Elastic scattering of excitons by excitons in semiconducting quantum-well structures: Finite confining-potential model

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We have calculated the cross sections of excitons due to elastic scattering by other excitons in semiconducting quantum-well structures of various widths using a finite confining-potential model. In quantum wells whose widths are comparable to the exciton Bohr radius, the behavior of the elastic-scattering cross sections shows trends similar to predictions based on a two-dimensional (2D) model. However, interesting quasi-3D features are revealed in narrow quantum wells. [S0163-1829(97)08916-9]

As an important feature of the optical spectra related to excitonic transitions, the exciton linewidth in quantum-well structures has been extensively studied both theoretically and experimentally.[1–3] However, the linewidth broadening due to scattering of excitons by free carriers and excitons has not been adequately addressed, even though these mechanisms contribute significantly to the linewidth broadening in situations where high densities of free carriers and excitons are generated, and when the scattering of excitons by optical and acoustic phonons is reduced.[4–7]

Theoretical calculations have been carried out to investigate the exciton scattering problems using two-dimensional (2D) models,[8,9] and quasi-2D models with infinite[10] and finite[11] confining potentials for the free-carrier–exciton scattering problem. Since the exciton linewidth and the scattering cross section are strongly correlated, the obtained cross section is useful in understanding the linewidth broadening. In the present work, we extend our study to exciton-exciton (exc-exc) elastic scattering, using the finite confining-potential model (FCPM). We confine our calculation to a simple two-body problem, treated within the Born's approximation, the validity of which has been discussed before.[10] For a typical well width about the order of the exciton Bohr radius (a_B), the excitonic properties are dominated by the in-plane masses of the carriers. Therefore, in the present study of quasi-2D exciton collisions, though we have assumed an isotropic effective mass (in both the well and barrier regions) for simplicity, it should be approximately interpreted as the in-plane mass of the carrier. Following Elkomoss and Munschy[12] in their treatment of exc-exc scattering in bulk semiconductors, we will consider only the symmetry effect when the two excitons involved are identical, and neglect the exchange of carriers. While exchange effects have been shown to be unimportant in bulk exciton scattering,[13] one would expect the enhancement in exciton binding energy and reduction in exc-exc correlation[14] in the quantum-well structure to further reduce the probability of interexciton carrier exchange, especially for exc-exc elastic scattering.

The wave functions used for the excitons $A(1,a)$ and $B(2,b)$ (where 1,2 are electrons, a,b are holes) are

$$\psi_{ni}(\vec{r}_{ni},z_n,z_i)=\frac{1}{\sqrt{N_{ni}}}\phi_n(z_n)\phi_i(z_i)\phi_{ni}(\vec{r}_{ni},z_n,z_i) \quad (1)$$

in a well of width L, where $(n,i)=(a,1)$ for exciton A and $(b,2)$ for exciton B,

$$\phi_i(z_i)=\begin{cases}\cos(k_iz_i), & |z_i|\leq L/2\\ A_i\exp(-q_i|z_i|), & |z_i|>L/2\end{cases} \quad (2)$$

for $i=a,b,1,2$, and

$$\phi_{ni}(\vec{r}_{ni},z_n,z_i)=\exp(-\alpha_{ni}\sqrt{r_{ni}^2+\gamma_{ni}(z_n-z_i)^2}), \quad (3)$$

where α_{ni}, γ_{ni} are variational parameters, and the $\vec{r}$'s are in-plane vectors. The interaction potential can be written as

$$V_i=\frac{e^2}{\epsilon}\left(\frac{1}{|\vec{\rho}_{ab}|}+\frac{1}{|\vec{\rho}_{12}|}-\frac{1}{|\vec{\rho}_{a2}|}-\frac{1}{|\vec{\rho}_{b1}|}\right), \quad (4)$$

where the $\vec{\rho}_{li}$'s are 3D vectors between the particles l $(=a,1)$ and i $(=b,2)$.

Using the quasi-2D formalism,[10,11] the wave functions (1), and interaction potential (4), the elastic scattering amplitude can be written as the sum of contributions due to the interaction between the ith and lth particles :

$$f(\theta)=\sum_{l,i} f_{li}(\theta), \quad (5)$$

where

$$f_{li}(\theta)=\pm\frac{\mu e^2\exp(i\pi/4)}{\epsilon\hbar^2\sqrt{2\pi k}}\int d\vec{R}\exp[i(\vec{k}_0-\vec{k})\cdot\vec{R}]\left\langle\frac{1}{|\vec{\rho}_{li}|}\right\rangle, \quad (6)$$

and $\langle\ \rangle$ denotes integration over internal coordinates of both excitons. $\vec{k}_0$ and $\vec{k}$ are the relative wave vectors between the excitons before and after collision, respectively, and μ is the reduced mass of the two-exciton system.

The differential cross section is then given by

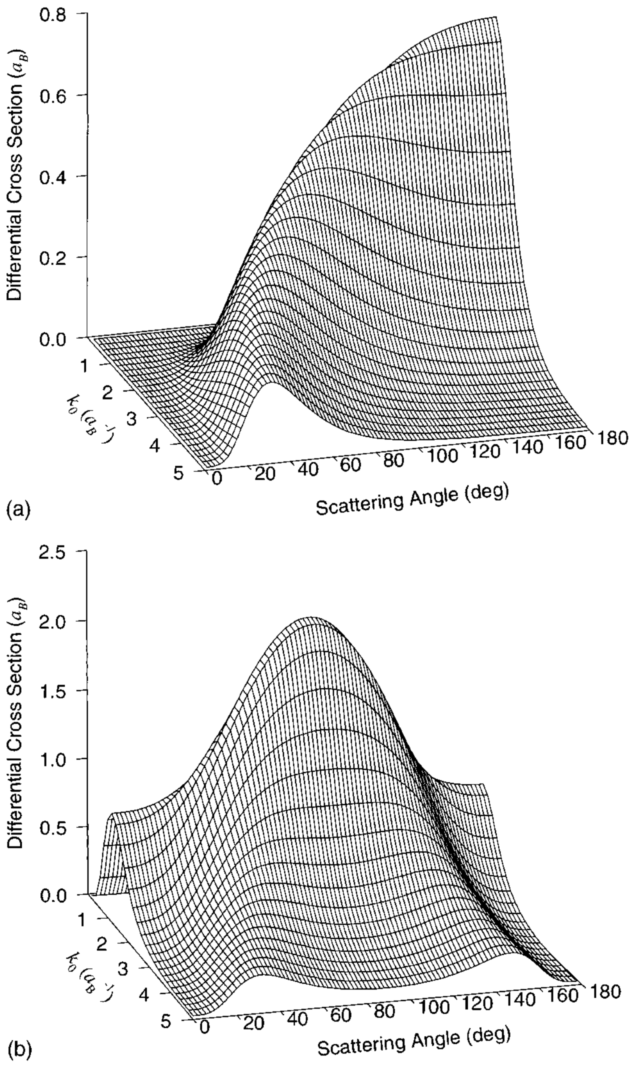

FIG. 1. The differential elastic cross sections without (a) and with (b) account of the symmetry effect, for scattering of identical excitons of mass ratio 0.15, are shown as a function of center-of-mass scattering angle θ and the initial relative wave vector k_0, for a well width of $1.0a_B$.

$$\sigma(\theta)=\frac{k}{k_0}\left|\sum_{l,i} f_{li}(\theta)\right|^2 \tag{7}$$

for two excitons that are distinguishable and

$$\sigma(\theta)=\frac{k}{k_0}\left|\sum_{l,i} f_{li}(\theta)+f_{li}(\pi-\theta)\right|^2 \tag{8}$$

if the two excitons are identical. The total elastic cross section is obtained by summing the differential cross section over all scattering angles numerically.

The differential cross section for scattering of identical excitons of electron-to-hole mass ratio (m_e/m_h) of 0.15, is shown in Fig. 1. When the symmetry effect is neglected, large-angle scattering dominates at low energies, and for higher energies, the differential cross section increases with increasing center-of-mass scattering angle (θ) until a peak is reached, after which it decreases with further increase in θ. The peak in the differential cross section shifts towards

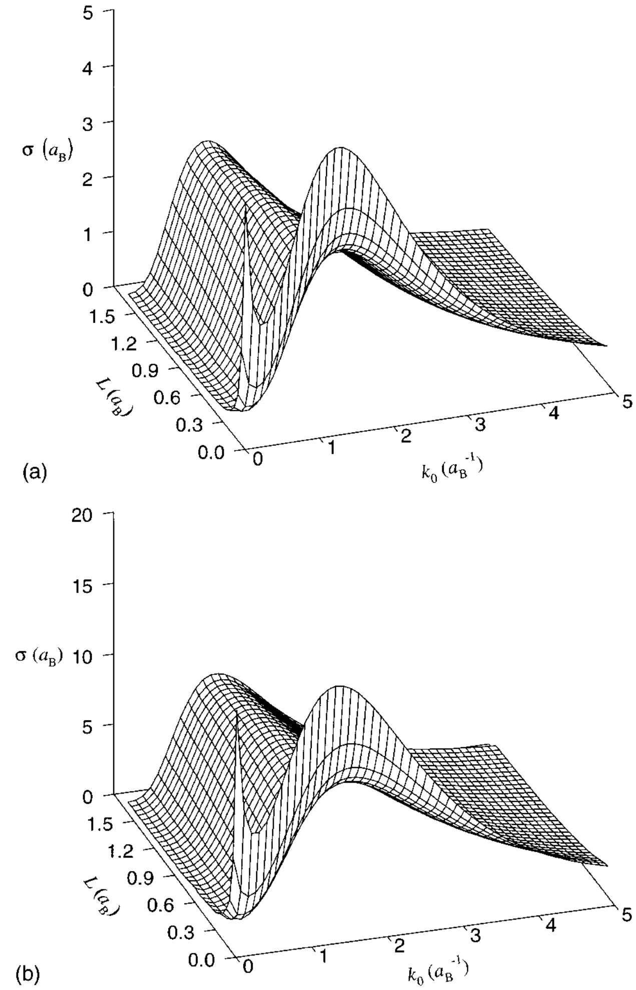

FIG. 2. The total elastic cross sections without (a) and with (b) account of the symmetry effect, for scattering of identical excitons of mass ratio 0.15, are shown as a function of well width L and initial relative wave vector k_0.

smaller θ as the initial energy increases. When the symmetry effect is considered, the differential cross section is symmetric about $\theta=\pi/2$ and are generally larger than that without the symmetry effect.

The corresponding total elastic cross sections are shown in Fig. 2, as functions of well width L and initial relative wave vector k_0. The total elastic cross sections are generally larger by a factor of $\sim$3–4 when the symmetry effect is considered. The behavior of the total cross section as a function of L and k_0, however, remains the same as in the case without the symmetry effect, except that the peak in the total cross section is slightly shifted towards higher incident energies. These characteristics of excitons under confinement are similar to that of bulk excitons.[12]

For typical well widths $L\sim(0.5-1.6)a_B$, a trend similar to previous calculations using the 2D model[9] is found for the total elastic cross section as a function of k_0. However, in the present FCPM, the position of the peak in the elastic cross section is found to be also dependent on L, and shifts towards smaller k_0 as L is increased.

The total cross section decreases with L until it reaches a minimum. At smaller well widths, the total cross section increases sharply with any further decrease in L. Such a phenomenon was also seen in the elastic cross section of excitons due to scattering by free carriers.[11] This is due to the fact that in very narrow wells, the exciton wave function penetrates into the barrier regions, allowing it to assume characteristics similar to that of bulk excitons in the barrier. It is also interesting to note the change in behavior of the total cross section, as it approaches a finite value when $k_0 \rightarrow 0$ and thus a minimum in the total cross section gradually emerges in the low-energy range, which is typical of 3D exc-exc elastic scattering.[12] We thus attribute these features in very narrow wells to the quasi-3D behavior of the excitons.

The exc-exc elastic cross section also depends on the electron-to-hole mass ratio. It was shown in the calculation based on the 2D model[9] that the cross section is a minimum when the mass ratio approaches unity, and is larger when the difference between the electron and hole masses is larger. Using the FCPM, the calculated cross sections for elastic scattering of identical excitons of mass ratio 0.8, including the symmetry effect, are shown in Fig. 3. Similar behaviors but smaller total cross sections are obtained for the scattering of excitons of mass ratio 0.8 when the symmetry effect is neglected, and thus not shown here. Comparisons of the cross sections shown in Figs. 2 and 3 reveal that the mass ratio plays an important role in exc-exc scattering. For scattering of identical excitons, the total cross section for a mass ratio of 0.15 is about 4 orders of magnitude larger than that for a mass ratio of 0.8. Also, the peak position in total cross section is found to shift to lower energy for the larger mass ratio. The cross section obtained for scattering of two excitons with mass ratios of 0.15 and 0.8 is intermediate in trends and magnitude between those for scattering of identical excitons, and is not shown here.

To better understand the behavior of the total cross section and the emergence of the quasi-3D behavior, we note that each term in the scattering amplitude given in Eq. (6) can be further written as

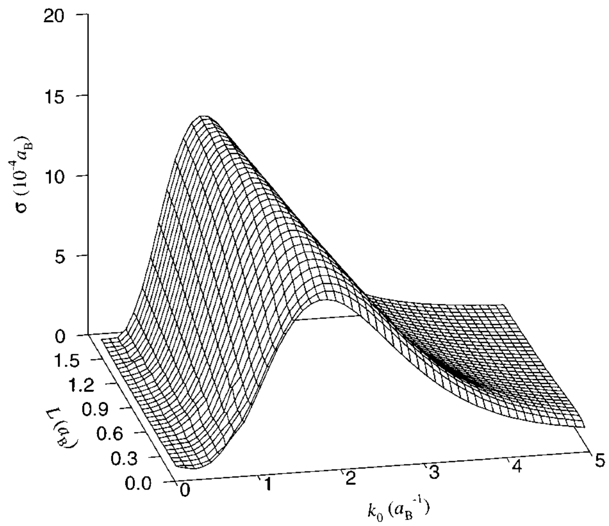

FIG. 3. The total elastic cross sections, with account of the symmetry effect, for scattering of identical excitons of mass ratio 0.8, are shown as a function of well width L and initial relative wave vector k_0.

$$f_{li}(\theta) \propto \frac{1}{\Delta k \sqrt{k}} \chi_{li}^{\parallel} \chi_{li}^{\perp}, \tag{9}$$

where Δk is the change in the relative wave vector and $\chi^{\parallel}$ and $\chi^{\perp}$ are obtained by integrating over the in-plane coordinates and z coordinates, respectively. For example,

$$\chi_{ab}^{\parallel} = \frac{4\alpha_{a1}\alpha_{b2}}{(k_{a1}k_{b2})^{3/2}} \tag{10}$$

and

$$\chi_{ab}^{\perp} = \int dz_1 dz_2 dz_a dz_b \phi_1^2(z_1)\phi_2^2(z_2)\phi_a^2(z_a)\phi_b^2(z_b)[1+\sqrt{\gamma_{a1}k_{a1}}|z_1-z_a|][1+\sqrt{\gamma_{b2}k_{b2}}|z_2-z_b|] \times \exp\{-\sqrt{\gamma_{a1}k_{a1}}|z_1-z_a| - \sqrt{\gamma_{b2}k_{b2}}|z_2-z_b|\}\exp(-\Delta k|z_b-z_a|), \tag{11}$$

where $k_{ni} = [4\alpha_{ni}^2 + (\Delta k m_i/(m_i+m_n))^2]$ $(i=1$ or $2)$.

The expressions for the other terms are similar, with the only differences being the mass factors and the argument of the last exponential factor in $\chi^{\perp}$. Therefore, $\chi^{\parallel}$ can be regarded as the contribution to the scattering amplitude due to the motion of the particles in the plane of the well, and $\chi^{\perp}$ due to the interactions and behavior of the particles in the growth direction. For typical well widths $\sim(0.5-1.6)a_B$, the exciton is confined almost entirely in the quantum well and its behavior is essentially two dimensional. The effect due to interactions along the growth direction is therefore less important. In the extreme case, we may ignore the differences in the $\chi^{\perp}$ terms such that they will contribute to the scattering amplitude only a multiplicative factor. Then the scattering amplitude for identical exciton scattering, neglecting the symmetry effect, can be written as

$$f(\theta) \propto \frac{1}{\Delta k \sqrt{k}} \chi^{\perp} \{k_e^{-3/2} - k_h^{-3/2}\}^2, \tag{12}$$

where $k_i = [4\alpha^2 + (\Delta k m_i/(m_e+m_h))^2]$ $(i=e,h)$. This is actually equivalent to approximating the confinement of the particles by an infinite well, such that no penetration of wave functions is allowed into the barrier regions and the particles can be characterized by similar wave functions along the direction of confinement.[10] We note that Eq. (12) is functionally similar to the elastic scattering amplitude in the 2D model,[9] differing only in the units used for Δk. This explains the similar behaviors in the total cross sections obtained using the 2D model and the FCPM for $L \sim (0.5-1.6)a_B$.

For very narrow wells in the quasi-3D range, the exciton wave function penetrates appreciably into the barrier regions along the direction of confinement, and the $\chi^{\perp}$ terms are no longer neccessarily the same. In the 2D model, the $\chi^{\parallel}$ terms cancel, leading to a vanishing total cross section when $\Delta k \rightarrow 0$. However, in the FCPM, the significant differences in the $\chi^{\perp}$ terms could surface when the effect of the $\chi^{\parallel}$ terms diminishes at small k_0, leading to increased cross sections and the emergence of a minimum in the total cross sections. We also see that in the case of scattering between excitons of larger mass ratios, due to the close values of the electron and hole masses, the difference in the $\chi^{\perp}$ terms becomes less significant. This results in a much smaller increase in total cross section at small k_0, and hence the minimum is not prominent.

When the present total cross section is compared with that due to scattering by free carriers,[11] it is found that the cross section for identical exc-exc scattering (both with and without the symmetry effect) is larger than that for electron-exciton scattering, but smaller than that for hole-exciton scattering, for a mass ratio of 0.15, in agreement with predictions from the 2D model.[8,9] The smaller exc-exc scattering cross sections compared to hole-exciton scattering could be caused by cancellation of the scattering amplitudes between the electron and hole within the incident exciton. For the case of scattering of identical excitons of mass ratio 0.8, the cancellation in the scattering amplitude is more severe, due to the close values of the electron and hole masses, and thus leads to much smaller cross sections.

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