CONTRIBUTION TO THE THEORY OF THE MOTT EXCITON IN A STRONG MAGNETIC FIELD

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Submitted March 16, 1967

Zh. Eksp. Teor. Fiz. 53, 717–722 (August, 1967)

The dependence of the energy of a Mott exciton on its transverse momentum is calculated in the case when the exciton is in a strong magnetic field (the distance between the Landau levels $e\hbar H/\mu c$ exceeds the Coulomb energy $\mu e^4/\varepsilon^2\hbar^2$, where μ is the reduced mass and ε the dielectric constant). The dependence of the probability for exciton production on the transverse component of the photon momentum and on the electric field is also determined.

THE theory of a Mott exciton in a strong magnetic field was developed by Elliott and Loudon[1] and by Hasegawa and Howard,[2] who confined themselves, however, to the case of a zero exciton momentum. We shall investigate the influence of the exciton motion on its spectrum and on the production probability.

In a strong magnetic field, when the distances between the Landau levels $eH\hbar/\mu c$ (μ = reduced mass) exceed the Coulomb energy $\mu e^4/\varepsilon^2\hbar^2$ (ε = dielectric constant), the question arises of separating the motion of the exciton mass center. Although such a problem was solved in principle by Lamb,[3] its exposition is very intricate. We therefore present here a more lucid derivation of Lamb's result, and use the derivation to obtain formulas for the exciton production probability.

We confine ourselves to the case of an isotropic dispersion law for electrons and holes. Then the Hamiltonian $\hat{\mathscr{H}}$ of an exciton situated in homogeneous electric and magnetic fields $\mathscr{E}$ and H is

$$\frac{1}{2m_1}\left(-i\hbar\nabla_1+\frac{e}{c}\mathbf{A}_1\right)^2+\frac{1}{2m_2}\left(-i\hbar\nabla_2-\frac{e}{c}\mathbf{A}_2\right)^2+e\mathscr{E}(\mathbf{r}_1-\mathbf{r}_2)-\frac{e^2}{\varepsilon|\mathbf{r}_1-\mathbf{r}_2|}=\hat{\mathscr{H}}. \quad (1)$$

We introduce the vector operator

$$\hat{\mathbf{P}}=-i\hbar\nabla_1-i\hbar\nabla_2+\frac{e}{c}(\mathbf{A}_1-\mathbf{A}_2)-\frac{e}{c}[\mathbf{H},\mathbf{r}_1-\mathbf{r}_2], \quad (2)^*$$

which plays the role of the momentum of the exciton in a magnetic field. It is easy to verify that the operator $\hat{\mathbf{P}}$ commutes with the Hamiltonian (1)[1)] and, moreover, all three of its components commute with one another. This circumstance makes it possible to obtain the dependence of the eigenfunctions of $\hat{\mathscr{H}}$ on the coordinate of the center of gravity of the exciton:

$$\mathbf{R}=(m_1\mathbf{r}_1+m_2\mathbf{r}_2)/(m_1+m_2).$$

Without loss of generality we can choose a definite gauge for **A**:

$$\mathbf{A}={}^1/_2[\mathbf{Hr}].$$

Then (2) takes the form

$$\hat{\mathbf{P}}=-i\hbar\nabla_{\mathbf{P}}-\frac{e}{2c}[\mathbf{Hr}],\quad \mathbf{r}=\mathbf{r}_1-\mathbf{r}_2. \quad (3)$$

The eigenfunctions of (3) are

$$\Psi_{\mathbf{P}}(\mathbf{r}_1,\mathbf{r}_2)=\exp\left\{i\left(\mathbf{P}+\frac{e}{2c}[\mathbf{Hr}]\frac{\mathbf{R}}{\hbar}\right)\right\}\Psi_{\mathbf{P}}(\mathbf{r}), \quad (4)$$

where $\Psi_{\mathbf{P}}(\mathbf{r})$ is an arbitrary function of **r**, and **P** is the exciton momentum. Finally, substituting (4) in (1) we obtain the equation of relative motion of the electron and hole:

$$\left\{-\frac{\hbar^2}{2\mu}\Delta+\frac{ie\hbar}{2\mu c}\gamma\mathbf{H}[\mathbf{r}\nabla]+\frac{e^2}{8\mu c^2}[\mathbf{Hr}]^2+\frac{e}{Mc}[\mathbf{PH}]\mathbf{r}+e\mathscr{E}\mathbf{r}-\frac{e^2}{\varepsilon r}+\frac{\mathbf{P}^2}{2M}\right\}\Psi_{\mathbf{P}}(\mathbf{r})=E\Psi_{\mathbf{P}}(\mathbf{r}). \quad (5)$$

Here

$$\mu=\frac{m_1m_2}{m_1+m_2},\quad M=m_1+m_2,\quad \gamma=\frac{m_2-m_1}{m_2+m_1}. \quad (6)$$

The quantity **P** which enters in this equation has all the properties of a momentum. In particular, the average exciton velocity **V** is determined from the usual relation

$$\mathbf{V}=\partial E/\partial\mathbf{P}. \quad (7)$$

For the proof we note that, according to footnote [1)]

$$\hat{\mathbf{P}}=M\hat{\mathbf{V}}-\frac{e}{c}[\mathbf{Hr}],$$

where $\hat{\mathbf{V}}=d\mathbf{R}/dt$ is the operator of the c.m.s. velocity. On the other hand, $\hat{\mathbf{V}}$ coincides with the derivative of the Hamiltonian of (5), $\mathscr{H}_{\mathbf{P}}$, with respect to the momentum

$$\frac{\partial\mathscr{H}_{\mathbf{P}}}{\partial\mathbf{P}}=\frac{1}{M}\left(\hat{\mathbf{P}}+\frac{e}{c}[\mathbf{Hr}]\right)=\hat{\mathbf{V}}.$$

We shall henceforth confine ourselves to the case of an electric field and momentum perpendicular to the magnetic field; the latter will be assumed directed along the z axis. The transverse components will be designated by the index ρ.

$^*[\mathbf{H},\mathbf{r}_1-\mathbf{r}_2]\equiv\mathbf{H}\times(\mathbf{r}_1-\mathbf{r}_2)$.

1)To this end it is sufficient to note that $\hat{\mathbf{P}}=m_1\hat{\mathbf{v}}_1+m_2\hat{\mathbf{v}}_2-ec^{-1}\mathbf{H}(\mathbf{r}_1-\mathbf{r}_2)$, where $\hat{\mathbf{v}}_{1,2}$ are the electron and hole velocity operators, and to write the operator equations of motion

$$m_1\frac{d\hat{\mathbf{v}}_1}{dt}=-e\mathscr{E}+\frac{e}{c}[\mathbf{H}\hat{\mathbf{v}}_1],\quad m_2\frac{d\hat{\mathbf{v}}_2}{dt}=e\mathscr{E}-\frac{e}{c}[\mathbf{H}\hat{\mathbf{v}}_2],$$

from which it follows directly that $d\hat{\mathbf{P}}/dt=0$.

By using the transformation

$$\Psi(\mathbf{r}) = \Phi(\mathbf{r} - \rho_0)\exp(i\gamma\mathbf{r}\mathbf{P}'/2\hbar), \tag{8}$$

where

$$\mathbf{P}' = \mathbf{P} + \frac{Mc}{H^2}[\mathbf{H}\mathscr{E}], \quad \rho_0 = \frac{c}{eH^2}[\mathbf{H}\mathbf{P}'], \tag{9}$$

we can reduce (5) to the form

$$\Big\{-\frac{\hbar^2}{2\mu}\Delta_\rho + \frac{ie\hbar}{2\mu c}\gamma\mathbf{H}[\rho\nabla] - \frac{e^2}{8\mu c^2}H^2\rho^2 - \frac{\hbar^2}{2\mu}\frac{d^2}{dz^2} - \frac{e^2}{\varepsilon[(\rho+\rho_0)^2+z^2]^{1/2}} + \frac{\mathbf{P}^2}{2M} - \frac{\mathbf{P}'^2}{2M}\Big\}\Phi = E\Phi. \tag{10}$$

In the case of a strong field we can neglect in the zeroth approximation the Coulomb interaction. Then the dependence of the energy on $\mathbf{P}$ and $\mathscr{E}$ is determined by the expression

$$\frac{\mathbf{P}^2 - \mathbf{P}'^2}{2M} = -\frac{c}{H^2}\mathbf{P}[\mathbf{H}\mathscr{E}] - \frac{Mc^2}{2}\frac{\mathscr{E}^2}{H^2}.$$

From this follow the physically obvious relations for the drift velocity

$$\mathbf{V} = \frac{c}{H^2}[\mathscr{E}\mathbf{H}] \tag{11a}$$

and for the dipole moment of the exciton

$$\mathbf{d} = \frac{Mc^2}{H^2}\mathscr{E} + \frac{c}{H^2}[\mathbf{P}\mathbf{H}]. \tag{11b}$$

As expected, the total effective mass of the free electron and hole, corresponding to motion across the field, is infinite. On the other hand, the nonzero values of the momentum (in the absence of $\mathscr{E}$) describe the average distance between particles

$$\rho_0 = -d/e.$$

A finite transverse mass occurs only when the Coulomb interaction is taken into account.

As shown by Elliott and Loudon,[1] the wave function of the exciton Φ from (10) can be represented in first approximation in the small parameter of the theory $(\mu e^4/\varepsilon^2\hbar^2)/(eH\hbar/\mu c)$ in the form

$$\Phi(\mathbf{r}) = \varphi(\rho)\psi(z),$$

where $\varphi(\rho)$ describes free transverse motion, and $\psi(z)$ satisfies the equation that results from the averaging of (10) with the aid of $\varphi(\rho)$.

We confine ourselves to an exciton in the zeroth Landau band. Then

$$\varphi_0(\rho) = \frac{1}{\sqrt{2\pi}\, r_0}\exp\Big\{-\Big(\frac{\rho^2}{4r_0^2}\Big)\Big\}, \tag{12}$$

where $r_0 = \sqrt{c\hbar/eH}$. The function $\psi(z)$ satisfies the equation

$$\Big\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dz^2} + U(z)\Big\}\psi = W\psi, \tag{13}$$

where

$$U(z) = -\frac{e^2}{2\pi\varepsilon r_0^2}\int\frac{d\rho}{[(\rho+\rho_0)^2+z^2]^{1/2}}\exp\Big\{-\frac{\rho^2}{2r_0^2}\Big\}. \tag{14}$$

The energy of the exciton (with allowance for the spin) is written here in the form

$$E = \Delta + \frac{\mathbf{P}^2 - \mathbf{P}'^2}{2M} + \frac{e\hbar H}{2\mu c} + W, \tag{15}$$

where Δ is the distance between the electron and hole bands.

Equation (13) can be easily solved by the method used in [2]. For the exciton ground state we obtain

$$W_0 = -\frac{\hbar^2}{2\mu r_B^2}\lambda^2, \quad r_B = \frac{\varepsilon\hbar^2}{\mu e^2}, \tag{16}$$

where λ is the solution of the equation

$$\lambda = 2\ln\Big(\frac{r_B}{\sqrt{2}\lambda r_0}\Big) - C - \Lambda\Big(\frac{r_0^2P'^2}{2\hbar^2}\Big); \tag{17}$$

$$\Lambda(x) = \int_0^x dy e^{-y}\ln\frac{x}{y}, \tag{18}$$

with $\Lambda(x) \approx x$ as $x \to 0$ and $\Lambda(x) = \ln x - C$ as $x \to \infty$; C is Euler's constant.

The excited states of the discrete spectrum are given by the formula ($\nu = 1, 2, \ldots$)

$$W_\nu = -\frac{\hbar^2}{2\mu r_B^2}\frac{1}{\nu^2} + \frac{\hbar^2}{2\mu r_B^2}\frac{1}{\nu^3}v_\nu, \tag{19}$$

$$\frac{1}{v_\nu} = \ln\Big(\frac{r_B\nu}{\sqrt{2}\,r_0}\Big) - \psi(\nu) - \frac{1}{2\nu} - \frac{3}{2}C - \frac{1}{2}\Lambda\Big(\frac{r_0^2P'^2}{2\hbar^2}\Big) \tag{20}$$

with Λ from (18). Here $\psi(\nu)$ is the ψ-function.

In addition, the exciton has a hydrogen series of levels, corresponding to wave functions that are antisymmetrical in z.[2] All the states are not degenerate with respect to the momentum.

At small momenta P' $(r_0P'/\hbar \ll 1)$, the P'-dependent addition to W_0 is equal to

$$\delta W_0 = \frac{1}{2\mu}\frac{r_0^2}{r_B^2}\lambda_0 P'^2 \equiv \frac{P'^2}{2M_0}, \quad M_0 = \mu\frac{r_B^2\lambda_0}{r_0^2}, \tag{21}$$

where λ_0 is the solution of (17) with $P' = 0$. The corresponding addition to W_ν is

$$\delta W_\nu = \frac{1}{4\mu}\frac{r_0^2}{r_B^2}v_{\nu_0}^2\frac{P'^2}{\nu^3} \equiv \frac{P'^2}{2M_\nu}, \quad M_\nu = 2\mu\frac{r_B^2}{r_0^2}\frac{\nu^3}{v_{\nu_0}^2}; \tag{22}$$

$v_{\nu 0}$ is given by formula (20) with $P' = 0$.

At large momenta $(r_0P'/\hbar \gg 1)$, Eq. (17) takes the form

$$\lambda = 2\ln\Big(\frac{r_B\hbar}{\lambda r_0^2P'}\Big) - 2C, \tag{23}$$

and formula (20) for v_ν goes over into

$$\frac{1}{v_\nu} = \ln\frac{\nu\hbar r_B}{r_0^2P'} - \psi(\nu) - \frac{1}{2\nu} - 2C. \tag{24}$$

All the foregoing formulas are valid for momenta that are not too large: $r_0^2P'/\hbar \ll r_B$.

At small values of P', the part of the energy that depends on the momentum $\mathbf{P}$ and on the electric field $\mathscr{E}$ is ($\nu = 0, 1, 2, \ldots$)

$$\delta E_\nu = \frac{\mathbf{P}^2 - \mathbf{P}'^2}{2M} + \frac{\mathbf{P}'^2}{2M_\nu} = \frac{\mathbf{P}^2}{2M_\nu} - \Big(1 - \frac{M}{M_\nu}\Big)\frac{c}{H^2}[\mathbf{H}\mathscr{E}]\mathbf{P} - \frac{1}{2}\Big(1 - \frac{M}{M_\nu}\Big)\frac{Mc^2}{H^2}\mathscr{E}^2, \tag{25}$$

where M_ν is given by (21) and (22). For the velocity and the dipole moment we have

$$\mathbf{V}=\frac{\mathbf{P}}{M_\nu}+\left(1-\frac{M}{M_\nu}\right)\frac{c}{H^2}[\mathscr{E}\mathbf{H}],$$
$$\mathbf{d}=\left(1-\frac{M}{M_\nu}\right)\frac{Mc^2}{H}\mathscr{E}+\left(1-\frac{M}{M_\nu}\right)\frac{c}{H^2}[\mathbf{PH}]. \tag{26}$$

From (26) we get the polarizability at a specified exciton momentum $\mathbf{P}$:

$$\alpha_P=\left(1-\frac{M}{M_\nu}\right)\frac{Mc^2}{H^2}. \tag{27}$$

Its order of magnitude is $\varepsilon r_0^4/r_B$, i.e., it is very small. The polarizability at a specified velocity α_ν, which coincides with the polarizability of the exciton at rest, is

$$\alpha_\nu=\frac{(M_\nu-M)c^2}{H^2}\approx\frac{M_\nu c^2}{H^2}. \tag{28}$$

Its order of magnitude is $\varepsilon r_0^2 r_B$, as expected from physical considerations.

We present one more formula for the addition to the energy, expressed in terms of $\mathbf{V}$ and $\mathscr{E}$:

$$\delta E_\nu=\frac{1}{2}M_\nu\mathbf{V}^2-\frac{1}{2}\alpha_\nu\mathscr{E}^2\approx\frac{1}{2}M_\nu\left(\mathbf{V}^2-\frac{c^2}{H^2}\mathscr{E}^2\right).$$

At large values of P', the dependence of the exciton energy on the momentum and on $\mathscr{E}$ has a more complicated form. We present the corresponding expression for the ground state only:

$$\delta E_0=-\frac{2\hbar^2}{\mu r_B^2}\ln^2\left(\frac{r_B\hbar}{r_0^2P'}\right)+\frac{\mathbf{P}^2-\mathbf{P}'^2}{2M} \tag{29}$$

(the formula is given with logarithmic accuracy). When $P'\ll\hbar/r_B$, the principal term is the logarithmic one. To the contrary, when $P'\gg\hbar/r_B$ the logarithmic term becomes a small addition.

In conclusion, let us discuss the dependence of the probability of exciton production on the electric field and on the momentum of the absorbed photon. As is well known (see, e.g., [4]), this dependence is determined by a factor $|\Psi(0)|^2$, where $\Psi(\mathbf{r})$ is the wave function of the relative motion of the exciton (8). According to (8), (9), and (12) we have in the zeroth Landau band

$$|\Psi_\nu(0)|^2=\varphi_0(\rho_0)^2\psi_\nu^2(0)=\frac{1}{2\pi r_0^2}\exp\left\{-\frac{r_0^2P'^2}{2\hbar^2}\right\}\psi_\nu^2(0). \tag{30}$$

The expressions for $\psi_\nu^2(0)$ can be readily obtained by the same method.[2] For the ground state we have

$$|\Psi_0(0)|^2=\frac{\lambda}{2\pi r_0^2r_B}\exp\left\{-\frac{r_0^2P'^2}{2\hbar^2}\right\}, \tag{31}$$

and for the excited states (ν = 1, 2, ...)

$$|\Psi_\nu(0)|^2=\frac{1}{2\pi r_0^2r_B}\frac{v_\nu^2}{\nu^3}\exp\left\{-\frac{r_0^2P'^2}{2\hbar^2}\right\} \tag{32}$$

with λ and v_λ from (17) and (20).

$\mathbf{P}'$ is given by formula (9), in which we must substitute for $\mathbf{P}$ the transverse component of the photon wave vector $\hbar\mathbf{k}_\perp$:

$$\mathbf{P}'=\hbar\mathbf{k}_\perp+\frac{Mc}{H^2}[\mathbf{H}\mathscr{E}]. \tag{33}$$

The dependence of $|\Psi(0)|^2$ on the momentum and on $\mathscr{E}$ is determined essentially by the exponential factor. In the absence of an electric field, it takes the form ($\lambda\!\!\!^{-}$ is the photon wavelength)

$$\exp\left\{-\frac{2\pi^2r_0^2}{\lambda^2}\sin^2\theta\right\} \tag{34}$$

where θ is the angle between the magnetic field and the photon direction. In the optical band, the numerical value of the argument of the exponential is $(1-0.5)H^{-1}$ (H is in kOe). Thus, in fields on the order of several kOe and weaker, the exponential factor plays an important role.

The influence of the electric field comes into play for fields

$$\mathscr{E}\sim2\pi\hbar H/\lambda Mc$$

or (when M is on the order of the mass of the free electron)

$$\mathscr{E}\ [\text{в/см}]\sim H\ [\text{кэ}].$$

In still stronger field, the exponential takes the form

$$\exp\left\{-\frac{M^2c^3}{2eH^3\hbar}\mathscr{E}^2\right\}, \tag{35}$$

and the intensity starts to decrease exponentially. The numerical value of the argument of the exponential is $\sim0.5\mathscr{E}^2/H^2$ ($\mathscr{E}$ in V/cm, H in kOe, M is of the order of the electron mass).

We are grateful to E. I. Rashba for valuable discussions.

[1] R. J. Elliott and R. Loudon, J. Phys. Chem. Solids **15**, 196 (1960).

[2] H. Hasegawa and R. E. Howard, J. Phys. Chem. Solids **21**, 179 (1961).

[3] W. Lamb, Phys. Rev. **85**, 259 (1952).

[4] J. Elliott and R. Loudon, Phys. Chem. Solids **8**, 382 (1959).

Translated by J. G. Adashko
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