Numerical simulation of a phase transition in the nuclear spin system of gallium arsenide with adiabatic demagnetization

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The results of a calculation of the phase-transition temperature (T_c), of the ground state of the nuclear spin system of GaAs, and of the process of adiabatic demagnetization of this system in the temperature range below T_c are presented.

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At ultralow temperatures $T \approx 10^{-7}$–10^{-8} K, the interaction between nuclear spins in a solid leads to their ordering.[1] Such temperatures are attained by adiabatic demagnetization of a strongly polarized nuclear spin system. The theory of adiabatic demagnetization is developed in the high-temperature approximation in Ref. 2. In this approximation, the polarization of nuclei in the starting state is known to be insufficient to obtain an ordered spin state after adiabatic demagnetization.

Thus existing analytic models do not permit determining the minimum polarization in a strong field, beginning with which adiabatic demagnetization leads to spontaneous ordering of spins. At the same time, it is desirable to know the value of this polarization before setting up an experiment. Under such circumstances, numerical simulation of the process of adiabatic demagnetization on a computer is important.

As the object of the study we chose GaAs, where appreciable nuclear polarization of the order of several tens of oersted can be obtained under conditions of optical orientation.[3] The limiting value of the polarization in these experiments can reach 70%.[4] A calculation was performed using Monte Carlo cells consisting of 96 Ga^{69} nuclei and 96 As^{75} nuclei (magnetic moments $\mu_{As} \approx 1.4\mu_N, \mu_{Ga} = 2.0\mu_N$, where μ_N is the nuclear magneton) with periodic boundary conditions. In actuality, we simulated the situation when the entire volume of the macroscopic crystal is separated into equal parts containing 192 nuclei (Monte Carlo cells) and having identical states of nuclear spin polarization. Only the magnetic dipole interaction between nuclear spins was included and the nuclear spins were assumed to be classical. It was assumed that the macroscopic crystal has a cubic shape.

Without going into the details of the computational procedure, we note that the calculations were performed in two stages. In the first stage we modeled the state of the nuclear spin system placed in a thermostat with temperature T. The external magnetic field here was assumed to be zero. The scheme for calculating this state is physically analogous to that in Ref. 5. In the second stage the interaction with the thermostat was switched off and the field H was slowly increased to a value $H_{max} \approx 4.5$ Oe. The adiabatic magnetization of the system was thereby simulated. In order to monitor the adiabaticity of the process, subsequent demagnetization was per-

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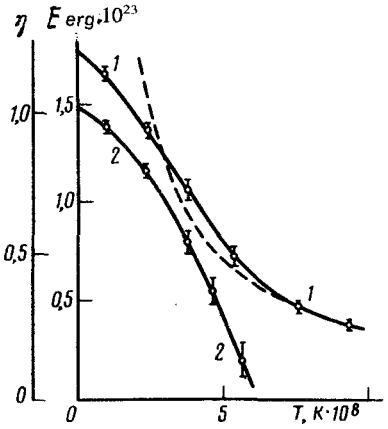

FIG. 1. Temperature dependence of the average energy of a single nuclear spin (1) and parameter (2). The dashed line shows the calculation using the high-temperature equation.

formed in a zero external field. The rate of change $\dot{H}$ was chosen to be so small that the change in the temperature after the magnetization–demagnetization cycle did not exceed 5×10^{-9} K.

The basic results obtained in the numerical experiment reduced to the following.

1. In the ground state of the system, corresponding to $T=0$, the nuclear spins are ordered in an antiferromagnetic manner in each sublattice (Ga and As). All spins are parallel or antiparallel to the axis [111]. In addition, for nuclei of one type lying in a single plane $(11\bar{2})$, the spins are parallel, while for neighboring planes they are antiparallel. The As sublattice was obtained from the Ga sublattice by a displacement with the vector $(-1/4,1/4,1/4)$.

2. The dependence of the average energy of a single nuclear spin on temperature T is shown in Fig. 1 (curve 1). For values $T\gtrsim 8\times10^{-8}$ K, this dependence is well approximated by the high-temperature equation $E\approx(\bar{\mu}^2H_L^2)/(3T)$, where $H_L^2\approx2.0$ Oe^2 is the average value of the square of the local field, acting on the nuclear spin from the side of neighboring nuclei, while $\bar{\mu}=1.7\mu_N$ is the average value of the nuclear magnetic moment. For $T<5\times10^{-8}$ K, the high-temperature approximation does not work. In the range of values $T\approx(5\pm2)\times10^{-8}$ K, the heat capacity of the system is maximum. However, the inadequate accuracy in determining the average energy ($\sim8\%$) does not permit finding the exact value of the phase-transition temperature from the discontinuity in the derivative dc/dT.

The same figure shows the temperature dependence of the amplitude of the maximum Fourier component of the spatial distribution of nuclear spin polarization (order parameter). This amplitude has highest value at $T=0$ and becomes negligibly small for $T>6\times10^{-8}$ K. This permits a more accurate estimate of the phase transition temperature 6×10^{-8} K $>T_c>5\times10^{-8}$ K. We note that the calculation with the Weiss field model gives the value $T_c\approx6\times10^{-8}$ K.

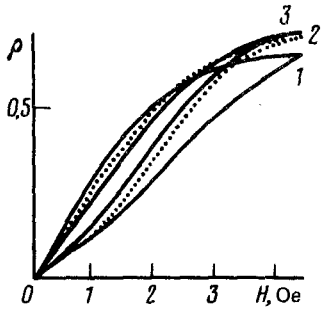

FIG. 2. Magnetization cycles of the nuclear spin system in the absence of heat exchange with the thermostat.

3. The results of the calculation of adiabatic magnetization and demagnetization processes are presented in Figs. 2 and 3. Figure 2 shows the dependence of the average nuclear spin on the magnitude of the magnetic field in the cycle $0 \rightarrow H_{max} \rightarrow 0$ for starting temperature $T = 4 \times 10^{-8}$ K. The rates of change of the magnetic field ($\dot{H}$) in cycles 1, 2, and 3 form the ratio 5:2.5:1. It is evident that as $\dot{H}$ decreases the magnetization ($0 \rightarrow H_{max}$) and demagnetization ($H_{max} \rightarrow 0$) branches approach each other, which corresponds to a decrease in irreversible energy loss due to heating of the nuclear spin system. In cycle 3 the increase in the average energy was $\approx 7\%$. In other words, after magnetization and demagnetization the temperature of the system increased by not more than 0.5×10^{-8} K. Keeping in mind the error in the calculation of the T dependence of E, such a rate of change of H can be viewed as sufficient to model the adiabatic process.

Figure 3 shows the dependence of the temperature of the system after adiabatic demagnetization (from the field $H_{max} \approx 4.5$ Oe) on the starting polarization ρ of nu-

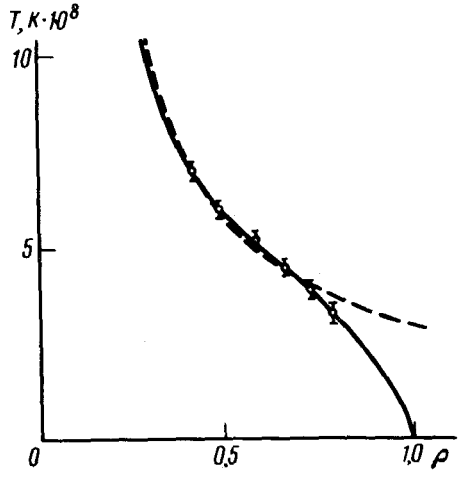

FIG. 3. Dependence of the temperature after demagnetization on the starting polarization in a field $H_{max} \approx 4.5$ Oe. The dashed line shows the high-temperature approximation.

clear spins. For $\rho < 0.45$ the curve $T(\rho)$ is well approximated by the high-temperature equation

$$T = \frac{\bar{\mu} H_{max}}{3\rho} \sqrt{\frac{H_L^2}{H_{max}^2 + H_L^2}} \,. \tag{1}$$

In the region $\rho \approx 0.5 (T \approx 5.5 \times 10^{-8}\text{K} \approx T_c)$ an inflection is observed in the computed function, which is naturally related to the transition of the demagnetized system into an ordered state. From this value of ρ, the quantitative disagreements between the computed dependents $T(\rho)$ and the high-temperature equation increase rapidly and for $\rho > 0.8$ (1) are no longer useful even for rough estimates. It is surprising that (1) describes $T(\rho)$ fairly well right up to the phase-transition temperature.

Starting from the results obtained, we can conclude that by combining optical orientation and adiabatic demagnetization it is possible to attain ultralow temperatures, at which the nuclear spins are ordered in an antiferromagnetic manner. As the minimum polarization in a strong field we can take the approximate value $\rho_{\min} \approx 50\%$, which is 20% less than the theoretical limit attainable with optical orientation.

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