Knight shift in quasi-1D disordered systems with an Anderson localization of electrons

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The Knight-shift distribution is calculated for a 1D system in the Anderson insulator state. As a result of cooling, the distribution broadens and becomes asymmetric. The NMR line has a similar shape at low temperatures.

1. The spatial distribution of electron spin density in disordered systems can be determined directly by measuring the Knight shift. We have calculated the distribution of the Knight shift, K, in systems with an Anderson localization of electrons. The distribution function K depends on a single parameter $\rho = 4TV_lN(E_F)$, where V_l is the localization volume, T is the temperature, and $N(E_F)$ is the average density of the electronic states at the Fermi level. With decreasing ρ, the distribution K becomes asymmetric and broadens. At sufficiently low temperatures, the Knight-shift distribution begins to affect the NMR lineshape, from which the electron localization radius can be determined directly.

We analyze below a 1D system of electrons, keeping in mind the interpretation of the experimental studies of the NMR in a quasi-1D conductor with a pronounced disorder, $Qn(TCNQ)_2$.

2. The Knight shift is proportional to the spin density of electrons at the nucleus, $\sigma(\mathbf{r})$. Disregarding the electron interaction, we find

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$$\sigma(\mathbf{r}) = \sum_{\nu} |\varphi_{\nu}(\mathbf{r})|^2 \frac{\partial f}{\partial \epsilon}\Big|_{\epsilon=\epsilon_{\nu}} 2\mu_B H, \tag{1}$$

where $f(\epsilon)$ is the Fermi electron-distribution function, and $\mu_B H$ is the Zeeman energy. The index ν specifies the localized states with energies ϵ_ν and wave functions $\varphi_\nu(\mathbf{r})$ with the localization center at the point $\mathbf{r}_\nu$; the wave functions decrease exponentially with increasing $|\mathbf{r}-\mathbf{r}_\nu|$. In the 1D case, we will approximate $|\varphi_\nu(r)|^2$ by using the function $(4R_l)^{-1}\cosh^{-2}[(r-r_\nu)/2R_l]$.

From Eq. (1) we then find

$$\kappa = \frac{K}{\overline{K}} = \rho^{-1} \sum_{\nu} \cosh^{-2} x_\nu \cosh^{-2} y_\nu, \tag{2}$$

where K is average (with respect to the volume) Knight shift which is proportional to $N(E_F)$, and $x_\nu = |r-r_\nu|/2R_l$ and $y_\nu = |E_F - \epsilon_\nu|/2T$. For $\rho\kappa \geqslant 1$ the distribution of κ depends on the function $\varphi_\nu(r)$ near $r = R_l$, and the description based on (2) has a model nature. At $\rho\kappa \ll 1$, the region $r \gg R_l$ determines the principal contribution to the distribution of κ, and the results which we obtain below for the systems are common to all systems.

The distribution of κ depends on the distribution of random quantities x_ν and y_ν in the x, y plane; the average density of the points ν is equal to ρ (we assume $E_F \gg T$). It follows from the calculations in Ref. 2 that x_ν and y_ν are distributed uniformly and independently of each other at $x_\nu > 1$. At shorter range, level repulsion accounts for the fact that small values of y_ν occur more likely when the values of x_ν are small ($x_\nu < 1$). This effect is unimportant at $\rho\kappa \ll 1$, and we will assume below that the distributions of x_ν and y_ν are independent of each other and uniform. We then find from (2) the following expression for the distribution function

$$W(\kappa) = \int_{-\infty}^{+\infty} \frac{dp}{2\pi} \exp\{ip\kappa + \rho \int_0^{\infty} dx \int_0^{\infty} dy \,[\exp(ip\rho^{-1}\cosh^{-2}x \cosh^{-2}y) - 1]\}. \tag{3}$$

At $\rho \gg 1$ expression (3) yields a Gaussian distribution

$$W(\kappa) = \sqrt{\frac{9\rho}{8\pi}} \exp\left[-\frac{9}{8}\rho(\kappa-1)^2\right], \quad \rho \gg 1. \tag{4}$$

To the extent it applies to the discussion above, asymptotic expression (4) can be used to only estimate the distribution width of κ.

For $\rho\kappa \ll 1$ the functions $\cosh^{-2}x$ and $\cosh^{-2}y$ can be replaced by exponential functions, since large values of x and y are dominant in the integral, and (3) becomes

$$W(\kappa) = \pi^{-1}\rho \exp\left(\frac{5\pi^2\rho}{12}\right) \int_0^{\infty} dt \sin(\pi\rho \ln\gamma t) \exp(-\kappa\rho t - \frac{1}{2}\rho \ln^2 \gamma t), \tag{5}$$

$$\gamma = e^C, \quad C = 0{,}577.$$

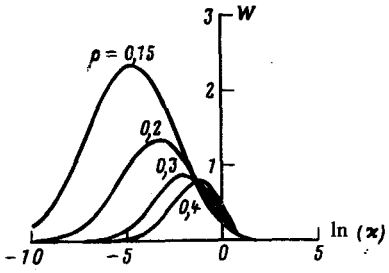

FIG. 1.

The plots of the function $W(\kappa)$ vs $\ln\kappa$ are shown in Fig. 1. From (5) we find a Gaussian distribution of the logarithm of κ in the limit $\rho \to 0$,

$$W(\kappa) = \rho \exp\left[\frac{1}{2\rho} - C - \frac{1}{2}\alpha(\ln\kappa - \ln b)^2\right], \tag{6}$$

$$\ln b = -\frac{1}{\rho} - \ln\rho, \quad \alpha^{-1} = \rho^{-1} - \ln(\pi/2\gamma^2\rho).$$

With decreasing ρ, the peak of the function $W(\kappa)$ decreases to $\rho\kappa \ll 1$, and description (6) for $\rho \ll 1$ is an exact description for nearly all κ, with the exception of the remote right wing, where the function $W(\kappa)$ is very small. With decreasing ρ, the true Knight-shift distribution width, $\Delta\kappa$, which is determined from half the maximum, first increases, reaching a maximum width at $\rho \approx 1$, and then falls off in proportion to

$$\rho^{-1}\exp\left[-\frac{1}{\rho} + \left(\frac{2\ln 2}{\rho}\right)^{1/2}\right]$$

as $\rho \to 0$. In the case of small values of ρ, the NMR lineshape may therefore depend on other broadening sources which are different from the nonuniform Knight shift. If the contribution from these sources to the line width is γ, then the Knight shift is dominant as $\Delta\kappa > \gamma$. In modern high-resolution NMR spectroscopy, the dipole-dipole broadening has been eliminated and the ratio $\gamma/\bar{K} \approx 0.02$ is well within reach in $Qn(TCNQ)_2$ single-crystal samples.[1] In this case, the Knight shift determines the lineshape at $\rho > 0.1$.

3. In our discussion above, we have disregarded the electron repulsion. At low temperatures, the electron repulsion gives rise to the appearance of states near the Fermi surface which are occupied by a single electron. As a result, the paramagnetic susceptibility χ increases in accordance with a power law as $T \to 0$, and we must use another approach to calculate the Knight shift (see Ref. 3). In $Qn(TCNQ)_2$, the paramagnetic susceptibility χ begins to increase below 20 K, and at $T > 20$ K χ is approximately constant and corresponds to the susceptibility of a degenerate electron gas. At 295 K, the measurements carried out in Ref. 1 have shown that the Knight shift plays a dominant role in forming the NMR line. This line is asymmetric, and its width corresponds, according to (4) or (5), to $\rho \approx 5$. From the data on χ we find $N(E_F) = (\pi v_F)^{-1} \approx 8.4 \times 10^3$ K$^{-1}\cdot$cm^{-1}, and R_l can be as large as approximately

15 intermolecular separations along the *TCNQ* stack. The reciprocal collision time is $\tau^{-1} = 2\,v_F/R_l \approx 150$ K, consistent with the values estimated in Ref. 4. As a result of cooling to 85 K, the line broadens and the peak shifts toward $K = 0$, consistent with the calculations. In this case ρ decreases by a factor of approximately 4; i.e., the localization length R_l is nearly independent of temperature over the interval 85–295 K. In the polycrystalline samples studies in Ref. 1, the value of γ is determined primarily by the anisotropy of the shift, and $\gamma/\overline{K} \approx 0.4$, irrespective of T. Since the Knight shifts in samples of the sort is dominant at $\rho \gtrsim 1$, only single-crystal samples can be used to study it at smaller values of ρ (below 85 K).

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