The change in the energy spectrum of an exciton moving transverse to a magnetic field

I. P. Ipatova, A. Yu. Maslov, and A. V. Subashiev

A. F. Ioffe Physicotechnical Institute, Academy of Sciences of the USSR
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When an exciton moves transversely to a magnetic field the center of relative motion undergoes a shift ρ_0 away from the center of the Coulomb potential and increases with the momentum P of the exciton. It is shown that in a definite magnetic-field interval having an upper limit the magnitude of ρ_0 increases abruptly when the momentum of the exciton reaches $P = P_c$. The corresponding value of ρ_0, $\rho_0 = \rho_c$ considerably exceeds the transverse dimension of the exciton state and, depending on the magnetic field strength, can be either smaller or larger than the Bohr radius.

Gor'kov and Dzyaloshinskiĭ[1] have shown that in a magnetic field the motion of the center of gravity of an exciton affects on its internal motion. In Ref. 1 they studied the dependence of the energy of an exciton on the momentum of the center of gravity for the case of magnetic fields that satisfy the condition

$$r_0/r_B \ll (\mu/M)^{1/2}, \tag{1}$$

where $r_0 = (\hbar c/eH)^{1/2}$ is the magnetic length, $r_B = \hbar^2\varkappa/\mu e^2$ is the Bohr radius, $\mu = m_+m_-/M$, $M = m_+ + m_-$, and m_- and m_+ are the masses of the electron and hole, respectively. For a large difference in mass between the electron and hole, the inequality (1) is stronger than the usual condition for a strong magnetic field

$$r_0/r_B \ll 1. \tag{2}$$

It was shown that the wave function of the relative motion is concentrated near the center of the magnetic oscillator located at a distance $\rho_0 = Pr_0^2/\hbar$ from the center of the Coulomb well. The value of ρ_0 increases monotonically with the exciton momentum P. In Ref. 2 the characteristic spectrum was determined for large P when the distance ρ_0 becomes larger than the Bohr radius.[1)] This state is characterized by a large dipole moment.

In this investigation we examine the case of magnetic fields that satisfy the inequality opposite to (1)

$$r_0/r_B \gg (\mu/M)^{1/2}. \tag{3}$$

This condition takes in both the case $r_0 \ll r_B$ for greatly differing electron and hole masses and the case of weak fields. We show that when expression (3) holds, the behavior of the system undergoes a qualitative change that consists of the following: for small momenta the wave function is concentrated near the Coulomb center and shifts only slightly with increasing momentum. In this region the energy of the system depends quadratically on the momentum up to some threshold value $P = P_c$. At $P \gtrsim P_c$ their is an abrupt shift of the center of the wave function by an amount ρ_0. The corresponding value $\rho_0 = \rho_c = P_c r_0^2/\hbar$, depending on H, can be either larger or smaller than the Bohr radius. When condition (3) holds, the distance between the centers of the two regions of possible relative motion ($\rho \approx 0, \rho \approx \rho_0$) turns out to be considerably larger than the radii of the wave functions of the corresponding states. This allows us to study the change of the spectrum in the region where it undergoes the change. In the problem of exciton absorption this transition can show up in a large change in the exciton lifetime as a function of energy.

The Schrödinger equation for the internal motion of the electron and hole has the form[1]

$$\left\{-\frac{\hbar^2}{2\mu}\Delta - \frac{ie\hbar}{2\mu c}\gamma\mathbf{H}[\mathbf{r}\times\nabla] + \frac{e^2[\mathbf{H}\times\mathbf{r}]^2}{8\mu c^2} + \frac{e[\mathbf{P}\times\mathbf{H}]\mathbf{r}}{Mc} - \frac{e^2}{\varkappa r}\right\}\Psi = \left(E - \frac{P^2}{2M}\right)\Psi, \tag{4}$$

where

$$\gamma = (m_+ - m_-)/M, \quad \mathbf{r} = \mathbf{r}_- - \mathbf{r}_+,$$

and the vector potentials $\mathbf{A}$ is taken in the gauge $\mathbf{A} = (1/2)\mathbf{H}\times\mathbf{r}$.

The second term in the curly brackets introduces considerable difficulty in the solution of Eq. (4) because it does not permit the separation of the potential energy in which the relative motion occurs. Actually, the projection of the momentum in the direction of the magnetic field is not a good quantum number of the Hamiltonian (4). However, for states that are close to the ground state it is possible to select a region of finite motion where this quantity is approximately conserved. In the case of strong magnetic fields, where (2) holds, for sufficiently small P we can use, for the zero-order wave functions, the functions

$$\Psi_{nm\nu} = e^{im\varphi}\Phi_{nm}(\rho)\chi_\nu^{(n,m)}(z), \tag{5}$$

which correspond to an immobile exciton, the spectrum of which is well known.[3] The functions (5) describe the motion relative to the center of the Coulomb well. Here n is the radial magnetic quantum number and ν enumerates the states of the Coulomb series. We shall use perturbation theory to deal with the term

$$V = e[\mathbf{P}\times\mathbf{H}]\mathbf{r}/Mc \tag{6}$$

in the Hamiltonian (4). It should be noted that in the range of magnetic fields that we are considering, $1 \ll r_B^2/r_0^2 \ll M/\mu$, and the excited states close to the ground state are not the

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excited states of the Coulomb series with $n=m=0$ and $\nu=1,2,3,\dots$ as was the case in Ref. 1, but states with $n=\nu=0$ and $m=-1,-2,\dots$. Therefore we shall write down the dependence $E(\mathbf{P})$ for these states as well.

To second order in V we have (for $\mathbf{P}\perp\mathbf{H}$)

$$E_{0,m,\nu}(\mathbf{P})=E_{0,m,\nu}(0)+\frac{P^2}{2M}-\frac{\mu P^2}{2M^2}\hbar\omega_c\left[\frac{|m|+1}{(\mu/M)\hbar\omega_c+E_B\lambda_\nu/(|m|+1)}-\frac{|m|}{(\mu/M)\hbar\omega_c+E_B\lambda_\nu/|m|}\right], \quad (7)$$

where

$$m=0,-1,-2,\dots,\quad E_B=\hbar^2/2\mu r_B^2,\quad \omega_c=eH/\mu c,$$
$$\lambda_0\approx\ln(r_B^2/r_0^2),\quad \lambda_\nu\approx[\nu^3\ln^2(r_B^2/r_0^2)]^{-1},\quad \nu=1,2,3\dots \quad (8)$$

The equations for finding the exact values of $\lambda\nu$ are given in Refs. 1 and 3.

The reciprocal of the coefficient of P^2 in (7) gives the magnetic field dependence of the transverse mass of the exciton. Thus, for the ground state we have

$$M_H=M[1+(\mu/M)(\hbar\omega_c/E_B\lambda_0)]. \quad (9)$$

Formula (9) is a generalization of the formula derived in Ref. 1 for the dependence on H of the mass of the exciton in the entire region where the inequality (2) holds. For strong magnetic fields that satisfy inequality (1), the term 1 that appears in the square brackets in (9) can be neglected. In this case expression (9) goes over to (21) of Ref. 1.

If we assume that for large values of the momentum the motion also takes place only in the vicinity of the Coulomb well, then in studying the ground state the quantity V in (6) can be taken into account by perturbation theory up to values of the momentum for which V becomes about as large as the spacing between the levels of the immobile exciton:

$$V\leqslant\frac{\mu}{M}\hbar\omega_c+E_B\lambda_0 \quad\text{or}\quad P<\frac{\hbar}{r_0}\left(\frac{M}{\mu}\frac{r_0^2\lambda_0}{r_B^2}\right). \quad (10)$$

For the exciting states the momentum range in which the corrections associated with V are small is bounded by somewhat smaller values of momentum than in (10). However, as will be shown below, even for small values of the momentum the energetically more favorable states are those that correspond to another potential well for the internal motion of the exciton, where the center of this well is shifted relative to the center of the Coulomb well.

To study this state we examine the spectrum in the range of quite large values of P, where the function (5) should be replaced by

$$\varphi(\mathbf{r})=\exp(i\gamma\boldsymbol{\rho}\mathbf{P}/2\hbar)\Psi(\mathbf{r}+\boldsymbol{\rho}_0), \quad (11)$$

the argument of which is shifted by $\boldsymbol{\rho}_0$ relative to the center of the Coulomb well.[1]

Substituting (11) into (4) we obtain

$$\left\{-\frac{\hbar^2}{2\mu}\Delta-\frac{ie\hbar}{2\mu c}\gamma\mathbf{H}[\mathbf{r}\times\nabla]+\frac{e^2H^2\rho^2}{8\mu c^2}-\frac{e^2}{\varkappa(z^2+\rho_0^2)^{1/2}}+V_1(z,\rho)\right\}\varphi=E\varphi, \quad (12)$$

where

$$V_1(z,\rho)=\frac{e^2}{\varkappa}\left[\frac{1}{(z^2+\rho_0^2)^{1/2}}-\frac{1}{(z^2+(\rho+\rho_0)^2)^{1/2}}\right]+\mathbf{b}\rho+\frac{Mc^2b^2}{2e^2H^2}. \quad (13)$$

The term $e^2/\varkappa(z^2+\rho_0^2)^{1/2}$ in (12) corresponds to a potential produced by the Coulomb center in the region of the second potential well, while the contribution of V_1 at large momenta is small. We estimate this contribution below by perturbation theory. The quantity $\mathbf{b}$ is determined from the condition that (13) have no term linear in $\boldsymbol{\rho}$.

In zero order in V_1 the variables in Eq. (12) are separable. The solutions for one-dimensional equation of motion in the z direction

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dz^2}-\frac{e^2}{\varkappa(z^2+\rho_0^2)^{1/2}}\right\}\chi(z)=E_\parallel\chi(z) \quad (14)$$

are known[1,2] and for the ground state of the Coulomb series they have the form

$$E_\parallel=-E_B\lambda^2 \quad\text{for}\quad \rho_0<r_B, \quad (15)$$

where $\lambda=2\ln(r_B\hbar/\lambda r_0^2P)-2C$, $C=0.5772\dots$, and

$$E_\parallel=-2E_B\frac{r_B}{\rho_0}\left[1-\frac{1}{2}\left(\frac{r_B}{\rho_0}\right)^{1/2}\right] \quad\text{for}\quad \rho_0>r_B. \quad (16)$$

The equation of motion in the (ρ,φ) plane corresponds to an oscillator whose spectrum is

$$E_\perp={}^1/_2\hbar\omega_c[n+{}^1/_2(|m|+\gamma m+1)], \quad (17)$$

and is independent of P. The total energy of the exciton in this case has the form

$$E=E_\parallel(P)+E_\perp. \quad (18)$$

An estimate of the contribution from V_1 by perturbation theory shows that, as regards the ground state energy, this contribution can be neglected for momentum

$$P>\frac{\hbar}{r_0}\left(\frac{M}{\mu}\frac{r_0^2}{r_B^2}\lambda_0\right)^{1/2}. \quad (19)$$

This defines the lower limit of applicability of formulas (15), (16), and (18). Because of the parameter (3) the regions in which inequalities (10) and (19) hold overlap, so that in the range of momentum

$$\left(\frac{M}{\mu}\frac{r_0^2}{r_B^2}\lambda_0\right)^{1/2}<\frac{Pr_0}{\hbar}<\frac{M}{\mu}\frac{r_0^2}{r_B^2}\lambda_0 \quad (20)$$

both solutions, (7) and (18), exist. We note that these solutions were obtained under the assumption that the wave function is concentrated entirely in one of the two potential wells. For the excited states the interval (20) becomes narrower as the energies of the states increase.

The ground state of the exciton is described by either solution (7) or (18) depending on which corresponds to the energy minimum. For some vaue $P \approx P_c$ these two energies are equal. If

$$\left(\frac{r_0}{r_B}\right)^4 < \frac{\mu}{M},$$

then $P_c = \frac{\hbar}{r_B}\left[\frac{M}{\mu}\lambda_0 \ln\left(\frac{M}{\mu}\frac{r_0^2}{r_B^2}\right)\right]^{1/2}, \quad \rho_c < r_B,$

and the energy of the exciton in the second well is described by formula (15). For

$$(r_0/r_B)^4 > \mu/M \tag{21}$$

the distance between the centers of the two wells is greater than r_B and there is a transition into the state with energy (16). In this case

$$P_c = (\hbar/r_B)(M/\mu)^{1/2}\lambda_0.$$

In the range of momentum near P_c it is necessary to take both potential wells into account. In the transition region the wave functions are a superposition of solutions (5) and (11), and the expression for the spectrum is given by the usual perturbation theory formulas for a twofold degenerate state. The width of this region is

$$\Delta E \approx E_B \exp\left[-\left(\frac{P_c r_0}{2\hbar}\right)^2\right],$$

$$\Delta P \approx \frac{\hbar}{r_B}\left(\frac{M}{\mu}\right)^{1/2} \exp\left[-\frac{1}{2}\left(\frac{P_c r_0}{2\hbar}\right)^2\right]. \tag{22}$$

From this it can be seen that the restructing of the spectrum from (7) to (18) takes place in an exponentially narrow region. This circumstance justifies the use of a superposition of wave functions corresponding to separate potential wells.

A similar spectrum restructuring corresponding to a crossing of levels occurs also, for instance, when the ground state level of one of the wells coincides with an excited state level of the other well. In the case, because of the exponential smallness of the overlap integrals, the pair of intersecting levels can be considered independent of the others. However, as was noted above, when the energy of the excited state increases the momentum range (20) in which nearly independent states coexist in the two wells becomes narrower and can vanish altogether. Therefore this treatment is not applicable for excited states beyond a certain point.

The change described above in the exciton spectrum with change in the momentum of the center of gravity occurs in the entire range of magnetic fields that satisfy condition (3), i.e., also in the region of weak fields. The most important difference that arises when the magnetic field is decreased is that for small momentum the expression for the H-dependent effective mass of the exciton differs from (9). In particular, in the limit of weak magnetic fields[4]

$$M_H = M\left[1 + \frac{9\mu}{8M}\left(\frac{\hbar\omega_c}{E_B}\right)^2\right]. \tag{23}$$

In the entire range of fields that satisfy inequality (21) the distance between the centers of the wells is greater than r_B. However, it should be noted that the binding energy of an exciton in the second well, even for $P \approx P_c$, is small ($E = \hbar\omega_c(\mu/M)^{1/2}$), which can make it difficult to observe experimentally in the case of weak magnetic fields.

Thus, the dependence of the energy of an exciton on the momentum of its center of gravity has a singular behavior near $P \approx P_c$. This behavior is manifest in a strong change in the derivative dE/dP for small variation of the momentum ΔP given by (22).

In a momentum range of width ΔP near P_c there is an abrupt increase from $\rho_1 = \mu r_B^2 P / M\hbar$ to $\rho_2 \approx P r_0^2/\hbar$ in the average distance between the electron and the hole. The average distance between the particles determines the dipole moment and the polarizability of the moving exciton.[1] In the range we are considering the polarizability increases from $\alpha_1 = \varkappa r_0^2 r_B$ to $\alpha_2 = \varkappa r_0^4 M/\mu r_B$ as the momentum increases. This jump in the polarizability can be observed experimentally by measurements of polarizability by the microwave methods of Refs. 5 and 6.

The abrupt change in the dependence of the energy on the momentum also leads to singularities in the density of states, and these can show up in the frequency dependence of the absorption coefficient. However, this topic requires a special investigation. Let us only note that the singularity in the total density of states is somewhat smoothed out because the dependence of the energy on the component of momentum parallel to H does not have singularities.

The magnetic mass, defined by formula (9) can be evident in phenomena associated with the localization of the exciton as a whole in potentials produced by defects[7] or by fluctuations in the composition of solid solutions.[8,9]

[1]) In Ref. 2 the problem that was studied was that of a stationary hydrogen-like system in crossed electric and magnetic fields. This problem is equivalent to that of a particle with momentum P because a field $\vec{\mathscr{E}} = \mathbf{P} \times \mathbf{H}/Mc$ appears in the coordinate frame attached to the particle.

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