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Excitons with anisotropic effective mass

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Abstract. We present a simple analytic scheme for calculating the binding energy of excitons in semiconductors that takes full account of the existing anisotropy in the effective mass, as a complement to the qualitative treatment in most textbooks. Results obtained for excitons in gallium nitride form the basis for a discussion of the accuracy of this approach.

Zusammenfassung. Wir präsentieren ein einfaches analytisches Verfahren zur Berechnung der Bindungsenergie von Exzitonen in Halbleitern, das die vorhandene Anisotropie in der effektiven Masse vollständig miteinbezieht, in Ergänzung zu der qualitativen Betrachtung in den meisten Lehrbüchern. Ergebnisse für Exzitonen in Galliumnitrid bilden die Grundlage für eine Diskussion der Genauigkeit dieser Methode.

I. INTRODUCTION

The traditional one-particle theory of semiconductors as taught in undergraduate courses is that of a material with a finite energy gap separating the highest occupied from the lowest unoccupied electronic state. In this picture the minimum energy for an elementary excitation is that required to raise a valence band electron into the conduction band, and is thus equal to the gap E_g. However, the electron and the hole, which is created in the same process, need not separate completely and can instead form a bound pair under the influence of their mutual Coulomb attraction [1]. Such bound electron-hole pairs, which transport energy and momentum but no charge, are called *excitons*. They are, in fact, the truly lowest elementary excitations of a pure semiconductor and their influence on the optical properties of a material is profound. Most importantly, the occurrence of excitons lowers the threshold for photon absorption to $E_\mathrm{g} - E_\mathrm{b}$, where E_b denotes the internal binding energy of the electron-hole pair.

Because of their practical significance excitons feature in all textbooks on solid state physics, but the discussion is usually restricted to some qualitative arguments based on formal similarities to the hydrogen atom problem, which is modified only by a dielectric constant to account for the surrounding medium and by empirical effective masses for the electron and hole [2]. The latter are always assumed to be isotropic, but while there certainly are textbook examples such as CdS for which this condition is nearly satisfied and hydrogenic absorption series have indeed been observed [3], in most semiconductors the anisotropy in the effective mass is so large that it cannot be ignored in a quantitative treatment. In this paper we present a variational scheme for calculating the binding energy E_b of excitons in realistic materials that takes full account of the existing anisotropy. Our priority has been to maintain a universally applicable and strictly analytic approach suitable for teaching purposes.

II. VARIATIONAL EXCITON WAVEFUNCTION

Most semiconductors used for modern electronic devices crystallize in the diamond (e.g. Si, Ge), zincblende (e.g. GaAs) or wurtzite (e.g. GaN) structure, for which the constant energy surfaces $E(\mathbf{k})$ about the valence band maximum and conduction band minimum are ellipsoidal in shape, yielding distinct longitudinal electron and hole effective masses $m_\parallel^\mathrm{e}$ and $m_\parallel^\mathrm{h}$ along one principal axis, and transverse effective masses $m_\perp^\mathrm{e}$ and $m_\perp^\mathrm{h}$ in the plane perpendicular to it. Here we will focus on this geometry, although the method is readily generalized. Taking the principal axis in the z-direction, the Hamiltonian for the relative motion of the electron-hole pair is

$$H = -\frac{\hbar^2}{2\mu_\perp}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right) - \frac{\hbar^2}{2\mu_\parallel}\frac{\partial^2}{\partial z^2} - \frac{e^2}{4\pi\epsilon_0\epsilon\sqrt{x^2+y^2+z^2}} \tag{1}$$

where $\mu_\perp = m_\perp^\mathrm{e} m_\perp^\mathrm{h}/(m_\perp^\mathrm{e}+m_\perp^\mathrm{h})$ and $\mu_\parallel = m_\parallel^\mathrm{e} m_\parallel^\mathrm{h}/(m_\parallel^\mathrm{e}+m_\parallel^\mathrm{h})$ denote the reduced transverse and longitudinal effective mass, respectively, and ϵ is a suitable dielectric constant. The anisotropy destroys the spherical symmetry of the hydrogen Hamiltonian, yielding a wavefunction with a different characteristic localization along the principal axis and in the transverse plane. We therefore choose a generalization of the hydrogen ground-state wavefunction with ellipsoidal symmetry

$$\psi(x,y,z) = \left(\frac{\beta^3}{\lambda\pi}\right)^{1/2} \exp\left(-\beta\sqrt{x^2+y^2+(z/\lambda)^2}\right) \tag{2}$$

where the two parameters β and λ can be varied independently to control the transverse and longitudinal extension. The wavefunction, of course, becomes exact in the isotropic case $\mu_\parallel = \mu_\perp$ with $\lambda = 1$ and $\beta^{-1} = a_0\epsilon m/\mu_\perp$, where $a_0 = 0.529\,\text{Å}$ denotes the Bohr radius and m is the free electron mass, but it remains an excellent approximation even when the anisotropy is large. A wavefunction

of the type (2) was originally proposed in [4] to describe shallow donor impurity states in Si and Ge, but treated numerically and evaluated only for the mathematically distinct case $\lambda < 1$, reflecting the fact that the longitudinal effective mass is greater than the transverse one for electrons at the bottom of the conduction band in both materials. No such restriction will be made in this paper.

Given the explicit form of the wavefunction (2) the calculation of the kinetic energy is straightforward, using the substitution $z' = z/\lambda$ and a subsequent transformation to spherical coordinates. We obtain

$$\begin{aligned} -\frac{\hbar^2}{2\mu_\perp}\int\psi\frac{\partial^2}{\partial x^2}\psi\,\mathrm{d}^3r &= -\frac{\hbar^2}{2\mu_\perp}\int\psi\frac{\partial^2}{\partial y^2}\psi\,\mathrm{d}^3r \\ &= \frac{\hbar^2}{6\mu_\perp}\beta^2 \end{aligned} \tag{3}$$

for the contribution in the transverse isotropic plane, and similarly

$$-\frac{\hbar^2}{2\mu_\parallel}\int\psi\frac{\partial^2}{\partial z^2}\psi\,\mathrm{d}^3r = \frac{\hbar^2}{6\lambda^2\mu_\parallel}\beta^2 \tag{4}$$

for the relative motion along the principal axis. To calculate the potential energy we use the same transformation to spherical coordinates. The integrals over the radial variable and the azimuth angle are readily evaluated, leaving

$$\begin{aligned} &-\frac{e^2}{4\pi\epsilon_0\epsilon}\int\psi\frac{1}{\sqrt{x^2+y^2+z^2}}\psi\,\mathrm{d}^3r \\ &\quad= -\frac{e^2}{8\pi\epsilon_0\epsilon}\beta\int_0^\pi\frac{\sin\theta\,\mathrm{d}\theta}{\sqrt{1+(\lambda^2-1)\cos^2\theta}}\,. \end{aligned} \tag{5}$$

The evaluation of the remaining integral over the polar angle depends on the sign of the factor $\lambda^2 - 1$. If $\lambda > 1$ we substitute $t = \sqrt{\lambda^2-1}\cos\theta$, otherwise we use the substitution $t = \sqrt{1-\lambda^2}\cos\theta$ to obtain an elementary integral, which is solved by

$$\begin{aligned} I(\lambda) &= \frac{1}{2}\int_0^\pi\frac{\sin\theta\,\mathrm{d}\theta}{\sqrt{1+(\lambda^2-1)\cos^2\theta}} \\ &= \begin{cases} \dfrac{\operatorname{arcsinh}\sqrt{\lambda^2-1}}{\sqrt{\lambda^2-1}} & \text{for } \lambda > 1 \\ \dfrac{\arcsin\sqrt{1-\lambda^2}}{\sqrt{1-\lambda^2}} & \text{for } \lambda < 1. \end{cases} \end{aligned} \tag{6}$$

While we have to make this formal case distinction, we emphasize that the energy function is smooth, with both branches of $I(\lambda)$ approaching unity in the limit $\lambda \to 1$.

Collecting the kinetic and potential contributions, we thus obtain the expression

$$E(\beta,\lambda) = \frac{\hbar^2}{6}\beta^2\left(\frac{2}{\mu_\perp}+\frac{1}{\lambda^2\mu_\parallel}\right) - \frac{e^2}{4\pi\epsilon_0\epsilon}\beta I(\lambda) \tag{7}$$

for the ground state energy, which must be minimized with respect to the parameters β and λ. The kinetic term is quadratic in β while the potential term is linear, so the respective partial derivative is readily performed. The condition $\partial E/\partial\beta = 0$ then yields a relation between the two parameters at the energy minimum

$$\beta = 3\left(\frac{e^2}{4\pi\epsilon_0\epsilon\hbar}\right)^2\left(\frac{2}{\mu_\perp}+\frac{1}{\lambda^2\mu_\parallel}\right)^{-1} I(\lambda) \tag{8}$$

which, when substituted in (7), allows us to rewrite the energy as a function of λ only

$$E(\lambda) = -\frac{3}{2}\left(\frac{e^2}{4\pi\epsilon_0\epsilon\hbar}\right)^2\left(\frac{2}{\mu_\perp}+\frac{1}{\lambda^2\mu_\parallel}\right)^{-1} I(\lambda)^2. \tag{9}$$

The energy minimum is found at the stationary point for which $\partial E/\partial\lambda = 0$ and through simple mathematical rearrangement we can express this condition in the form

$$\frac{\mu_\perp}{\mu_\parallel} = 2\lambda^3\frac{1-\lambda I(\lambda)}{I(\lambda)-\lambda} \tag{10}$$

which may be solved graphically. The important point to note is that the right-hand side of (10) is a universal function $f(\lambda)$ that does not depend on the material properties, so the same plot can be used for all semiconductors to determine λ. In practice, however, the reduced transverse and longitudinal effective mass will often not differ by more than a factor of three and in this value range the function on the right-hand side of (10) is accurately approximated by its lowest-order polynomial term $f(\lambda) \approx \lambda^3$. The parameter λ is then explicitly given by

$$\lambda = \left(\frac{\mu_\perp}{\mu_\parallel}\right)^{1/3}. \tag{11}$$

This simplification allows for a very efficient analytic calculation of the material-specific binding energy E_b, which is given by the modulus of the ground state energy according to (9). It is still exact in the isotropic limit $\mu_\parallel = \mu_\perp$, yielding the correct binding energy $E_\mathrm{b} = R_\infty m/(\mu_\perp\epsilon^2)$ where $R_\infty = 13.6\,\mathrm{eV}$ is the hydrogenic Rydberg energy. The wavefunction itself, required for instance to calculate the optical absorption coefficient, is given by the original variational expression with β defined through the relation (8).

III. NUMERICAL RESULTS FOR GaN

In order to illustrate the numerical quality of our scheme, we now consider the case of gallium nitride as an explicit example for excitonic binding energies in a realistic semiconductor. In GaN the valence band maximum comprises three almost degenerate subbands, giving rise to three distinct hole types that can partake in the formation of excitons. Conventionally, these are referred to as light holes, heavy holes and split-off holes, reflecting their different effective masses. Within the same material we can study excitons for which the reduced longitudinal

TABLE I. Comparison between approximate and numerically calculated binding energies E_b for excitons in GaN, formed with holes of different effective mass m^h from the three nearly degenerate subbands at the valence band maximum. The analytic approximation is accurate even when the anisotropy $\mu_\perp/\mu_\parallel$ is very different from unity.

				E_b (meV)	
Hole type	$m^\mathrm{h}_\perp$	$m^\mathrm{h}_\parallel$	$\mu_\perp/\mu_\parallel$	approx.	numer.
Light hole	0.15	1.10	0.483	15.456	15.458
Heavy hole	1.65	1.10	0.959	24.809	24.809
Split-off hole	1.10	0.15	1.805	18.939	18.941

effective mass is greater than the transverse as well as excitons for which it is smaller, and test the accuracy of the approximate treatment in either case.

The effective mass of the electron at the bottom of the conduction band is $m^\mathrm{e}_\perp = 0.18$ in the transverse and $m^\mathrm{e}_\parallel = 0.20$ in the longitudinal direction, given in units of the free electron mass m, while corresponding parameters for the three hole types are listed in table I. All values are quoted from [5]. Next the calculated anisotropy factors $\mu_\perp/\mu_\parallel$ are given. For excitons formed with heavy holes this is close to unity, indicating a rather small perturbation from the isotropic case, but the ratio is substantially smaller with light holes and larger with split-off holes, respectively. The fifth column in table I lists the binding energies E_b obtained analytically from (9) with $\lambda = (\mu_\perp/\mu_\parallel)^{1/3}$. These are compared with results that we obtained by exact diagonalization of the Hamiltonian (1) using standard numerical techniques. The applicable value of the static dielectric constant is the low-frequency limit $\epsilon = 9.5$ of GaN.

The excellent agreement between the approximate and numerical results in all cases confirms the validity of the variational wavefunction (2) as well as the accuracy of the additional simplification (11) that makes the approach strictly analytic. Comparison with experimental data is more problematic because it is very difficult to extract accurate binding energies from optical spectra. Nevertheless, the recently published values of 21 meV for excitons with light and heavy holes and 23 meV for excitons with split-off holes in GaN are probably quite reliable [6]. The discrepancy with the results obtained here is due to the underlying model Hamiltonian (1), however, not the analytic approximations introduced to solve it. While the anisotropy in the effective mass is treated adequately, other important features such as the mixing of states at the threefold degenerate valence band maximum or the spatial variation of the dielectric function are still neglected. A more involved quantitative scheme will also have to incorporate these in order to reproduce experimental binding energies for real materials.

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