RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 43, NUMBER 17 15 JUNE 1991-I

Interband absorption spectra and Sommerfeld factors of a one-dimensional electron-hole system

Tetsuo Ogawa and Toshihide Takagahara
NTT Basic Research Laboratories, 3-9-11 Midori-cho, Musashino-shi, Tokyo 180, Japan
(Received 5 February 1991)

Optical absorption spectra are exactly calculated for direct interband transitions in a one-dimensional (1D) electron-hole system within the effective-mass approximation. We employ a modified Coulomb potential between an electron and a hole to avoid the well-known divergence problem in the 1D system. The Sommerfeld factor, which is the absorption intensity ratio of the unbound exciton to the free electron-hole pair above the band edge, is found for the first time to be less than unity for the direct allowed transition in striking contrast to the three- and two-dimensional cases. This feature can be understood in terms of anomalously strong concentration of oscillator strength on the lowest 1D exciton state.

There is growing interest in semiconductor nanostructures having quantum confinement in more than one dimension such as quantum wires and quantum boxes not only from the viewpoint of fundamental physics but also from the expectation of their potential applications to various optical and electronic devices. As for quantum wires, an interesting optical anisotropy in the photoluminescence excitation spectra was observed,[1] and a stimulated emission from quantum-wire heterostructures was successfully observed.[2] Quantum wires offer a good stage where electrons and holes are free to move in only one spatial dimension (two-dimensional confinement). It is very interesting and important to investigate physical properties peculiar to the one-dimensional (1D) systems. One of the most striking features of the 1D system is the inverse-square-root divergence of the joint density of states at the energy of the fundamental optical gap (the band edge). This feature will be manifested most remarkably in optical properties. The singularity in the density of states is expected to appear above the band edge, namely in the *interband* absorption spectra. Thus it is of great importance to study the linear absorption spectra both below and above the band edge in order to clarify the characteristic features of the 1D system. In this paper, we examine analytically electron-hole envelope functions and absorption spectra of a 1D electron-hole system in comparison with three- and two-dimensional cases, and clarify for the first time peculiar behaviors of the Sommerfeld factor, which is the absorption intensity ratio of the unbound exciton to the free electron-hole pair above the band edge.

An ideal limit of the 1D electron-hole system, namely the limit of infinitesimal wire cross section and perfect confinement, has been treated as a "one-dimensional hydrogen atom" problem.[3] Bound states of this system were studied by Elliott and Loudon[4] who clarified pathological features[3] of 1D excitons below the band edge. Recently, Abe[5] examined the oscillator strength of 1D excitons in Peierls systems and found the concentration of oscillator strength on the lowest exciton state. Contrary to the bound states, there are few studies on continuous (unbound) states of a 1D electron-hole pair which contributes directly to the interband absorption. Because there exist well-known singular characteristics in the 1D Coulomb system, it is desirable to study the system rigorously without the use of approximate tools, e.g., variational methods and WKB methods, to avoid ambiguities. Therefore, we shall study an exactly solvable model for an electron-hole system confined in pure one dimension with a modified Coulomb interaction. Taking inorganic semiconductors into consideration, we employ the effective mass and envelope-function approximations in the band picture.

The relative motion of a 1D electron-hole pair is described by the 1D Schrödinger equation. The attractive potential is assumed to be a long-range Coulomb potential with a cusp-type cutoff $z_0 \geq 0$,[3] in order to make the problem analytically solvable; that is

$$V_{\text{long}}(z) \equiv -e^2/\epsilon(|z|+z_0)\,, \tag{1}$$

where z is a relative coordinate of the electron-hole pair and the dielectric constant is denoted by ϵ. The dielectric effect arising from the difference in the dielectric constant between the quantum wire and the surrounding material is not considered here. This is a standard model of an ideal limit of semiconductor quantum wires. The feasibility of this model will be discussed afterwards.

Because attention is focused on the interband transition, the unbound wave function of the pair is relevant. The energy of the interband transition has a continuous spectrum and is positive ($E>0$); it is scaled by a wave number k as $E \equiv \hbar^2 k^2/2m$ (m is a reduced mass). The origin of energy E is the band gap E_g of the material. Introducing an independent variable $x \equiv 2ik(|z|+z_0)$, the 1D Schrödinger equation is reduced to the Whittaker equation, i.e.,

$$\frac{d^2\phi(x)}{dx^2} - \left(\frac{1}{4}+\frac{i\alpha}{x}\right)\phi = 0\,, \tag{2}$$

where $\phi(x)$ is an envelope function of the pair and $\alpha = (a_B^* k)^{-1}$ with the bulk Bohr radius $a_B^* = \epsilon\hbar^2/me^2$. Two independent solutions of Eq. (2) are given as

$$W^{(j)}_{-i\alpha,1/2}(x) \equiv \Gamma(1 \pm i\alpha)\, x e^{-x/2}[F(1+i\alpha,2;x) \pm G(1+i\alpha,2;x)]\,, \tag{3}$$

for $j=1$ (2) corresponding to the + (−) sign on the right-hand side, where $\Gamma(x)$ is the gamma function and $F(1+i\alpha,2;x)$ and $G(1+i\alpha,2;x)$ are two basis solutions of the confluent hypergeometric equation. Explicit forms of the solutions will be listed elsewhere.[6] In the following, Eq. (3) is abbreviated as $W^{(1)}(x)$ and $W^{(2)}(x)$, respectively.

Corresponding to the twofold degeneracy of a level in the continuous energy spectrum, there are two wave functions with different parities, i.e., "gerade" and "ungerade."[4] Derivative of the former wave function at the origin vanishes $[d\phi_k^g(0)/dz=0]$, while the latter one becomes zero at the origin $[\phi_k^u(0)=0]$. Because our model potential in Eq. (1) is symmetric with respect to $z=0$, these two functions form a basis set of the problem. Only the gerade component is relevant to the optically allowed transition, whereas the ungerade component corresponds to the forbidden one.

Normalization of the wave function of a continuous state is of peculiar importance in calculating the absorption strength because the value of the wave function at the origin ($z=0$) is required. We employ the k-scale normalization[7] which imposes the relation

$$\int_{-\infty}^{\infty}\phi_k^*(z)\phi_{k'}(z)dz=\delta(k-k')\,. \tag{4}$$

Then the normalized wave functions with gerade and ungerade parities are written down as

$$\phi_k^g(z)=\left(\frac{e^{\pi\alpha}}{2\pi}\right)^{1/2}\frac{D_0^{(2)}W^{(1)}(x)-D_0^{(1)}W^{(2)}(x)}{[|D_0^{(1)}|^2+|D_0^{(2)}|^2]^{1/2}}\,, \tag{5a}$$

$$\phi_k^u(z)=\mathrm{sgn}(z)\left(\frac{e^{\pi\alpha}}{2\pi}\right)^{1/2}\frac{W_0^{(2)}W^{(1)}(x)-W_0^{(1)}W^{(2)}(x)}{[|W_0^{(1)}|^2+|W_0^{(2)}|^2]^{1/2}}\,, \tag{5b}$$

where $W_0^{(j)}\equiv W^{(j)}(2ikz_0)$ and $D_0^{(j)}\equiv dW^{(j)}(x)/dx|_{x=2ikz_0}$ for $j=1$ or 2. Now we are at the position to discuss the absorption spectra. We shall discuss separately two types of interband transitions, i.e., direct allowed and direct forbidden transitions.

(a) Direct allowed transition.—The optical-absorption coefficient for the direct allowed transition is defined as [8,9]

$$K_a(\omega)=\frac{1}{c\eta'}\frac{4\pi^2e^2}{m_0\omega}|\langle f|e^{i\eta' kr}\varepsilon P|i\rangle|^2\rho(\hbar\omega)\,, \tag{6}$$

where $\rho(\hbar\omega)$ is the joint density of states, η' the real part of refractive index, ε the polarization vector of light,[10] P the total momentum of electrons, m_0 the free-electron mass, and ω is the frequency of incident light. For the allowed transition where $\langle c|\varepsilon p|v\rangle\neq 0$, we have used

$$|\langle f|e^{i\eta' kr}\varepsilon P|i\rangle|^2=m_0^2\omega^2|\phi_k^g(0)|^2|\langle c|\varepsilon r|v\rangle|^2\,,$$

with a *gerade* wave function. Thus the intensity of the allowed transition is proportional to the probability for creating an electron and a hole at the same position. A characteristic feature of 1D systems is the band-edge divergence of the density of states ρ_{1D} due to the Van Hove singularity, i.e.,

$$\rho_{1D}(\hbar\omega)=\frac{2m}{\pi\hbar^2k}\Theta(\hbar\omega-E_g)=\frac{\sqrt{2m}}{\pi\hbar(\hbar\omega-E_g)^{1/2}}\Theta(\hbar\omega-E_g)\,, \tag{7}$$

where $\Theta(x)$ is the Heaviside step function. This is reflected in a *free*-carrier absorption spectrum, i.e., $K_a^{1D,\mathrm{free}}(\omega)\propto\rho_{1D}(\hbar\omega)$.

Taking account of the attractive interaction [Eq. (1)] between an electron and a hole, the absorption intensity above the band edge is modified to

$$K_a^{1D}(\omega)=C_ae^{\pi\alpha}\frac{w+E_g/Ry^*}{\sqrt{w}}\frac{|D_0^{(2)}W_0^{(1)}-D_0^{(1)}W_0^{(2)}|^2}{|D_0^{(1)}|^2+|D_0^{(2)}|^2}\,, \tag{8}$$

where the photon energy is scaled by $w=(\hbar\omega-E_g)/Ry^*$ with $Ry^*=me^4/2\hbar^2\epsilon^2$, and

$$C_a=\frac{m_0Ry^*}{c\eta'\hbar}|\langle c|\varepsilon r|v\rangle|^2\,. \tag{9}$$

Figure 1(a) shows optical absorption spectra above E_g for

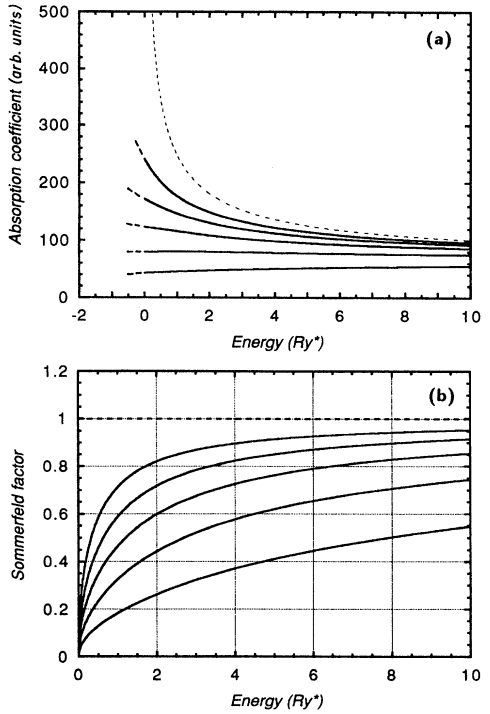

FIG. 1. (a) Absorption spectra due to a direct allowed transition are plotted by solid curves as a function of photon energy $w=(\hbar\omega-E_g)/Ry^*$ for several values of the cutoff length, i.e., $z_0/a_B^*=2.0$, 1.0, 0.5, 0.2, and 0.05 (from top to bottom). The dashed curve indicates the free-carrier absorption spectrum showing the band-edge divergence of the 1D systems. Discrete exciton absorption lines below E_g ($w<0$) are not shown here. (b) Sommerfeld factors for the allowed transition for the same values of the cutoff as (a). These factors in any cases are less than unity indicating suppressed absorption.

various values of the cutoff z_0/a_B^*. Absorption intensities due to bound states below E_g are omitted here but will be reported elsewhere.[6] We find from Fig. 1(a) that the absorption strengths are *smaller* than the free-carrier absorption $K_a^{1D,\text{free}}$ for any value of z_0 and that the band-edge singularity is removed. More remarkably, the smaller the cutoff z_0 is, the weaker the absorption intensity becomes. As the cutoff length decreases ultimately to zero ($z_0 \to 0$), where the attractive potential approaches the bare Coulomb potential, the interband absorption vanishes and the material becomes transparent even for the photon energy above the band gap.

These anomalous features can be seen more clearly in terms of the Sommerfeld factor. This factor, which is the ratio of the absorption coefficient of the unbound exciton to the free-carrier absorption, is given as

$$S_a^{1D}(\omega) \equiv \frac{K_a^{1D}(\omega)}{K_a^{1D,\text{free}}(\omega)} = \frac{e^{\pi\alpha}}{8} \frac{|D_0^{(2)}W_0^{(1)} - D_0^{(1)}W_0^{(2)}|^2}{|D_0^{(1)}|^2 + |D_0^{(2)}|^2}, \tag{10}$$

which is plotted in Fig. 1(b). The most striking features are $S_a^{1D}(\omega) < 1$ for all $\hbar\omega > E_g$ and $S_a^{1D}(0) = 0$ at the band edge. Comparison with two-dimensional (2D) and three-dimensional (3D) cases will be made later.

(b) Direct forbidden transition.—In the case of forbidden transition, on the other hand, $\langle c|\varepsilon p|v\rangle = 0$. Here we employ

$$|\langle f|e^{i\eta' kr}\varepsilon P|i\rangle|^2 = \frac{\hbar}{2m_0^2}\left|\frac{d\phi_k^{\mu}(0)}{dz}\right|^2 |\langle c|M|v\rangle|^2$$

with an *ungerade* wave function, where an explicit form of $|\langle c|M|v\rangle|^2$ was given in Ref. 9. Then the absorption coefficient is calculated as

$$K_f^{1D}(\omega) = C_f e^{\pi\alpha} \frac{\sqrt{w}}{w + E_g/Ry^*} \frac{|W_0^{(2)}D_0^{(1)} - W_0^{(1)}D_0^{(2)}|^2}{|W_0^{(1)}|^2 + |W_0^{(2)}|^2}, \tag{11}$$

where

$$C_f = \frac{1}{c\eta'} \frac{4\hbar\sqrt{m}}{m_0^3 a_B^* (2Ry^*)^{1/2}} |\langle c|M|v\rangle|^2. \tag{12}$$

The results are illustrated in Fig. 2(a) for several values of the cutoff z_0. Contrary to the direct allowed case, the absorption becomes stronger than the free-carrier absorption $K_f^{1D,\text{free}}$ for any z_0. Therefore, the Sommerfeld factor

$$S_f^{1D}(\omega) \equiv \frac{K_f^{1D}(\omega)}{K_f^{1D,\text{free}}(\omega)} = \frac{e^{\pi\alpha}}{2} \frac{|W_0^{(2)}D_0^{(1)} - W_0^{(1)}D_0^{(2)}|^2}{|W_0^{(1)}|^2 + |W_0^{(2)}|^2} \tag{13}$$

is larger than unity as shown in Fig. 2(b). As the cutoff z_0 is reduced, the absorption intensity for the forbidden transition becomes divergingly large in contrast with the allowed case. At the band edge, the Sommerfeld factor diverges because $K_f^{1D,\text{free}}(0) = 0$.

To facilitate the following discussion, results of three- and two-dimensional cases are briefly reviewed here. In

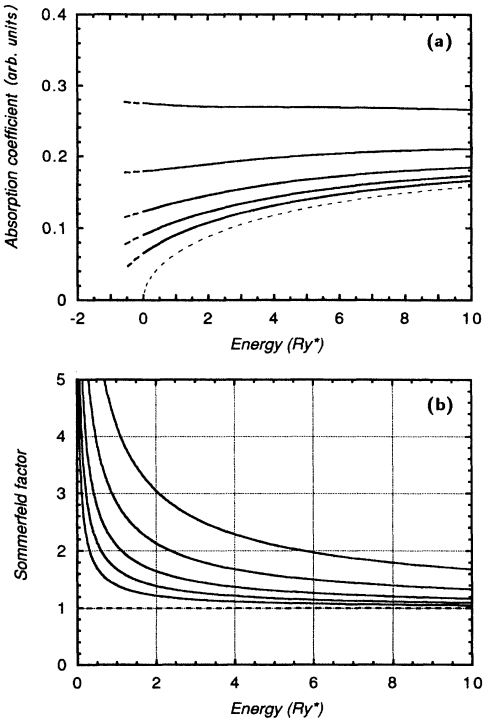

FIG. 2. (a) Absorption spectra due to a direct forbidden transition are plotted by solid curves as a function of w for several values of cutoff, i.e., $z_0/a_B^* = 2.0$, 1.0, 0.5, 0.2, and 0.05 (from bottom to top). The dashed curve indicates the free-carrier absorption spectrum. Discrete exciton absorption lines below E_g ($w < 0$) are not shown here. (b) Sommerfeld factors for the forbidden transition for the same values of cutoff as (a).

isotropic bulk (3D) systems,[8] the Sommerfeld factors for allowed and forbidden transitions are $S_a^{3D} = \pi\alpha e^{\pi\alpha}/\sinh(\pi\alpha)$ and $S_f^{3D} = (1+\alpha^2)\pi\alpha e^{\pi\alpha}/\sinh(\pi\alpha)$, respectively, where $\alpha = (a_B^* k)^{-1} = w^{-1/2}$. These are always larger than unity indicating that the Coulomb attraction between an electron and a hole *enhances* optical absorption for both allowed and forbidden transitions. This also holds for the 2D system,[9] where the Sommerfeld factors are $S_a^{2D} = e^{\pi\alpha}/\cosh(\pi\alpha)$ and $S_f^{2D} = (1+4\alpha^2)e^{\pi\alpha}/\cosh(\pi\alpha)$. This is the reason why the Sommerfeld factor has also been called the "Coulomb enhancement factor."

This is not the case in the 1D system. As seen in Fig. 1, the Coulomb interaction between an electron and a hole *suppresses* the allowed interband absorption intensity. Moreover, the allowed interband absorption vanishes completely in the case of the bare Coulomb attraction (with zero cutoff, $z_0 = 0$). These anomalous results can be understood qualitatively by considering the absorption due to bound states below E_g. As Loudon pointed out,[3] the binding energy of the lowest exciton (which has an even parity) in the 1D systems becomes very large and its wave function becomes a δ function. Therefore, the oscillator strength of the lowest exciton state becomes very huge and almost the entire oscillator strength concentrates on this bound state,[5] resulting in a very weak interband absorption. This is a remarkable feature of a purely

one-dimensional Coulomb system in striking contrast to the 3D and 2D systems.

In order to clarify influences of potential shape on the absorption intensity, we have also investigated[6] analytically a case of a short-range attractive potential, i.e., $V_{\text{short}}(z) = -V_0 \cosh^{-2}(z/\zeta)$ with parameters $V_0 > 0$ and $\zeta > 0$. Global characteristics of the interband absorption spectra are the same as those in the long-range case [Eq. (1)], namely, the Sommerfeld factor for allowed (forbidden) transition is smaller (larger) than unity for any photon energy $\hbar\omega > E_g$. Thus, these features can be considered as universal in the one-dimensional system.

Now we shall discuss the feasibility of the modified Coulomb potential with a cusp-type cutoff given in Eq. (1). Cutoff has been introduced at first only to avoid the difficulty of divergence and to make the problem analytically solvable, and several types of cutoff have been employed.[3-5] Among them, the potential in Eq. (1) is the most effective in discussing the optical properties of a semiconductor wire structure. The reason is as follows. An effective 1D Coulomb potential was estimated[11] in cylindrical and square semiconductor wires assuming perfect confinement. Their results can be fitted very well by Eq. (1) and the cutoff z_0 is found to be proportional to the cross-section size of the wires. Thus the cusp-type Coulomb potential has the simplest form enabling analytical solutions and also describes rather well the actual potential in the quantum-wire structures.

Last, we mention the observability in experiments. Not only artificial 1D systems (inorganic semiconductor wires) but also "natural quantum wires" are candidates for observing features peculiar to the 1D system in optical-absorption spectra clarified in this paper. Organopolysilanes (Si-polymers) and polydiacetylenes are good examples. In fact, they exhibit very strong exciton absorption and weak interband absorption,[12] which can be interpreted by considering our results.

In summary, the linear optical-absorption spectra of a 1D electron-hole system were studied analytically and peculiar behaviors of the Sommerfeld factor were clarified. This is in striking contrast to the 3D and 2D cases. These new findings will be of great significance in the interpretation of experimental results. Our 1D model system is too simple to be applied to a strongly coupled electron-lattice system. As far as semiconductor wire structures are concerned, however, our model calculation may serve as a standard model for the optical-absorption properties.

The authors thank Dr. H. Kanbe, Dr. N. Uesugi, Dr. H. Ando, Dr. Y. Horikoshi, and Dr. T. Kimura for their discussions and encouragement.

[1] M. Tsuchiya, J. M. Gaines, R. H. Yan, R. J. Simes, P. O. Holts, L. A. Coldren, and P. M. Petroff, Phys. Rev. Lett. **62**, 466 (1989); D. Gershoni, J. S. Weiner, S. N. G. Chu, G. A. Baraff, J. M. Vanderberg, L. N. Pfeiffer, K. West, R. A. Logan, and T. Tanbun-Ek, Phys. Rev. Lett. **65**, 1631 (1990); M. Tanaka and H. Sakaki, Appl. Phys. Lett. **54**, 1326 (1989).

[2] E. Kapon, D. M. Hwang, and R. Bhat, Phys. Rev. Lett. **63**, 430 (1989).

[3] R. Loudon, Am. J. Phys. **27**, 649 (1959).

[4] R. J. Elliott and R. Loudon, J. Phys. Chem. Solids **8**, 382 (1959); **15**, 196 (1960).

[5] S. Abe, J. Phys. Soc. Jpn. **58**, 62 (1989).

[6] T. Ogawa and T. Takagahara (unpublished).

[7] In calculating the normalization constant of wave functions, n_0-scale normalization has been employed in the literature [H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957), p. 22 and M. Shinada and S. Sugano, J. Phys. Soc. Jpn. **21**, 1936 (1966)] where n_0 is the number of states within a phase volume of length k in the k space. In one-dimensional systems, n_0 is proportional to k. Therefore, the k-scale normalization coincides with the n_0-scale version aside from a constant factor.

[8] R. J. Elliott, Phys. Rev. **108**, 1384 (1957).

[9] M. Shinada and S. Sugano, Ref. 7.

[10] In our model, the polarization characteristics become isotropic because no mixing among valence subbands is taken into account.

[11] Ladis Bányai, Ian Galbraith, Claudia Ell, and Hartmut Haug, Phys. Rev. B **36**, 6099 (1987); H. Ando (unpublished).

[12] P. Trefonas, R. West, R. D. Miller, and D. Hofer, J. Polym. Sci. Polym. Lett. Ed. **21**, 823 (1983); H. Tachibana, Y. Kawabata, S. Koshihara, and Y. Tokura, Solid State Commun. **75**, 5 (1990).