
Planar (Ref. 11)	$\Delta\sum_{i=1}^{2}\hat{\xi}_i^L\hat{\xi}_i^S$	$\epsilon_k^2 + \vert\Delta\vert^2[1 - (\hat{k}\cdot\hat{\xi}^L)^2]$ $\hat{\xi}^L \equiv \hat{\xi}_1^L \times \hat{\xi}_2^L$	$\hat{\xi}^S\hat{\xi}^S + \frac{1}{2}(1+Y)(\overleftrightarrow{1} - \hat{\xi}^S\hat{\xi}^S)$ $\hat{\xi}^S \equiv \hat{\xi}_1^S \times \hat{\xi}_2^S$
Axial (Ref. 13)	$\Delta(\hat{\xi}_1^L + i\hat{\xi}_2^L)\hat{\xi}^S$	$\epsilon_k^2 + \vert\Delta\vert^2[1 - (\hat{k}\cdot\hat{\xi}^L)^2]$	$Y\hat{\xi}^S\hat{\xi}^S + (\overleftrightarrow{1} - \hat{\xi}^S\hat{\xi}^S)$
Isotropic (Ref. 11)	$\Delta\sum_{i=1}^{3}\hat{\xi}_i^L\hat{\xi}_i^S$	$\epsilon_k^2 + \vert\Delta\vert^2$	$(\frac{2}{3} + \frac{1}{3}Y)\overleftrightarrow{1}$

staneous energy minimum. Granted Eqs. (9) and (10), however, they can be solved so as to eliminate $\hat{\xi}^S$ from Eq. (8), so that

$$\dot{\vec{S}} = \gamma\vec{S}\times\vec{H} + 2V_d^{(a)}[(1+\alpha)^2 - 4(\hat{\xi}^L\cdot\hat{S})^2]^{-1/2}\hat{\xi}^L\cdot\hat{S}\hat{\xi}^L\times\hat{S}\,, \quad (11)$$

where

$$\alpha \equiv \frac{V_d^{(a)}}{|\vec{S}|^2(\chi_\parallel^{-1} - \chi_\perp^{-1})}\,. \quad (12)$$

For unsaturated resonance Eq. (11) may be linearized in the deviations of $\hat{S}$ from $\hat{H}$. Then $\vec{S}$ is found to precess harmonically about $\vec{H}$ with frequency

$$\omega = [\omega_0^2 + (2\gamma V_D^{(a)}/\chi_\parallel)(1+\alpha)^{-1}]^{1/2}\,; \quad (13)$$

there is no longitudinal resonance. These results are the same[18] as those of Anderson. It is also possible to reduce Eq. (12) directly to quadrature, from which it may be predicted in the saturated resonance case that transverse absorption also occurs at odd harmonics of the fundamental, while longitudinal absorption develops at even harmonics but not at the fundamental itself. Thus pulsed-NMR experiments may be another critical test of the assumptions (9) and (10) of Anderson, along with a check of the dependence of ω on α as per Eq. (13), leading at low fields to $\omega \propto H$.

Leggett's analysis is also equivalent to the assumption that $\hat{\xi}^L$ are locked rigidly to their equilibrium position; i.e., Eq. (9) is assumed; on the other hand, the motion of $\hat{\xi}^S$ is not given by Eq. (10). The "classical" equation giving Leggett's result is

$$\frac{d}{dt}\hat{\xi}^S = \hat{\xi}^S \times \left(\frac{\partial(\delta F - \vec{S}\cdot\vec{H})}{\partial\vec{S}}\right). \quad (14)$$

This equation leads to a clearer understanding of the physics behind Leggett's quantum-mechanical analysis, for it says that the field acting on $\hat{\xi}^S$ is the same as the field acting on $\vec{S}$. Clearly this must be true if $\vec{S}$ is the generator of rotations in spin space. From Eqs. (8), (9), and (14), one can solve for the transverse and longitudinal frequencies in the linear approximation. One again finds the transverse frequency given by Eq. (13); however, there is now a longitudinal resonance at a frequency given by

$$\omega_L = \left[\left(\frac{2\gamma V_D^{(a)}}{\chi_\parallel}\right)\frac{1}{(1+\alpha)}\right]^{1/2}. \quad (15)$$

For the isotropic case, one can use Eqs. (7), (9), and (14) for each component i and find transverse resonance frequency to be zero, but find a longitudinal frequency given by Eq. (15), with $\alpha = 0$ and $\chi_\parallel = \chi$.

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[17]From Eq. (3) we confirm Leggett's statement (Ref. 10) that δF is minimized in the isotropic state when $\overleftrightarrow{d}$ is proportional to a matrix of rotation through the angle $\cos^{-1}(-\frac{1}{4})$ about an arbitrary axis.
[18]Reference 9, however, is based upon the planar rather than the axial state.