Diamagnetic susceptibility of indirect excitons in deformed germanium

T. G. Tratas and V. M. Édel'shteĭn

Institute of Solid State Physics, USSR Academy of Sciences
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The diamagnetic susceptibility of indirect excitons in Ge uniaxially compressed along the axis [100] or [111] is calculated. It is shown that despite the large anisotropy of the effective masses, the main contribution to the susceptibility comes from the Hamiltonian term that is quadratic in the external magnetic field (the Langevin term).

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1. INTRODUCTION

The Hamiltonian that describes the relative motion of an electron with an effective-mass tensor m^e_{ik} and of a hole with m^h_{ik}, which form an exciton with zero gravity-center momentum, is of the form[1]

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1+\mathcal{H}_2, \quad \mathcal{H}_0=\frac{1}{2}\hat{\mathbf{p}}\mu^{-1}\hat{\mathbf{p}}-e^2/\varepsilon_0 r,$$

$$\mathcal{H}_1=\frac{e}{c}[\mathbf{A}^e(\mathbf{r})m_e^{-1}-\mathbf{A}^h(\mathbf{r})m_h^{-1}]\hat{\mathbf{p}}, \tag{1}$$

$$\mathcal{H}_2=\frac{e^2}{2c^2}[\mathbf{A}^e(\mathbf{r})\mathbf{m}_e^{-1}\mathbf{A}^e(\mathbf{r})+\mathbf{A}^h(\mathbf{r})\mathbf{m}_h^{-1}\mathbf{A}^h(\mathbf{r})]+\frac{3e^2}{2c^2}\mathbf{A}(\mathbf{r})\mathbf{M}^{-1}\mathbf{A}(\mathbf{r}),$$

where

$$\mathbf{A}^{e,h}={}^1/_2[\mathbf{H},\ (\mu\mathbf{m}^{-1}_{e,h}\ \mathbf{r})], \quad \mathbf{A}=\mathbf{A}^e+\mathbf{A}^h, \quad \mu^{-1}=\mathbf{m}_e^{-1}+\mathbf{m}_h^{-1}, \quad \mathbf{M}=\mathbf{m}_e+\mathbf{m}_h$$

and it is assumed that the products of the coordinates and momenta have been symmetrized in $\mathcal{H}_1$. It is seen that an energy correction quadratic in the magnetic field results not only from $\mathcal{H}_2$ in first-order perturbation theory (the Langevin diamagnetism), but also from $\mathcal{H}_1$ in second order (the van Vleck orbital paramagnetism). In the case of isotropic masses, $\mathcal{H}_1$ goes over into[2]

$$\frac{e\hbar}{2\mu c}\frac{m_h-m_e}{m_h+m_e}\mathbf{H}\hat{\mathbf{L}}.$$

The relative-motion angular momentum $\hat{\mathbf{L}}$ is conserved, and $L=0$ in the ground state. There is therefore no orbital paramagnetism in the isotropic limits.

In uniaxially deformed germanium, the degeneracy of the hole band is lifted, the spin motion is separated with good accuracy from the orbital motion, and the latter is described by Hamiltonian (1).

2. COMPRESSION ALONG THE [001] AXIS

For the sake of argument, we consider an electron valley located along the [111] axis of the crystal. We choose an orthogonal basis $\mathbf{e}_1^0\mathbf{e}_2^0\mathbf{e}_3^0$ such that $\mathbf{e}_3^0 \parallel [001]$, and the plane $\mathbf{e}_2^0\mathbf{e}_3^0$ passes through the [111] axis. In this basis[3]

$$m_{h1}{}^0=m_{h2}{}^0=0{,}1095m_0, \quad m_{h3}{}^0=0.0457m_0. \tag{2}$$

The electron-mass matrix is diagonal in the basis $(\mathbf{e}_1'\mathbf{e}_2'\mathbf{e}_3')$, which is obtained by rotation around the $\mathbf{e}_1^0$ axis through an angle $\varphi=\tan^{-1}2^{1/2}$, and is equal to[3]

$$m_{e1}{}'=m_{e2}{}'=0{,}0815m_0, \quad m_{e3}{}'=1.588m_0. \tag{3}$$

It is convenient to carry out the calculations in the basis $(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3)$ that diagonalizes the reduced-mass matrix μ. It is obtained by rotating $(\mathbf{e}_1^0\mathbf{e}_2^0\mathbf{e}_3^0)$ around $\mathbf{e}_1^0$ through an angle $\alpha\approx\tan^{-1}3.33$, in which case

$$\mu_1=0.047m_0, \quad \mu_2=0.031m_0, \quad \mu_3=0.083m_0. \tag{4}$$

The ground state of the exciton can be obtained by a variational method. Measuring the length in units of $a_B=\hbar^2\varepsilon_0/\mu_3e^2$ and of energy $R=\mu_3e^4/2\hbar^2\varepsilon_3^2$, and using the wave function

$$\psi_0=(\pi abc)^{-1/2}\exp\{-[x^2/a^2+y^2/b^2+z^2/c^2]^{1/2}\},$$

we obtain

$$a=1.74, \quad b=2.02, \quad c=1.42, \quad E_0=-0.58. \tag{5}$$

In absolute units $aa_B=170$ Å, $ba_B=198$ Å, $ca_B=139$ Å, and $RE_0=-2.78\times10^{-3}$ eV. We reduce all the matrices in (2) to the basis $(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3)$, substitute in $\mathcal{H}_2$ and, using the numerical values in (2), (3), and (4), obtain

$$\delta E_L=(\mathcal{H}_2)_{00}=(e^2a_B^2/2m_0c^2)(25H_x^2+17H_y^2-8H_yH_z+41H_z^2). \tag{6}$$

If $|n^*\rangle$ is the first excited state of the exciton at which $(\mathcal{H}_1)_{0n^*}=0$, then the van Vleck correction satisfies the inequality

$$|\delta E_{VV}|=\sum_n{}'|(\mathcal{H}_1)_{0n}|^2/E_n-E_0\leqslant(\mathcal{H}_1^2)_{00}/E_{n^*}-E_0. \tag{7}$$

To estimate E_{n^*} we note that the first excited states corresponding to the $2p$-hydrogen states, are of the form

$$(c_1x+c_2y+c_3z)\psi(x^2, y^2, z^2)$$

and cause $(\mathcal{H}_1)_{0n}$ to vanish. It seems plausible that in higher states, e.g., $3d$, the quantity $E_{n^*}-E_0$ is equal to $|E_0|$ with sufficient accuracy. Indeed, in the hydrogenlike case $E_{3d}-E_0\approx0.9\ |E_0|$, and in our case the anisotropy of μ in (4) is of the order of unity. It is possible to refine the value of E_{n^*}, e.g., by a variational method, but there is no need for it since δE_{VV} is of the order of several percent of δE_L:

$$|\delta E_{VV}|\leqslant(2\hbar^2\varepsilon_0{}^2/m_0{}^2c^2|E_0|\mu_3e^2)(4H_x^2+0.7H_y^2-0.2H_yH_z+0.3H_z^2). \tag{8}$$

We write down now the diamagnetic-susceptibility tensor in the standard coordinate system of the crystal, i.e., $X\parallel(100)$, $Y\parallel(010)$, and $Z\parallel(001)$

$$\chi^L_{ik}\left[\frac{\text{erg}}{\text{G}^2}\right]=-10^{-24}\begin{pmatrix}8.3 & 1.6 & 1.9\\ 1.6 & 8.3 & 1.9\\ 1.9 & 1.9 & 5.7\end{pmatrix}. \tag{9}$$

The diamagnetic correction to the energy is given by

$$\delta E_L=-{}^1/_2\chi_{ik}{}^LH_iH_k, \quad i, k=1, 2, 3,$$

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where $H=(H_x H_y H_z)$ for an electron valley directed along the [111] axis, $H=(H_y, -H_x H_z)$ for the valley along [−1, 1, 1], $H=(-H_y, H_x, H_z)$ for the valley along [1, −1, 1], and $H=(-H_x, -H_y, H_z)$ for the valley along [−1, −1, 1]. The magnetic-field components H_x, H_y, and H_z are defined here in terms of the standard crystallographic coordinate system.

3. COMPRESSION ALONG THE [111] AXIS

It is known that compression decreases the energy of the electron valley located on the compression axis. We confine ourselves to this valley, i.e., to a "cold" exciton. In this case the [111] axis is the axial-symmetry axis and all the results can be clearly represented in analytic form. In a basis with $\mathbf{e}_3$ axis along [111] we have $m_{h\perp}=0.13m_0$ and $m_{h\parallel}=0.04m_0$ (Ref. 3), so that $\mu_\perp=0.05m_0$ and $\mu_\parallel=0.04m_0$. We express the length and energy in units $a_{B\perp}=\hbar\varepsilon_0/\mu_\perp e^2$ and $R_\perp=\mu_\perp e^4/2\hbar^2\varepsilon_0^2$ respectively, and choose the trial wave function of the ground state in the form

$$\psi_0=(\pi a_\perp^2 a_\parallel)^{-1/2}\exp\{-[(x^2+y^2)/a_\perp^2+z^2/a_\parallel^2]^{1/2}\}.$$

The energy corresponding to such a wave function was obtained in Ref. 4 and at the given values of $\mu_{\perp,\parallel}$ we obtain $a_\perp=1.06$, $a_\parallel=1.18$, and $E_0=-0.91$. In absolute units $a_\perp a_{B\perp}=172$ Å, $a_\parallel a_{B\perp}=191$ Å, and $R_\perp E_0=-2.62\times10^{-3}$ eV. In analogy with Sec. 2, it can be shown that $\mathcal{H}_2$ leads to a diamagnetic susceptibility

$$\chi_\perp^{\,L}=-\frac{e^2}{4c^2}a_{B\perp}^2\left\{a_\parallel^2\left[\frac{3}{M_\perp}+\frac{1}{M_\parallel^2}\left(\frac{m_{h\parallel}^2}{m_{e\perp}}+\frac{m_{e\parallel}^2}{m_{h\perp}}\right)\right]+(\perp\leftrightarrow\parallel)\right\},$$
$$\chi_\parallel^{\,L}=-e^2a_{B\perp}^2a_\perp^2/2\mu_\perp c^2. \qquad (10)$$

The Hamiltonian $\mathcal{H}_1$ leads only to a contribution to $\chi_\perp$. Arguments similar to the preceding ones lead to the estimate

$$|\chi_\perp^{\,VV}|\leqslant\frac{e^2}{c^2}\mu_\parallel\mu_\perp(m_{e\parallel}^{-1}m_{e\perp}^{-1}-m_{h\parallel}^{-1}m_{h\perp}^{-1})^2\times\frac{\hbar^2}{5R_\perp|E_0|}\left[\frac{\mu_\parallel}{\mu_\perp}\left(\frac{a_\parallel}{a_\perp}\right)^2+\frac{\mu_\perp}{\mu_\parallel}\left(\frac{a_\perp}{a_\parallel}\right)^2-2\right], \qquad (11)$$

which amounts in this case to less than 2% of χ_1^L. The numerical values are $\chi_1^L=-7.3\times10^{-24}$ and $\chi_\parallel^L=-8.3\times10^{-24}$ erg/G^2.

4. CONCLUSION

In both considered cases the contribution made to the susceptibility by $\mathcal{H}_1$ turned out to be numerically very small, and the anisotropy of χ^L substantial. The first circumstance is due principally to the small anisotropy of μ (for strongly anisotropic m_e and m_h), and also to the appearance, in the estimate of χ^{VV}, of small numbers, e.g., when averaging on a hydrogen ground-state function we have $(x^2\nabla_x^2)_{00}=0.2$. The second circumstance is due to the fact that the electrons and holes contribute to the Langevin susceptibility for the most part independently, and their contributions are determined separately by their masses.

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