s-Band State Density at the Fermi Energy in NbN

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Nb^{93} spin-lattice relaxation-time measurements in NbN show that the niobium 5s contribution to the total state density at the Fermi energy is less than 10%. This result is considered in terms of electronic band models for NbN.

It was suggested a few years ago that the high-transition-temperature superconductor NbN ($T_c \approx 16\,^\circ K$) is a s-p-band superconductor.[1] This suggestion was supported mainly by the unusually low values of the electronic-heat-capacity coefficient and the magnetic susceptibility which indicated a very low electronic density of states at the Fermi energy. This low value of the state density is similar to that of lead and an order of magnitude smaller than those of Nb_3Sn and V_3Si, for example, which are d-band superconductors with nearly the same T_c as NbN. Recently, Mattheiss has calculated the electronic energy bands of NbN making use of the augmented-plane-wave (APW) scheme.[2] Mattheiss has found that the energy bands near the Fermi energy are predominantly d like and that the s character there is very small. It is thus of interest to perform an experiment which can distinguish between d- and s-like character and to determine experimentally the character of the electrons at the Fermi energy. A measurement of the niobium nuclear spin-lattice relaxation time (T_1) could serve in such a direction since, due to the large difference in the hyperfine field of s and d electrons, T_1^{-1} for s-band electrons should be ~2 orders of magnitude larger than T_1^{-1} for d-band electrons with the same density of states at the Fermi energy.

We have measured the Nb^{93} spin-lattice relaxation in $NbN_{0.91}$ at 77 and 20.3 °K by observation of the recovery of the spin-echo amplitude as a function of the time after saturating the system by a comb of rf pulses. It was found that for these two temperatures $T_1 T = 5 \pm 1$ (sec °K). This value may be used now to put an upper bound to the s density of states at the Fermi energy since $(T_1^{-1})_{meas} \geq (T_1^{-1})_s$, where $(T_1^{-1})_s$ is the relaxation rate caused by the s electrons alone. $(T_1^{-1})_s$ is given by[3]

$$(T_1^{-1})_s = 4\pi\gamma_n^2 \hbar k_B T[H_{hf}(s)\eta_s]^2,$$

where $H_{hf}(s)$ is the hyperfine field per electron due to the s electrons, and η_s is the s density of states per atom at the Fermi energy. Assuming $H_{hf}(5s) = 2.5\times 10^6$ Oe,[3] it turns out that $\eta_s \leq 0.03\,eV^{-1}$ (Nb atom)$^{-1}$. The bare density of states at the Fermi energy, analyzed from specific-heat data using McMillan's strong coupling formula,[4] is ~$0.3\,eV^{-1}$ (Nb atom)$^{-1}$.[1] Thus, it is concluded that the density of the niobium 5s states is less than 10% of the total density of states. This is in agreement with the Mattheiss[2] calculations which predict that the predominant part of the density of states at the Fermi energy comes from the 4d bands.

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[2]L. F. Mattheiss, this issue, Phys. Rev. B 5, 315 (1972).

[3]See, for example, Y. Yafet and V. Jaccarino, Phys. Rev. 133, A1630 (1964).

[4]W. L. McMillan, Phys. Rev. 167, 331 (1968).