Suppression of exciton-phonon scattering in quasi-one-dimensional systems

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Calculations have been made of the linewidth due to LO-phonon scattering of excitons in quasi-one-dimensional (Q1D) systems, which is thought to be the dominant factor in homogeneous broadening of excitonic absorption lines at room temperature. Three kinds of suppression effects for exciton-phonon scattering have been isolated, all of which appear to be achieved in the most pronounced manner in Q1D systems: first by fabricating smaller structures, second by the presence of a Coulomb field between electron and hole in the dissociated exciton, and third by possessing close mass values for electron and hole. It is demonstrated, in particular, as a hypothetical example that an exciton state can be achieved by combining the above effects, which is free from phonon scattering at room temperature.

I. INTRODUCTION

Recently, much interest has focused on low-dimensional electronic systems because of their anticipated new physical properties. So far, detailed studies have been carried out especially for two-dimensional (2D) systems using semiconductor layered structures of high quality. More recent progress in epitaxial growth and nanofabrication technology is now making it possible to fabricate 1D systems by laterally confining the 2D structures.[1-6]

Especially interesting from the standpoint of optical applications is the enhancement of excitonic effects by employing low-dimensional systems. In fact, it has been found that the performance of optical modulators and optical nonlinear devices is markedly improved by exploiting the enhanced excitonic effects in 2D systems: the pronounced change in the excitonic absorption coefficient due to the external perturbation (electric field and optical intensity, respectively).[7] As a practical matter, however, besides the above enhancement effects, it is essential that the excitonic absorption linewidth be made as small as possible. There are two kinds of factors responsible for the linewidth broadening: inhomogeneous and homogeneous factors. The former broadening factor results from distribution of excitonic resonance energy due to some imperfections of the system (structure fluctuations and band-gap fluctuations). The latter one is defined using the lifetime of the exciton due to phonon scattering in the homogeneous (nonfluctuating) structures. At the current state of technology, the former broadening factor is undoubtedly primarily responsible for the linewidth, especially in 1D systems. We believe, however, that this will be eliminated at least, in principle, by highly controlled fabrication technology in the future. At the same time, the latter broadening factor will not be excluded as long as the materials are retained at room temperature (the practical temperature for device operation). With these points in mind, the suppression of phonon scattering seems to be the inherent objective for improving the excitonic absorption linewidth.

Several papers have been published on the phonon scattering of 2D excitons.[8-10] To our knowledge, however, no report has addressed exciton-phonon scattering in 1D systems, although 1D electron-phonon scattering has been treated in several papers.[11-13]

This paper reports on LO-phonon scattering of quasi-one-dimensional (Q1D) excitons with a primary view to improving the excitonic absorption linewidth. Several exciton-phonon-scattering suppression effects are proposed, all of which appear to be achieved in the most pronounced manner in Q1D systems.

II. EXCITON WAVE FUNCTIONS

Within the framework of effective-mass and envelope-function approximations, an electron-hole pair in a Q1D system is described by the wave equation that is subject to the confinement potential and the Coulomb potential between these two particles. Here, we neglect the multiplicity of the valence band and treat it as a single band. Let our Q1D system be a quantum wire, the cross section of which is a rectangle with the sides of lengths L_x and L_y. Assuming a strong confinement, the wave function of this system is separable as follows:

$$\psi = f_e(\mathbf{r}_e) f_h(\mathbf{r}_h) L_\xi^{-1/2} e^{iK\xi} \phi(z) , \qquad (1)$$

where $\mathbf{r}_e = (x_e, y_e)$ represents the electron coordinates in the direction of confinement, $\mathbf{r}_h$ is for a hole, ξ is the center-of-mass coordinates in the direction of the Q1D axis, and z stands for the relative motion. Then, $f_e(\mathbf{r}_e)$ and $f_h(\mathbf{r}_h)$ are the envelope functions of electron and hole, respectively, both of which are presently assumed to be the fundamental quantum states in the confinement potential. Next, $\phi(z)$ describes the relative motion, which will have bound (discrete) and unbound (continuous) states (Secs. II A and II B). The plane-wave term in Eq. (1) describes the center-of-mass motion which is normalized in the length L_ξ. When the particles are weakly confined, as in actual Q1D systems, the wave function cannot be separated as simply as in Eq. (1) because of the coupled two-confinement directions.[2] For this reason, our study will concentrate on the simple case mentioned earlier. In this case, the wave function of relative motion has to satisfy the following equation:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dz^2}+V_{\text{eff}}(z)\right]\phi(z)=\varepsilon\phi(z) , \tag{2a}$$

where μ is the reduced mass ($\mu^{-1}=m_e^{-1}+m_h^{-1}$) and

$$V_{\text{eff}}(z)=-\frac{e^2}{\epsilon_r}\int d\mathbf{r}_e d\mathbf{r}_h \frac{|f_e(\mathbf{r}_e)|^2|f_h(\mathbf{r}_h)|^2}{[(\mathbf{r}_e-\mathbf{r}_h)^2+z^2]^{1/2}} \tag{2b}$$

is the effective Coulomb potential in the Q1D system. This is expressed as a formula in which the bare Coulomb interaction is averaged over the two confinement directions for electron and hole with the weight of the envelope functions. Within the confines of a pure 1D system (wire of infinitesimal widths), Eq. (2b) tends toward the bare Coulomb potential. This potential is known to show a pathological phenomenon owing to its singularity at the origin:[14,15] excitons have an infinitely deep binding energy due to the localization of the ground state toward the origin. The averaging procedure for the Q1D system shown in Eq. (2b) softens the behavior of the potential around the origin and as a result eliminates the anomalous phenomenon mentioned above. We do not consider here the dielectric effect arising from the difference in the dielectric constant between the Q1D system and the surrounding materials. The effective Coulomb potential $V_{\text{eff}}(z)$ can be well approximated by an analytical-model potential having a cusp at the origin

$$V_{ab}(z)=-\frac{e^2}{\epsilon_r}\frac{a}{|z|+b} , \tag{3}$$

which is fundamentally the same as the form proposed by Loudon,[15] except that Eq. (3) possesses two parameters (a and b) while the latter has only one parameter (b). This will enable us to approximate the effective potential $V_{\text{eff}}(z)$ by the model potential $V_{ab}(z)$ more accurately. These two parameters are determined such that Eq. (3) describes the numerically evaluated effective potential [Eq. (2b)] very precisely. However, the parameters thus determined depend upon the range of z values used. To avoid this, we determined the optimum a and b values through

$$\frac{\partial^2}{\partial a \partial b}\sum_j [V_{ab}(z_j)-V_{\text{eff}}(z_j)]^2|\phi_0^{ab}(z_j)|^2=0 , \tag{4}$$

where z_j are the points ranging from 0 to 200 Å. Here, $\phi_0^{ab}(z)$ is the ground-state wave function, which can be uniquely determined once the parameters (a and b) are given (Sec. II A). Equation (4) implies that the square sum of potential deviation with the weight of the ground state should be minimized. The model potential thus determined is expected to give a good picture at least of the ground state of Q1D excitons.

A. Discrete states

The wave equation [Eq. (2)] for discrete states (bound states, $\varepsilon<0$) is reduced to the following form:

$$\frac{d^2\phi}{d\zeta^2}-\frac{1}{4}\phi+\frac{\alpha}{\zeta}\phi=0 , \tag{5}$$

when we introduce an independent variable $\zeta=2k(|z|+b)$. Here, $k=e^2a\mu/\hbar^2\epsilon_r\alpha$ and $\varepsilon=-\hbar^2k^2/2\mu$. Equation (5), which we call the Whittaker equation, has two independent solutions denoted by $M_{\alpha,1/2}(\zeta)$ and $W_{\alpha,1/2}(\zeta)$.[16] Since the first solution shows a divergence at the infinite z, only the second solution $W_{\alpha,1/2}(\zeta)$ corresponds to bound states. Imposing a smooth continuation at the origin ($\zeta=2kb$) on the wave function, the equation

$$W'_{\alpha,1/2}(2kb)=0 , \tag{6a}$$

and

$$W_{\alpha,1/2}(2kb)=0 \tag{6b}$$

give discrete energy states ε_n of even ($n=0,2,4,\ldots$) and odd ($n=1,3,5,\ldots$) parity, respectively. The wave functions corresponding to these states are given by

$$\phi_n(z)=pC_nW_{\alpha_n,1/2}(\zeta) , \tag{7}$$

where C_n is a normalization constant and $\zeta=2k_n(|z|+b)$. Here, k_n and α_n are expressed using ε_n. For even states, $p=+1$ and for odd states, $p=+1$ at $z>0$ and $p=-1$ at $z<0$.

With the above analytical formulation, we investigated several discrete states through a variational approach. The ground-state wave function for relative motion was assumed to be

$$\phi_0(z)=C_0e^{-\sqrt{(z/\lambda_0)^2+\sigma_0^2}} , \tag{8a}$$

where λ_0 and σ_0 are variational parameters and C_0 is a normalization constant. This variational function was chosen to satisfy three basic requirements: first, it has even parity, second, it is a smooth function around the origin, and third, it behaves asymptotically as an exponentially decaying function, which is the same as the asymptotic behavior of the Whittaker function. Wave functions proposed so far do not satisfy all of these requirements,[17,18] and thus may lead to results different from those in the present paper. Since the first excited state is of odd parity, it must have the form

$$\phi_1(z)=C_1(z/\lambda_1)e^{-\sqrt{(z/\lambda_1)^2+\sigma_1^2}} , \tag{8b}$$

which is the simplest function satisfying this requirement. Here, parameters are defined similarly to those for $\phi_0(z)$. Since these two functions are orthogonal regardless of the choice of λ_j and σ_j ($j=0,1$), the optimization for $\phi_0(z)$ and $\phi_1(z)$ can be independently accomplished by minimizing the expectation value of the Hamiltonian [Eq. (2)]. Although higher excited states can be evaluated variationally in a similar manner, it may be sufficient to compare the results for the lowest two states with those obtained by the analytical method.

Figure 1 shows the Rydberg series of Q1D excitons as functions of wire width L. Here, we have employed a quantum wire of square cross section ($L_x=L_y=L$) as a

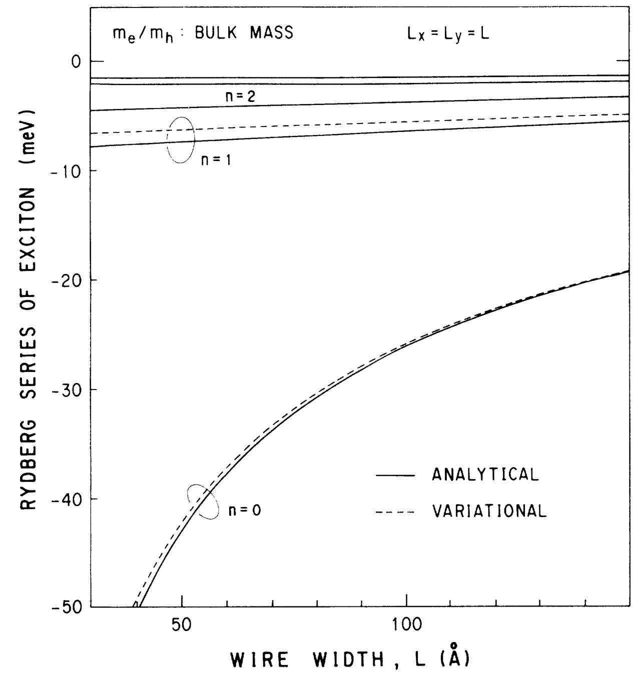

FIG. 1. Rydberg series of the exciton in a Q1D system, the cross section of which is a square with sides of length L. Solid lines indicate energy levels obtained analytically by using the model potential and dashed lines indicate energy levels obtained variationally.

Q1D system and used material parameters for bulk GaAs. Results obtained analytically (solid lines) are shown together with those obtained variationally (dashed lines) for a series ranging from the ground ($n=0$) to several excited states ($n\geq 1$). The variational results show good agreement with analytical results, indicating that the simple variational wave functions proposed in Eq. (8) describe well the excitonic behavior in Q1D systems. Here, it should be noted that the ground-state energy shows a pronounced decrease with narrowing L, while the excited states remain nearly constant. In the limit of pure 1D ($L\rightarrow 0$), the ground state comes to have infinitely deep energy, which is peculiar to the 1D exciton;[15] this is in contrast to the 2D system, in which the exciton has a ground-state energy only four times that of the bulk (3D) exciton.[19] The deep ground state of the Q1D exciton suggests the possibility that the scattering of the exciton from the ground to other states may be prohibited because of the absence of final states of scattering. This is possible in practice when we take into account the scattering by some dispersionless particles such as LO phonons. This will be discussed in detail later in the paper.

B. Continuous states

For continuous states (unbound states, $\varepsilon>0$), the wave equation is reduced to

$$\frac{d^2\phi}{d\zeta^2}-\frac{1}{4}\phi-\frac{i\alpha}{\zeta}\phi=0\ , \tag{9}$$

which resembles Eq. (5) for discrete states, introducing a complex independent variable $\zeta=2i\kappa(|z|+b)$. Here, we defined parameters similar to those for discrete states by $\kappa=e^2a\mu/\hbar^2\epsilon_r\alpha$ and $\varepsilon=\hbar^2\kappa^2/2\mu$. Independent solutions for Eq. (9) are given by the Whittaker functions of complex variables, $M_{-i\alpha,1/2}(\zeta)$ and $W_{-i\alpha,1/2}(\zeta)$.[16] It may be convenient to take the additional bases $\varphi_j(z)$ ($j=1,2$) by transforming the Whittaker functions as follows:

$$\varphi_j(z)=\tfrac{1}{2}\Gamma(1+i\alpha)e^{(\pi|\alpha|)/2}\times[T_{-i\alpha,1/2}(\zeta)\pm W_{-i\alpha,1/2}(\zeta)]\ , \tag{10a}$$

where Γ is the gamma function and $T_{-i\alpha,1/2}(\zeta)$ is defined by

$$T_{-i\alpha,1/2}(\zeta)=\frac{2e^{-\pi|\alpha|}}{\Gamma(1-i\alpha)}W_{-i\alpha,1/2}(\zeta)+M_{-i\alpha,1/2}(\zeta)\ , \tag{10b}$$

and we choose the upper (lower) sign for $j=1$ (2) in these equations. These bases have been taken so that their asymptotic behaviors are described by plane waves $[\exp(\pm i\kappa|z|)]$ with unit amplitude. The wave functions for continuous states are described by the linear combination of $\varphi_1(z)$ and $\varphi_2(z)$. Imposing a smooth continuation at the origin, the wave functions are obtained as follows:

$$\phi_e(z)=\frac{\varphi_2'(0)\varphi_1(z)-\varphi_1'(0)\varphi_2(z)}{[|\varphi_2'(0)|^2+|\varphi_1'(0)|^2]^{1/2}}\frac{i}{L_z^{1/2}} \tag{11a}$$

and

$$\phi_o(z)=p\frac{\varphi_2(0)\varphi_1(z)-\varphi_1(0)\varphi_2(z)}{[|\varphi_2(0)|^2+|\varphi_1(0)|^2]^{1/2}}\frac{1}{iL_z^{1/2}} \tag{11b}$$

for states of even and odd parity, respectively, where $p=+1$ at $z>0$ and $p=-1$ at $z<0$. Here, we normalized these functions in a length L_z, making use of the asymptotic forms of $\varphi_1(z)$ and $\varphi_2(z)$, i.e., plane waves with unit amplitude.[14] This normalization is possible because the $\varphi_j(z)$ values at smaller arguments contribute much less to the normalization integral than those at asymptotic arguments and, therefore, the former is neglected compared with the latter. An imaginary unit is inserted to adjust the phase of these functions appropriately. The wave function for a continuous scattering state is generally expanded in partial waves of different angular momenta. In the present case (Q1D), the partial waves have only two components, $\phi_e(z)$ and $\phi_o(z)$. Hence, we finally derive the general form of the wave function for the continuous state in the Q1D system as follows:

$$\phi_\kappa(z)=\frac{1}{\sqrt{2}}[\phi_e(z)+i\phi_o(z)]\ , \tag{12}$$

which is characterized by κ, the wave number of the continuous state. It is clear from the above discussion that this wave function converges at a one-dimensional plane wave, $L_z^{-1/2}\exp(i\kappa|z|)$, in the limit of the weak Coulomb field ($\alpha\rightarrow 0$) or in the asymptotic region ($|z|\rightarrow\infty$).

III. EXCITON-PHONON SCATTERING

The motion of an electron-hole pair (exciton) in the Q1D system can be separated into center-of-mass motion and relative motion. The first motion is characterized by parabolic dispersion and the second motion is quantized into an infinite number of discrete states (Rydberg series) that converge at the bottom of the continuum. The total energy of an exciton is the sum of these two energies. Figure 2 shows a schematic diagram of a Q1D exciton band, which depicts the total energy of the exciton vs the one-dimensional wave number (K) of the center-of-mass motion. Here, the electron and the hole constituting an exciton are assumed to occupy the fundamental quantum level in the confinement potential. The binding energy of the exciton is denoted by ε_b (which is also equal to $-\varepsilon_0$). With irradiation of light, an exciton is created at the bottom of the ground state ($n=0$ and $K=0$), since a photon has nearly zero momentum and the ground state has the largest oscillator strength. The exciton thus created may be scattered by phonons. In this paper, we investigate the exciton scattering by absorbing LO phonons, because this is thought to be the dominant process at room temperature; other processes in which acoustic phonons are involved seem to be weak.[20] Moreover, it is unnecessary to consider the phonon emission processes, since there are no final states for phonon emission. Here, we are concerned with bulk phonons; in other words, we do not take the separate modes arising from the anisotropy of the system into account. This treatment is partially justified by the sum rule elaborated by Mori and Ando,[21] which states that in a simple material such as GaAs the sum of interactions with various phonon modes coincides approximately with the interaction with bulk phonon mode (although they derived it for Q2D systems). Throughout this paper, LO phonons are assumed to have a single dispersionless energy $\hbar\omega_{\rm LO}$.

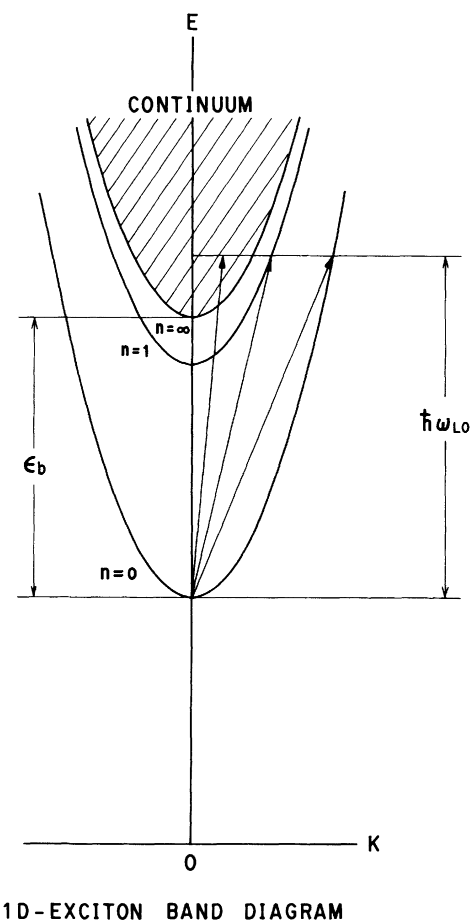

FIG. 2. Schematic diagram of the 1D exciton band. K is the wave number of center-of-mass motion and ε_b is the binding energy of the exciton. Several phonon-scattering processes for excitons created at the ground state are indicated by arrows.

Two kinds of scattering processes are possible, as indicated by arrows in Fig. 2. The first process is the scattering to discrete states. If this occurs as $0\rightarrow 0$, it is called intraband scattering, in which the center-of-mass motion is excited with no change in the internal state (0). If this occurs as $0\rightarrow n$ ($n\geq 1$), internal states are excited (interband scattering), together with the change in the center-of-mass motion. The second process is the scattering to continuum, in which the electron-hole pair dissociates, having some wave number and, at the same time, the center-of-mass motion is excited. It is apparent that the second process occurs only if $\varepsilon_b<\hbar\omega_{\rm LO}$. The total linewidth Γ is given by the sum of these scattering linewidths

$$\Gamma=\sum_{\nu}\Gamma_{\nu 0}\ , \tag{13}$$

where ν specifies the exciton band and extends over both discrete states ($n=0,1,2,\ldots$) and continuum (c). The exciton at the initial state of scattering ($n=0$ and $K=0$) is strongly coupled to the photon and, as a result, it actually exists as a polariton. However, we neglect this effect for simplicity and assume that it exists as a pure exciton. Since the phonon interacts only with the exciton component of the polariton, this approximation might overestimate the scattering linewidth.[22] This, however, does not substantially alter the conclusion of the present paper. The LO-phonon absorption by an exciton is described by the interaction Hamiltonian, which is the sum of Fröhlich interactions of an electron and a hole with an LO phonon. The linewidth (half width at half maximum) due to $0\rightarrow\nu$ scattering is calculated according to the first-order perturbation theory using the Fermi golden rule,

$$\Gamma_{\nu 0}=\pi|c|^2\sum_{\mathbf{Q}}Q^{-2}|U(\nu K:00)|^2\delta(E_{\nu K}-E_{00}-\hbar\omega_{\rm LO})\ , \tag{14}$$

where $\mathbf{Q}$ is the three-dimensional wave-number vector of the LO phonon and is denoted properly by (q_x,q_y,q_z), or $(\mathbf{q},q_z)$ hereafter. Here,

$$c=ie\,[2\pi\hbar\omega_{LO}(\epsilon_\infty^{-1}-\epsilon_0^{-1})]^{1/2}$$

is the coupling constant and $E_{\nu K}$ is the sum of energies for the νth exciton state and the center-of-mass motion of wave number K, which is given by

$$E_{nK}=E_{00}+\varepsilon_b+\varepsilon_n+\hbar^2K^2/2m$$

for discrete states ($\nu=n$) and

$$E_{cK}=E_{00}+\varepsilon_b+\hbar^2\kappa^2/2\mu+\hbar^2K^2/2m$$

for the continuous state ($\nu=c$ and is characterized by the wave number κ for the dissociative relative motion in one dimension), where $m=m_e+m_h$ is the mass of the exciton. The temperature-dependent part (Bose distribution function),

$$N_B=[\exp(\hbar\omega_{\rm LO}/kT)-1]^{-1}$$

is omitted in Eq. (14) and, therefore, the observable linewidth should be written as ΓN_B. Here, $U(\nu K:00)$ is the matrix element of the interaction Hamiltonian between the final (νK) and intial (00) states. Due to the momentum conservation in the direction of the Q1D axis, K should be q_z, the wave number of the phonon in the z direction. The integral for the envelope functions in this matrix element can be easily carried out and, finally, we obtain

$$U(\nu K:00)=\frac{\pi^2\sin\beta_x}{(\pi^2-\beta_x^2)\beta_x}\frac{\pi^2\sin\beta_y}{(\pi^2-\beta_y^2)\beta_y}V_{\nu0}(q_z)\ , \tag{15}$$

where $\beta_x=L_xq_x/2$ and $\beta_y=L_yq_y/2$ and,

$$V_{\nu0}(q_z)=\int_{-\infty}^{\infty}dz\ \phi_\nu^*(z)(e^{iq_zp_hz}-e^{-iq_zp_ez})\phi_0(z)\ . \tag{16}$$

Here, $p_e=m_e/m$ and $p_h=m_h/m$. To facilitate the later discussion, it may be convenient to rewrite the matrix element in a different form, depending on the parity of final states, as follows:

$$\int_{-\infty}^{\infty}dz\ \phi_\nu^*(z)[\cos(q_zp_hz)-\cos(q_zp_ez)]\phi_0(z)\ , \tag{17a}$$

for ν of even parity and

$$i\int_{-\infty}^{\infty}dz\ \phi_\nu^*(z)[\sin(q_zp_hz)+\sin(q_zp_ez)]\phi_0(z)\ , \tag{17b}$$

for ν of odd parity, since $\phi_0(z)$ has even parity. This relation holds for both the discrete states ($\nu=n$) and the continuum ($\nu=c$).

A. Scattering to discrete states

The linewidth for scattering to discrete states ($\nu=n\geq0$) can be expressed as follows,

$$\Gamma_{n0}=4\pi^6|c|^2|V_{n0}(q_{n0})|^2\times\int d\mathbf{q}\frac{1}{q^2+q_{n0}^2}\left\{\frac{\sin\beta_x}{(\pi^2-\beta_x^2)\beta_x}\frac{\sin\beta_y}{(\pi^2-\beta_y^2)\beta_y}\right\}^2\ , \tag{18}$$

after performing the integration over q_z. The matrix element term $[V_{n0}(q_{n0})]$ can be calculated using Eq. (16) and the wave functions of discrete states [Eq. (7) or Eq. (8)]. Here,

$$q_{n0}=\{2m[\hbar\omega_{\rm LO}-(\varepsilon_b+\varepsilon_n)]\}^{1/2}/\hbar$$

and therefore the scattering occurs to the states (n) which satisfy the relation, $\varepsilon_b+\varepsilon_n<\hbar\omega_{\rm LO}$.

Figure 3 shows the linewidth (Γ) for $0\rightarrow n$ scattering as functions of wire width (L) for three different geometries: (a) $L=L_x=L_y$, (b) $L=L_x$ ($L_y=40$ Å), and (c) $L=L_x$ ($L_y=65$ Å), where L_x and L_y are again the lengths of sides of a rectangular cross section. In this calculation, we have employed the bulk values for electron and hole masses. Solid lines indicate the results obtained using the analytical wave functions [Eq. (7)] and dashed lines using the variational wave functions [Eq. (8)]. The dash-dotted line indicates the sum of all the linewidths due to interdiscrete-states scattering. Results for these two different methods show good agreement: in particular, the results for $0\rightarrow0$ scattering coincide completely with each other. This again shows that our variational wave functions describe the Q1D excitonic behavior very well. There appears to be a general tendency that the scattering linewidth decreases with increasing n; finally, scatterings to higher excited states ($n\geq5$) come to be nearly negligible. One exception in this tendency is the $0\rightarrow1$ scattering, in which a sharp linewidth spectrum is observed around the critical wire width (which we tentatively call the scattering edge and it corresponds to the edge of the energy band). This seems to reflect the density of state of the 1D electronic system which has a sharp band edge and behaves like $(E-E_c)^{1/2}$. In addition, the linewidth ratio ($\Gamma_{n_o0}/\Gamma_{n_e0}$) between odd and even states was found to be proportional to $q_{n_o0}^1/q_{n_e0}^3$ in the vicinity of the band edge. These imply that the scatterings to odd states show sharp scattering edges compared with those to even states. Next, as shown in Fig. 3, the linewidth decreases with increasing L in the region far from the scattering edge. This phenomenon may be construed as follows. With the increase in L, the excitons come to be weakly localized. The exciton thus enlarged is more likely to be scattered by phonons of longer wavelength (i.e., smaller wave number) because the exciton interacts primarily with the phonons, the wavelengths of which are of the same order as the exciton size. This will make the interaction between them less effective. There seems to be no essential difference in the scattering linewidth among the structures shown in Figs. 3(a)–3(c). Owing to the difference in the exciton Rydberg series among these structures, however, some difference can be found in the scattering edge at which the interband transition sets in. Moreover, Fig. 3(a) ($L_x=L_y=L$), shows sharp spectra compared with the other two [Figs. 3(b) and 3(c)], in which the spectra are relatively broad. This results from the fact that the former structure receives the change in quantum states of two directions while the latter two receive that of only one direction. As we predicted in Sec. II A, scatterings to higher exciton states (interband scattering) are prohibited for smaller structures because of the disappearance of final states of scattering and as a result only the intraband ($0\rightarrow0$) scattering is observed. We have thus found that the LO-phonon scattering linewidth can be suppressed to a great degree by fabricating smaller structures.

B. Scattering to continuous state

The linewidth for scattering to the continuous state ($\nu=c$) can be expressed as follows:

$$\Gamma_{c0}=\pi^5|c|^2\frac{m}{\hbar^2 q_{00}}\int d\mathbf{q}\left\{\frac{\sin\beta_x}{(\pi^2-\beta_x^2)\beta_x}\frac{\sin\beta_y}{(\pi^2-\beta_y^2)\beta_y}\right\}^2 \times\int_0^{\kappa_0}d\kappa\frac{|V_{c0}(q_{00}\gamma(\kappa))|^2}{[q^2+q_{00}^2\gamma(\kappa)^2]\gamma(\kappa)}\,, \quad (19)$$

after performing the integration over q_z. The matrix element term $[V_{c0}(q_{00}\gamma(\kappa))]$ can be calculated using Eq. (16) and the wave functions of the continuous state [Eq. (12)] and ground state [Eq. (7)]. Here,

$$\gamma(\kappa)=(1-\varepsilon_b/\hbar\omega_{LO})^{1/2}(1-\kappa^2/\kappa_0^2)^{1/2}$$

and

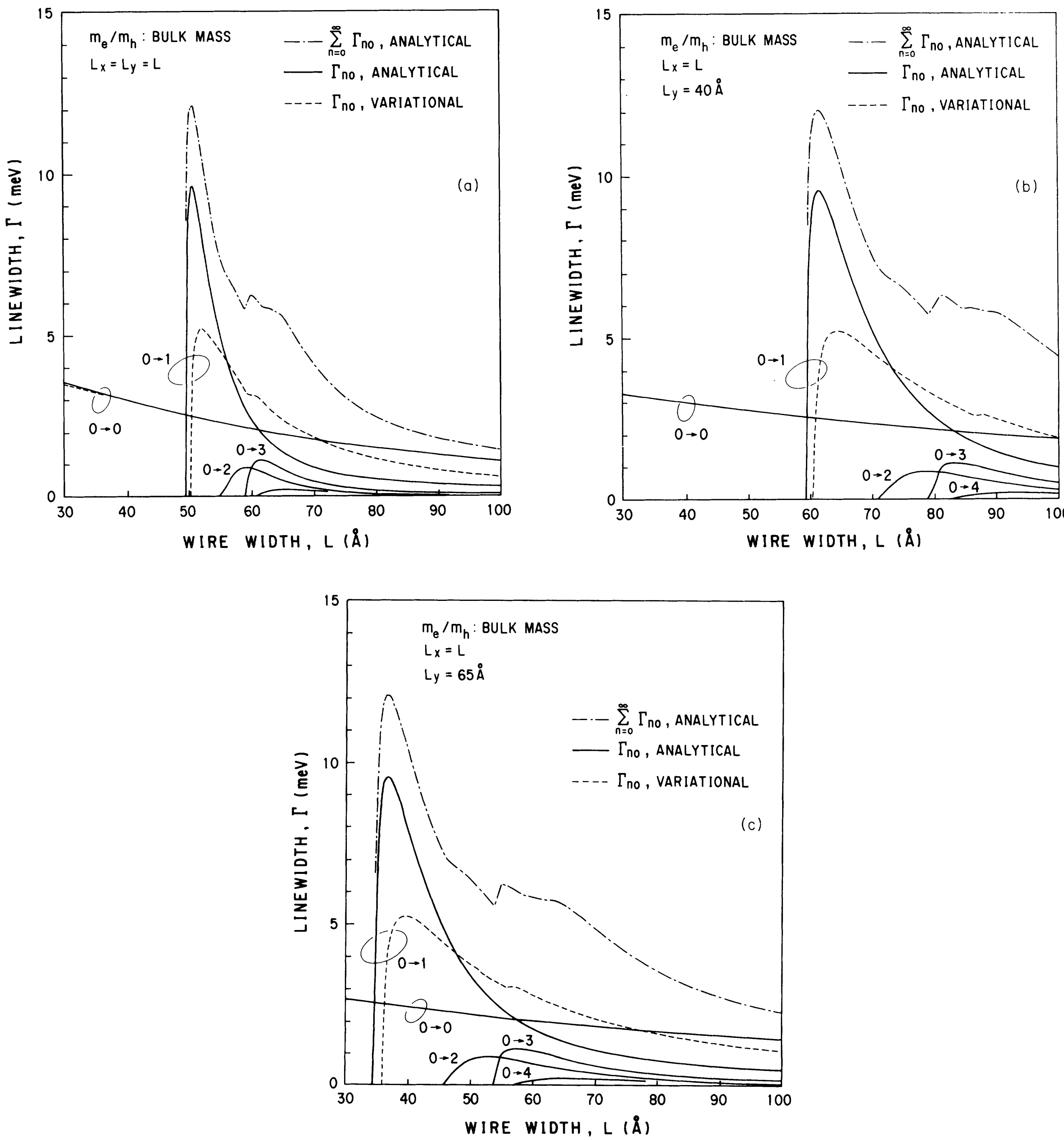

FIG. 3. Linewidths caused by phonon scattering of the exciton from the ground state (0) to discrete states (n) are plotted as functions of wire width (L) of the Q1D system. Its cross section is a rectangle with sides of lengths L_x and L_y for (a) $L=L_x=L_y$, (b) $L=L_x$ ($L_y=40$ Å), and (c) $L=L_x$ ($L_y=65$ Å). Bulk mass values are used for electron and hole.

$\kappa_0=(2\mu/\hbar^2)^{1/2}(\hbar\omega_{LO}-\varepsilon_b)^{1/2}$.

In the above calculation, the length L_z that appeared in Eq. (11) is canceled and hence we put $L_z=1$ in these equations. Note that Γ_{c0} exists only when $\varepsilon_b<\hbar\omega_{LO}$.

Figure 4 shows the linewidth for $0\rightarrow c$ (continuum) scattering as a function of (a) $L=L_x=L_y$, (b) $L=L_x$ ($L_y=40$ Å), and (c) $L=L_x$ ($L_y=65$ Å). These structures correspond to those in Fig. 3. The total scattering linewidth should be obtained by summing up these two kinds of linewidths (Figs. 3 and 4). Here again, we have employed the bulk masses for electron and hole in this calculation. Solid lines indicate the results obtained using the analytical wave functions [Eqs. (7) and (12)]. The re-

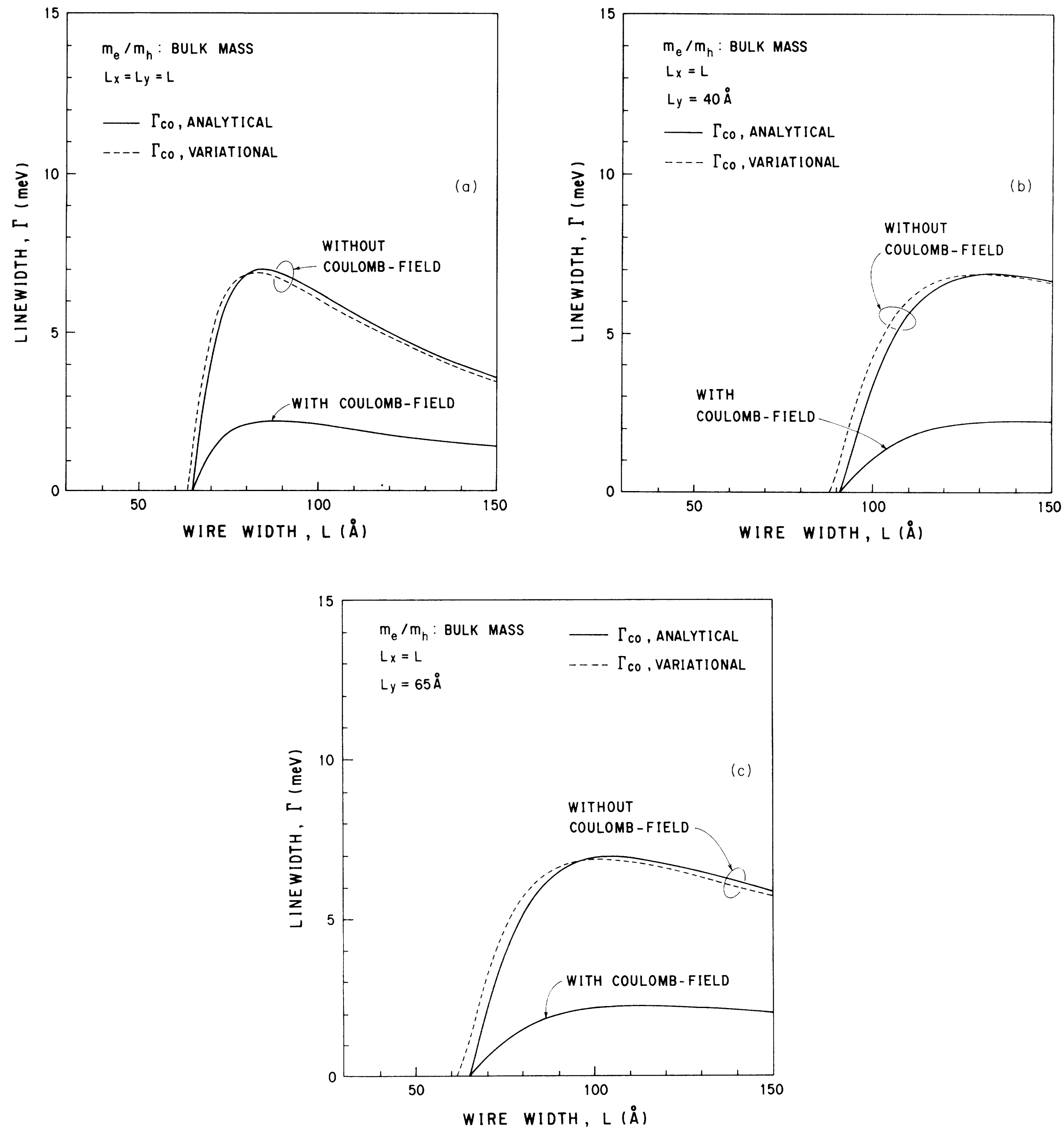

FIG. 4. Linewidths caused by phonon scattering of the exciton from the ground state (0) to continuous state (c) are plotted as functions of wire width (L) of the Q1D system. Its cross section is a rectangle with sides of lengths L_x and L_y for (a) $L=L_x=L_y$, (b) $L=L_x$ ($L_y=40$ Å), and (c) $L=L_x$ ($L_y=65$ Å). Bulk mass values are used for electron and hole.

sults taking the Coulomb field into account are shown together with those neglecting it: in the latter, the final state of scattering is described by a plane wave as discussed in Sec. II B. The dashed line indicates the result calculated using the variational wave function of the ground state [Eq. (8a)] and the plane wave for the final continuous state. The two results show close agreement. As clearly shown in Fig. 4, the scattering linewidth is found to be suppressed to a certain degree by the presence of the Coulomb field between electron and hole in the dissociated exciton.

IV. DISCUSSION

In the preceding section, we have shown that there are two kinds of suppression effects for the linewidth due to LO-phonon absorption by the Q1D exciton through (1) the size effect and (2) the Coulomb-field effect.

The first effect can be achieved by fabricating structures so small that the energy interval between the ground state and the excited states exceeds the LO-phonon energy. In order to attain this effect for structures of realistic size, it may be desirable to make the critical size for this effect larger. This could be accomplished by employing Q1D materials that produce a deeper Rydberg series (i.e., smaller dielectric constant) and have smaller phonon energy. This quideline has general utility in searching for optimum materials. We should note, however, that actually searching for such materials may not be very easy, because the two parameters presented above are known to be negatively correlated. Additional factors such as dielectric effects[23] and strain effects[24] may help to circumvent this difficulty. The above effect is observable not only in the Q1D system, but in Q2D and bulk systems as well, since it can be achieved provided that the energy interval of the Rydberg series exceeds the phonon energy. However, the latter two systems do not seem to be suitable to our purpose, because weak exciton binding in these systems compared with the Q1D system.[25] Moreover, as discussed in Sec. II A, the energy interval $\varepsilon_1-\varepsilon_0$, which determines this effect, is much larger in the Q1D system. In this context, it is evident that the Q1D system is the most probable material system to achieve the suppression effect due to its smaller structures.

The second effect is induced by the presence of the Coulomb field between electron and hole in the dissociated exciton. To confirm this effect, we carried out two kinds of calculations. First, we investigated this effect for larger L values. Since our analysis is applied only to the Q1D system, the wire width is not allowed to be very large. Then, we studied it in the region of large L in which this analyisis seems to be correct (<300 Å). In this region, the above effect tended to disappear with increasing L. Second, we studied this effect for a fixed structure ($L=100$ Å) assuming hypothetical very large phonon energy values ($\hbar\omega_{\mathrm{LO}}=1000-2000$ meV). In this region, the Coulomb-suppression effect was shown to disappear gradually with increasing $\hbar\omega_{\mathrm{LO}}$ value. The above two studies correspond to the calculation in which the Coulomb field can be nearly neglected compared with the kinetic-energy term. In order words, the final state of scattering can be regarded as a nearly free state. The convergence of linewidth to the value in free space shown above indicates that the Coulomb suppression effect is actually present in the structure region studied here. This effect resembles very closely the effect reported recently

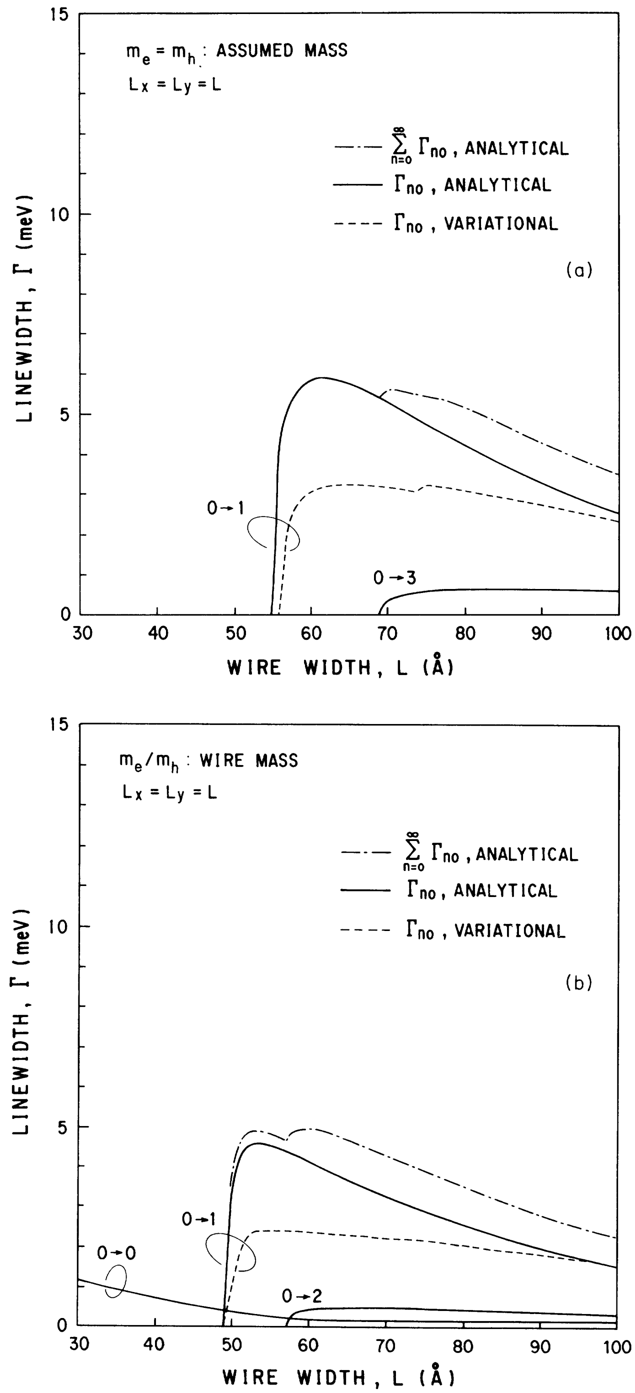

FIG. 5. Linewidths caused by phonon scattering of the exciton from the ground state (0) to discrete states (n) are plotted as functions of wire width (L) of the Q1D system. Its cross section is a square with sides of length L (a) assuming the same mass value for electron and hole, and (b) using the calculated Q1D mass values for electron and hole.

for the optical absorption due to unbound excitons in the 1D system:[26] the Sommerfeld factor assumes a value of less than unity in the 1D system, which is defined as the ratio of optical-absorption coefficients obtained considering, divided by those not considering, the Coulomb field between electron and hole in the dissociated exciton. They ascribed this Coulomb-reduction effect to the strong concentration of oscillator strength on the lowest 1D exciton state. The present Coulomb suppression effect in phonon scattering appears to be closely related to this phenomenon. A difference exists only in the matrix element for the transition: the former (phonon absorption) is determined by the $\phi_\kappa(z)$ values for the z region within the extension of the ground state [see Eq. (16)], whereas the latter (optical absorption) depends only upon $\phi_\kappa(0)$, the wave-function value at the origin. It is natural to predict, from the reduction in $\phi_\kappa(0)$ due to the Coulomb field, that the $\phi_\kappa(z)$ values may also be reduced similarly around the origin: this leads to the reduction in matrix element $[V_{c0}(q_{00}\gamma(\kappa))]$ amplitude due to the presence of this field. The two phenomena are thus found to arise from the same origin in the sense that both are determined by the continuous-state wave function in the vicinity of the origin.

In addition to the above two suppression effects, we have found a third similar effect as follows. As known from Eq. (17), if the electron mass and the hole mass in the direction of the Q1D axis have the same value ($m_e = m_h$, therefore, $p_e = p_h$), the scattering matrix element $V_{\nu 0}(q_z)$ vanishes for even ν states. This implies that in such a situation the $0 \rightarrow \nu$ (ν is even) scattering may be completely suppressed. On the other hand, the $0 \rightarrow \nu$ (ν is odd) scattering cannot be suppressed even in such a situation. This relation holds not only for discrete states but also for a continuous state. Moreover, it is apparent that the scattering may be suppressed in the general $\nu \rightarrow \nu'$ transitions provided that these (ν and ν') states have the same parity and the mass value for electron and hole is the same. An example of this hypothetical situation is shown in Fig. 5(a) for $L_x = L_y = L$, in which the same mass value is used for these particles (that is assumed to be the geometric mean of the bulk mass values for electron and hole). Note that there appears, for smaller structures, a state which is free from phonon scattering. This arises from the complete suppression of the $0 \rightarrow 0$ scattering, which could not be eliminated even by the first suppression effect (small size effect). The more realistic situation can be investigated by the aid of the actual mass values for the Q1D system. Recently, Arakawa, Yamauchi, and Schulman[27] have calculated the mass values of conduction and valence bands in the direction of the Q1D axis using the tight-binding method. They reported that the electron becomes heavier while the hole becomes lighter than those for bulk materials owing to the coupling among energy bands: in other words, the two masses tend to have close values. This change in the mass values will facilitate this third suppression effect. Figure 5(b) shows the results calculated using their masses. Results for larger structures ($L > 70$ Å) may contain some errors, since these were calculated using the masses extrapolated from the values for smaller structures. The results for smaller structures, however, may be sufficient to confirm the suppression effect for the linewidth. Note, in particular, that the $0 \rightarrow 0$ scattering linewidth is suppressed to one-third that obtained using the bulk mass values. This effect also suppresses the $0 \rightarrow c$ scattering because the scattering to the even-parity component of the continuous-state wave function [Eq. (12)] is suppressed due to the same mechanism. Moreover, if a more pronounced change in the mass values for electron and hole is to be achieved by, for example, employing strained Q1D systems,[28] it may be possible to completely suppress the phonon scattering of the exciton in the actual Q1D systems.

V. SUMMARY AND CONCLUSION

LO-phonon scattering is thought to be the dominant factor in mechanisms which are responsible for homogeneous broadening of excitonic absorption lines at room temperature (the practical temperature for device operation). In light of this, we have investigated the LO-phonon scattering of excitons in Q1D systems, with a primary view to suppressing it. Through this study, three kinds of suppression effects have been discovered, all of which seem to be achieved in the most pronounced manner in the Q1D system: first by fabricating smaller structures, second by the presence of a Coulomb field between electron and hole in the dissociated exciton, and third by possessing close mass values for electron and hole in the direction of the Q1D axis. We have demonstrated, in particular, as a hypothetical example (however, it may be achievable by the aid of strains, for example) that an exciton state can be realized by combining the above effects, which is free from phonon scattering at room temperature. These effects suggest the high potentiality of the Q1D system for achieving optical devices which exploit the sharp excitonic-absorption edge such as optical modulators and optical nonlinear devices.

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