Activation energy of the hopping conductivity of the δ-doped semiconductor in the low-density limit

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We consider the impurity band structure of a system of multiple donor sheets, spaced significantly farther apart than the average in-plane donor separation. In a low-density limit the overlap of the wave functions of neighboring donors is relatively small and the spread of the energy levels is governed by the Coulomb shifts produced by the charged acceptors and donors. The activation energy of the hopping conductivity in the regime of nearest-neighbor hopping is equal to the Fermi-level position with respect to the isolated donor level, which is calculated as a function of the two-dimensional concentration of donors and the interplane distance assuming that the small degree of compensation is provided by the acceptors, which are distributed randomly between the sheets.

I. INTRODUCTION

In a number of recent publications the electronic properties of δ-doped layers representing a plane of donors implanted into a semiconductor during the process of growth have been explored.[1-11] Most experiments were performed on GaAs samples doped with Si donors.[5-11] It was demonstrated that the arrangement of the electronic states in such a system depends strongly on the two-dimensional concentration n_d of donors in the plane. For n_d greater than some critical value n_c, which corresponds to the metal-insulator transition in two dimensions ($n_c \approx 1.3\times10^{11}$ cm^{-2} for GaAs), the donors unify their electrons and the electron gas screens the potential of the charged plane. The resulting potential has a V-shaped form. Therefore for $n_d > n_c$ the electronic spectrum consists of 2D quantum subbands and the low-temperature conductivity of such samples is metal-like. The treatment of the magnetotransport data permits the determination of the electronic occupations of each subband and the corresponding mobilities.[4,6,7]

For $n_d < n_c$ the donors in the sheets keep their individuality. The overlap of the wave functions of the neighboring donors is relatively small. Therefore the conductivity of such samples decreases rapidly with the decrease of temperature.[10,11] For the experimental study of transport properties of δ layers in the low-density limit, multilayered structures corresponding to a set of parallel δ layers spaced by some distance larger than the mean distance between the donors in the plane appears to be effective. Using the multilayer structure instead of a single δ-doping layer avoids the carrier depletion caused by the p-type background dopants.

In the range $10 \lesssim T < 77$ K the conductivity of the samples with $n_d < n_c$ involves excitation of electrons from the donors to the conduction-band edge. As shown in Ref. 11 below $T=10$ K the conductivity manifests the crossover to the regime of hopping transport. Note, however, that the hopping transport is impossible if all the donors are occupied. At low temperatures only the presence of some portion of acceptors can create the vacant positions in the impurity band and give rise to hopping conductivity.

Another significant consequence of the finite compensation is that after some electrons fall from the donors to the acceptors both acceptors and donors become charged and produce Coulomb shifts of the energy levels on the other donors. As a result, the density of states is smeared into the classical impurity band. (This term means[12,13] that the width of the band is not caused by an overlap of wave functions.) At low temperatures the Fermi level separates the energy levels of occupied and empty donors in the impurity band. If the compensation degree of the semiconductor $K=N_a/N_d=N_aD/n_d \ll 1$, the Fermi level should lie higher than the isolated donor level (Fig. 1). Here N_a and N_d are the bulk concentrations of dopants and D is the spacing between the sheets.

Under the condition $K \ll 1$ most of the donors are situated far from the acceptors and their energy levels are only slightly shifted by the charged impurities (Fig. 1). Then the occupation number of a typical donor is equal to $[1+\exp(\mu/T)]^{-1}$, where μ is the Fermi-level position measured from the isolated donor level. If the temperature is not extremely small, hopping conductivity is determined by typical pairs of the donors. The conductance of one pair is proportional to the small probability to have one of the donors empty, which is $\exp(-\mu/T)$ if $\mu \gg T$. Thus the temperature dependence of conductivity has a form

$$\sigma \propto \exp\left[-\frac{\varepsilon_3}{T}\right] \tag{1}$$

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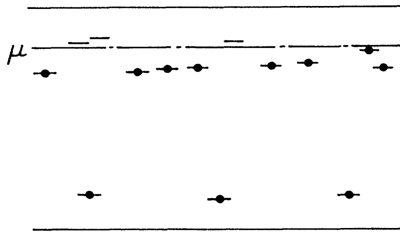

FIG. 1. Energy diagram of a weakly compensated semiconductor. The solid lines show the bottom of the conduction and the top of the valence band. The black dots represent electrons occupying the donor and acceptor levels. The Fermi level μ is shown by the dash-dotted line. The first acceptor from the left forms a 2 complex, the second a 1 complex, and the third a 0 complex.

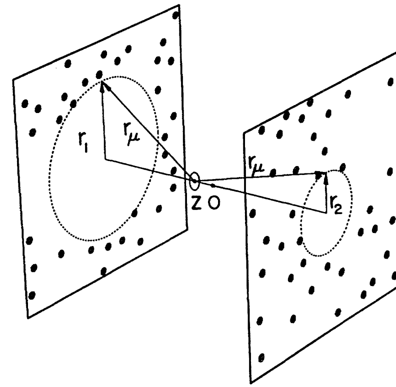

FIG. 2. Two neighboring donor planes and an acceptor (open circle) situated at a distance z from the midplane. The area enclosed by the dashed circles should contain no donors in order to form a 0 complex.

with an activation energy $\varepsilon_3=\mu$.

Therefore the calculation of the activation energy of hopping conductivity reduces to the evaluation of the Fermi-level position within the impurity band. This problem is the subject of the present paper in which the impurity band of a system of evenly spaced δ layers is studied theoretically. We show that the arrangement of donors in the separate sheets can strongly change the Fermi-level position and, consequently, the activation energy of hopping conductivity. This result can differ significantly from the prediction of the conventional theory,[12] developed for a uniformly doped bulk semiconductor. For the case when the distance between the sheets is much larger than the mean distance between donors in a sheet $n_d^{1/2}D \gg 1$, we obtain

$$\varepsilon_3=\mu=\frac{2e^2}{\kappa D}\ , \tag{2}$$

where e is the electron's charge and κ is the dielectric constant. Remarkably enough in this region ε_3 does not depend on n_d. In the opposite case $n_d^{1/2}D \ll 1$, the arrangement of donors in planes is of no importance and we can use the old result[13] for the Fermi-level position in a system of donors distributed randomly in space

$$\varepsilon_3=\mu=0.99\frac{e^2}{\kappa}N_d^{1/3}=0.99\frac{e^2}{\kappa}\left[\frac{n_d}{D}\right]^{1/3}\ . \tag{3}$$

A computer simulation was performed to obtain ε_3 for arbitrary D. Results can be approximated by Eq. (2) for $n_d^{1/2}D \geq 3$ and by Eq. (3) for $n_d^{1/2}D \leq 3$ with an accuracy better than 8%.

II. PRINCIPLE EQUATION

The theory of the impurity band structure of a lightly doped and low compensated three-dimensional semiconductor was developed in Refs. 12 and 13. We shall use here the main ideas of this theory.

Consider randomly distributed acceptors in the space between two δ layers (Fig. 2). Since the concentration N_a is less than n_d/D, all the acceptors are negatively charged. In the case $K \ll 1$ there are many donors between two acceptors. Normally the electron for the acceptor is provided by the closest donor, which then acquires a positive charge, so that the donor and acceptor constitute a neutral dipole. To remove the electron from the donor the acceptor should shift the donor's energy level above the Fermi level. The latter shift is equal to $e^2/\kappa r$, where r is the distance between the acceptor and the donor. The shift is greater than μ if the condition

$$r<\frac{e^2}{\kappa\mu}=r_\mu \tag{4}$$

is met. Since donors are randomly distributed within the planes, for any given μ a finite probability exists that for some of the acceptors there are voids on both of their neighboring planes, and no donors fulfill the condition (4) (Fig. 2). Following Ref. 13 these negatively charged configurations with no charged donors around an acceptor will be referred to as 0 complexes. Since a bulk semiconductor has to be electrically neutral, some acceptors must shift the energies of two neighboring donors above the Fermi level, thus creating a positively charged 2 complex. As shown in Ref. 13, for an appropriate location of donors, an acceptor can produce positive shifts of energy levels of two charged donors despite their mutual interaction, but configurations with one acceptor and three or more empty donors are prohibited. In principle, two close acceptors can hold three empty donors about them. However, since we have assumed that $K \ll 1$, the probability of such a configuration is much smaller than the probability of the formation of 0 and 2 complexes.

We see that the charged configurations in the system under study are negatively charged 0 complexes and positively charged 2 complexes; therefore the condition of total charge neutrality of the sample takes the form

$$N_0(\mu)=N_2(\mu)\ , \tag{5}$$

where $N_0(\mu)$ and $N_2(\mu)$ are the concentration of 0 and 2 complexes, respectively, for a given value of μ. Now in

order to determine the Fermi-level position one should calculate the concentrations N_0 and N_2 as functions of μ and solve Eq. (5). This program is realized in the following section.

III. CALCULATION OF THE FERMI-LEVEL POSITION

The expression for the concentration of 0 complexes can be derived using the fact that the probability of the formation of a void with the radius r in a system of donors randomly distributed in the plane is equal to $\exp(-\pi n_d r^2)$. Let the acceptor be at distance z from the midplane between two donor planes (Fig. 2). It will be a 0 complex if there are no donors at distances less than r_μ from the acceptor. Then the radii of the corresponding voids on both planes are

$$r_1(z,r_\mu)=\left[r_\mu^2-\left[\frac{D}{2}-z\right]^2\right]^{1/2}\Theta\left[r_\mu-\frac{D}{2}+z\right],$$

$$r_2(z,r_\mu)=\left[r_\mu^2-\left[\frac{D}{2}+z\right]^2\right]^{1/2}\Theta\left[r_\mu-\frac{D}{2}-z\right],\tag{6}$$

where $\Theta(t)$ is the step function. The step function is introduced here since, if the distance between the acceptor and one of the planes is greater than r_μ, no void is necessary to form a 0 complex. If r_μ fulfills the inequality

$$r_\mu < D ,\tag{7}$$

then voids on the two nearest planes are sufficient for creating a 0 complex, and the probability that the chosen acceptor is a 0 complex can be expressed as

$$p(z,r_\mu)=\exp[-\pi n_d r_1^2(z,r_\mu)-\pi n_d r_2^2(z,r_\mu)] .\tag{8}$$

The total concentration of 0 complexes can be obtained by averaging the probability $p(z,r_\mu)$ over the acceptor position

$$N_0(\mu)=N_a\int_{-D/2}^{D/2}p(z,r_\mu)\frac{dz}{D} .\tag{9}$$

Substituting (8) into (9) and performing the integration we get

$$N_0(\mu)=\frac{2N_a}{D}\left[\frac{D}{2}-r_\mu+r_dF\left[\frac{r_\mu}{r_d}\right]\right]\tag{10a}$$

if $r_\mu < D/2$ and

$$N_0(\mu)=\frac{2N_ar_d}{D}\exp\left[-2\pi n_dD\left[r_\mu-\frac{D}{2}\right]\right]\times\left[\frac{1}{\sqrt{2}}F\left[\frac{\sqrt{2}(r_\mu-D/2)}{r_d}\right]-F\left[\frac{D-r_\mu}{r_d}\right]\right]\tag{10b}$$

if $D/2 < r_\mu < D$, where $r_d \equiv (\pi n_d)^{-1/2}$ is a typical distance between donors in a plane and $F(t)=\exp(-t^2)\int_0^t\exp(x^2)dx$ is the Dawson integral.[14]

Now we turn to the calculation of the concentration of 2 complexes $N_2(\mu)$. A 2 complex can be constructed either from an acceptor and two donors on the nearest plane to the acceptor, or from an acceptor and two donors on different planes. The latter configuration is forbidden if r_μ meets inequality (7) because the largest energies of the donors reached when the acceptor is placed exactly between the planes and the donors are placed just opposite the acceptor are $2e^2/\kappa D - e^2/\kappa D < \mu$. So we will consider only 2 complexes of the first type.

The arrangement of 2 complexes depends strongly on the relation between r_μ and r_d. The analytical expression for $N_2(\mu)$ can be obtained only in the cases $r_\mu \ll r_d$ and $r_\mu \gg r_d$. Consider the first case. For $r_\mu \ll r_d$ 2 complexes are formed by the pairs of donors located anomalously close to the acceptor. Let the acceptor distance from the plane of a δ layer be h (Fig. 3). We denote by $\boldsymbol{\rho}_1$ and $\boldsymbol{\rho}_2$ the two-dimensional coordinates of the donors measured from the projection of the acceptor on the plane. Then the conditions for formation of a 2 complex can be written in the form

$$\varepsilon_1(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2)=\frac{e^2}{\kappa}\left[\frac{1}{(h^2+\rho_1^2)^{1/2}}-\frac{1}{|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}\right]>\mu ,\tag{11}$$

$$\varepsilon_2(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2)=\frac{e^2}{\kappa}\left[\frac{1}{(h^2+\rho_2^2)^{1/2}}-\frac{1}{|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}\right]>\mu .\tag{12}$$

Under these conditions the Coulomb shift of the energy levels of both donors is greater than μ. As is shown in Ref. 13 under the condition $r_\mu \ll r_d$, the concentration $N_2(\mu)$ is equal to the total concentration of donor pairs satisfying the conditions (11) and (12) (this is $N_2^>$ in the notation of Ref. 13),

$$N_2(\mu)=\frac{2N_an_d^2}{D}\int_0^{D/2}dh\int d\rho_1^2\int_{|\boldsymbol{\rho}_1|<|\boldsymbol{\rho}_2|}d\rho_2^2\Theta(\varepsilon_1-\mu)\times\Theta(\varepsilon_2-\mu) .\tag{13}$$

Here the factor of 2 takes into account the fact that the acceptor can be located both above and below the plane. The restriction $|\boldsymbol{\rho}_2|>|\boldsymbol{\rho}_1|$ reflects the fact that swapping the donor positions results in the same configuration. A straightforward but tedious evaluation of the integral (13) yields

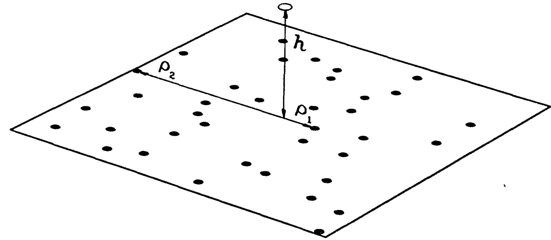

FIG. 3. A 2 complex formed by an acceptor at a distance h from a plane and two donors at positions $\boldsymbol{\rho}_1$ and $\boldsymbol{\rho}_2$ in the plane.

$$N_2(\mu)=C\frac{N_a n_d^2 r_\mu^5}{D}\ ,\quad r_\mu \ll r_d \tag{14}$$

where the dimensionless constant $C \approx 1.08\times10^{-2}$. Consider now the opposite case $r_\mu \gg r_d$. We will see later that under this condition the main contribution to the $N_2(\mu)$ comes from the acceptors situated at a distance $h \gg r_d$ from the donor plane. In this case there are normally many donors from which the acceptor can remove an electron. It can be shown that under the condition $h \gg r_d$ one electron is always removed form the closest one. A typical value of ρ_1 (Fig. 3) is then $\rho_1 \sim r_d$. For the formation of a 2 complex the coordinates $\boldsymbol{\rho}_2$ of the second donor have to obey the condition (12). It is obvious that in order to increase the distance between the donors the vector $\boldsymbol{\rho}_2$ should be antiparallel to $\boldsymbol{\rho}_1$. Then the condition (12) takes the form

$$\varepsilon_2(\rho_1,\rho_2)=\frac{e^2}{\kappa}\left[-\frac{h^2}{2\rho_2^3}+\frac{\rho_1}{\rho_2^2}\right]>\mu\ . \tag{15}$$

The energy $\varepsilon_2(\rho_1,\rho_2)$ as a function of ρ_2 has a maximum at $\rho_{2\max}=3h^2/\rho_1 \gg h$ with the value

$$\varepsilon_{2\max}=\frac{16}{27}\frac{e^2}{\kappa}\frac{\rho_1^3}{h^4}\ . \tag{16}$$

Since $\rho_{2\max} \gg h \gg r_d$, there is always a donor nearby this optimal point, so that for a given ρ_1 an acceptor produces a 2 complex if its distance from the plane of donors is less than $h_\mu(\rho_1)=(\frac{16}{27}\rho_1^3 r_\mu)^{1/4}$. Then the concentration of 2 complexes can be written in the form

$$N_2(\mu)=\frac{2N_a}{D}\int_0^\infty h_\mu(\rho_1)w(\rho_1)d\rho_1\ , \tag{17}$$

where $w(\rho_1)$ is the distribution density of ρ_1. Since the donor at $\boldsymbol{\rho}=\boldsymbol{\rho}_1$ is the nearest neighbor of the acceptor, we have $w(\rho_1)=2\pi\rho_1 n_d \exp(-\pi\rho_1^2 n_d)$ and, evaluating the integral, we obtain

$$\begin{aligned}N_2(\mu)&=\frac{4\Gamma(\frac{11}{8})N_a}{(9\pi)^{3/8}}\frac{r_\mu^{1/4}n_d^{-3/8}}{D}\\ &\approx 1.02\frac{r_\mu^{1/4}n_d^{-3/8}}{D}\ ,\quad r_\mu \gg r_d\ .\end{aligned} \tag{18}$$

In order to find the dependence $N_2(\mu)$ for intermediate values of $r_\mu \sim r_d$, a computer simulation was performed. The program generated a large number of random configurations of donors in the plane and an acceptor at some random distance from the plane. For every configuration the program looked for a critical value $\mu=\mu_2$ at which this configuration gives a 2 complex. Knowing the distribution function of μ_2, it is easy to calculate $N_2(\mu)$, which is obviously proportional to the fraction of configurations from which $\mu_2>\mu$.

In order to figure out μ_2 for a given configuration, the program calculated the Coulomb energy of the best 2 complex in it,

$$E_2=\frac{e^2}{\kappa}\min_{i,j}\left[-\frac{1}{r_i}-\frac{1}{r_j}+\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}\right]\ ,$$

where i and j are donors numbers and $\mathbf{r}_i$ is the distance between the donor and the acceptor and energy of the 1 complex $E_1=(e^2/\kappa)\min_i(-1/r_i)$. The 2 complex is more profitable in terms of energy if $E_2+\mu<E_1$, so μ_2 can be calculated first as $\mu_2=E_1-E_2$. The resulting dependence $N_2(\mu)$ fits perfectly with the asymptotes (15) and (18).

Let us turn now to the solution of Eq. (5). In the case of large spacing between the δ layers $D \gg n_d^{-1/2}$ it can be done analytically using the expression (10) and the asymptote (18). The result is

$$\mu=\frac{2e^2}{\kappa D}[1+0.85(n_d D^2)^{-3/8}]\ , \tag{19}$$

which is correct as long as the second term in the brackets is much smaller than 1. If we neglect this term, Eq. (19) coincides with Eq. (2). Another form of Eq. (2) is $r_\mu \simeq D/2$ for $n_d D^2 \gg 1$. The qualitative interpretation of this result is as follows. For $r_\mu \sim D$ and $n_d D^2 \gg 1$, we have $r_\mu \gg n_d^{-1/2}$. In such a limit only acceptors located at a distance $h \sim D/(n_d D^2)^{3/8} \ll D$ from the plane can produce a 2 complex. This means that $N_2 \sim N_a h/D \ll N_a$. Consequently, the concentration of 0 complexes N_0 should be much less than N_a. The 0 complexes for $n_d D^2 \gg 1$ are mostly provided by acceptors located close to the midplane between the donor planes, so that the spacing of acceptor from both neighboring planes exceeds r_μ. Therefore the concentration of 0 complexes can be estimated as

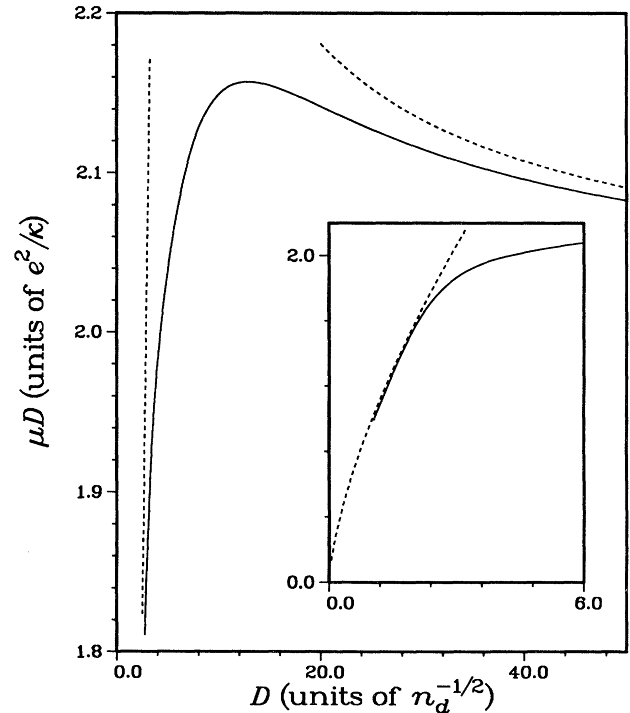

FIG. 4. The product μD as a function of D in the ranges $0<D<50$ and $0<D<6$ (inset). The small-D asymptote [Eq. (3)] and the large-D asymptote [Eq. (19)] are shown by dashed lines.

$$N_0=\frac{2N_a}{D}\left[\frac{D}{2}-r_\mu\right].$$

Since $N_0 \ll N_a$, we have $D/2-r_\mu \ll D/2$, i.e., $\mu \approx 2e^2/\kappa D$.

We also solved Eq. (5) numerically using the simulation results for N_2 and the expression (10) for N_0. The result is given in Fig. 4 together with the asymptotes (19) and (12). The curve begins at the point where $\mu\kappa D/e^2=1$ since for smaller D condition (7) is violated. Our simulation cannot give the dependence $\mu(D)$ for $D<n_d^{1/2}$, but at this point the exact solution is already surprisingly close to the asymptote (3), which can be used for smaller values of D.

IV. CONCLUSION

Hopping transport in samples constructed as multiple δ layers was studied experimentally in Refs. 10 and 11. The parameters of the samples used were $n_d=0.8\times10^{11}$ cm^{-2}, $D=1000$ Å. The degree of compensation with residual acceptors was estimated to be between 1% and 6%. For the value $n_dD^2=8$ the theory developed in the present paper predicts $\mu\approx1.85(e^2/\kappa D)$. Using the value $\kappa=12.5$ for GaAs we get $\mu\approx2.1$ meV. The activation energy of hopping conductivity obtained by fitting the experimental data[10,11] to the dependence (1) appears to be $\varepsilon_3=1.1$ meV. We suggest that the difference between the calculated and experimental values can be accounted for by the quantum-mechanical effects. Indeed the theory presented here should work only for $n_d \ll n_c$. In Refs. 10 and 11 $n_d\approx0.6n_c$, which is too large to expect quantitative agreement with our theory.

There are at least two reasons why the quantum-mechanical corrections lower the value of ε_3 obtained classically. First, the equality $\varepsilon_3=\mu$ does not take into account the fact that the energy level of the empty donor can be shifted due to the overlap of its wave function with the wave function of the closest occupied donor. Actually, the energy levels of the empty and the occupied donors are split and that causes a negative correction to the activation energy of the hop, which is of the order of the overlapping energy. Another correction to the classical result concerns the calculation of the concentration of a 0 complexes $N_0(\mu)$. For the formation of the 0 complex, we demanded the absence of donors at distances less than r_μ from the acceptor. Consider now a close pair of donors, such as a hydrogenlike molecule. It is known (see, for example, Ref. 15) that since the distance between the atoms in a molecule is less than $2.5a_B$ (a_B is the Bohr radius), the ionization potential of the molecule is greater than the Bohr energy. Therefore, if a close pair of donors is located at a distance even less than r_μ from the acceptor, the electron would not be removed from such a pair. In other words, pairs of donors separated by a distance less than $2.5a_B$ do not prevent the formation of 0 complexes. The Bohr radius in GaAs is 100 Å, while the average donor spacing is 350 Å. Hence the close pairs of donors may cause a significant increase of N_0. Since $N_0(\mu)$ is an increasing function of μ, the increase of N_0 lowers the Fermi level.

The indication that quantum-mechanical effects are important in the experimental situation of Refs. 10 and 11 is provided by the strong dependence of the activation energy on the magnetic field observed in these experiments. It is clear that the classical result is not sensitive to the magnetic field.

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