Phonon-mediated asymmetric Fano profiles in a semiconductor quantum well

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We predict, on the basis of a model calculation, that an asymmetric Fano-type line shape in the intersubband absorption spectrum will be produced by the electron–LO-phonon interaction in a suitably designed quantum well. The asymmetry parameter q, the broadening Γ, and the frequency shift $\Delta\omega_p$ in the Fano profile are varied with the change of the quantum-well structure parameters, and q is also altered by the variation of the doping density in the well.

I. INTRODUCTION

Quantum interference effects in the absorption of atoms and molecules have been investigated since they were originally studied by Fano.[1] Examples of Fano profiles may be found in all areas of atomic, molecular, and solid-state physics. Recent examples include interference between multiple absorption pathways in two-photon absorption[2] and in molecular dissociation.[3] The effect of Fano interference on the absorption and emission profiles has attracted considerable interest with regard to "lasting without inversion."[4] More recently, Fano interference in type-II semiconductor quantum-well structures,[5] in quasi-one-dimensional electron waveguides,[6] and in absorption in a coupled-quantum-well semiconductor[7] have been investigated. These Fano effects result from the coupling between an electronic discrete state and an energetically degenerate electronic continuum.

Fano interference occurs when transitions, whatever the excitation mechanism is,[1] couple a discrete state and continuum to a common ground state and when the discrete state is quantum-mechanically coupled to the continuum with matrix element V. Interference of LO phonons with an electronic continuum in Raman scattering was investigated in heavily doped p-type[8] and n-type[9] Si during the 1970s. We have recently studied the asymmetric Fano resonance in Raman scattering resulting from the electron–LO-phonon coupling in a semiconductor quantum well.[10]

In this paper, we analyze the asymmetric Fano profile of absorption caused by the electron–LO-phonon coupling in a semiconductor quantum well. We present the theoretical calculations for the asymmetry parameter q, broadening Γ, and frequency shift $\Delta\omega_p$ of Fano-type asymmetric line shapes for appropriately designed quantum-well structures.

II. THEORY

Fano resonances occur in a system containing two different transition channels, one belonging to a continuum and the other to a bound state which interferes with the continuum. Such an interference is known to lead to an asymmetric line shape.[1]

In the system shown in Fig. 1, there exists a ground state $|g\rangle$, an excited electronic state $|e\rangle$ with excitation energy E_e, and a one-phonon excited state $|p\rangle$ with energy $E_p=\hbar\omega_p$. The transition matrix elements connecting the latter two states to the ground state are T_e and T_p. The electron-phonon interaction matrix element is $V=\langle e|H_{ep}|p\rangle$.

Consider $|e\rangle$ to be one level in the continuum. We assume for simplicity, as in Ref. 11, that the transition matrix element T_e and the interaction matrix element V are both constant for each level $|e\rangle$ in the continuum. When an optical beam irradiates the system, with a formalism similar to that of Ref. 11 which describes the Fano profile of Raman scattering in heavily doped Si, we can deduce that the absorption intensity is proportional to

$$A(E)=\pi D(E)T_e^2\frac{(q+\epsilon)^2}{1+\epsilon^2}\ , \tag{1}$$

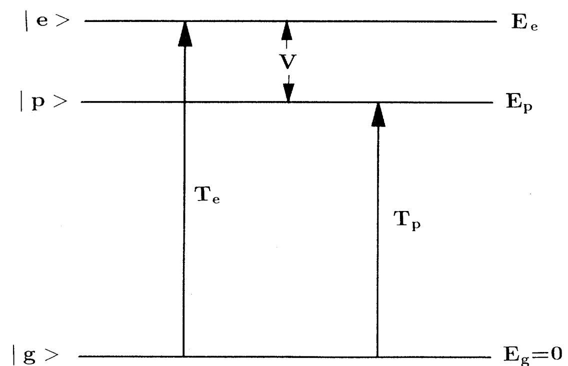

FIG. 1. System with an electronic excited state $|e\rangle$ and a one-phonon excited state $|p\rangle$ coupled by a matrix element V. The transition matrix elements connecting $|e\rangle$ and $|p\rangle$ to the ground state $|g\rangle$ are T_e and T_p, respectively.

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where

$$I(E)=\frac{|q+\epsilon|^2}{1+\epsilon^2} \tag{2}$$

is the Fano profile with

$$\epsilon=\frac{E-E_p-V^2R(E)}{\pi V^2 D(E)} \tag{3}$$

and

$$q=\frac{VT_p/T_e+V^2R(E)}{\pi V^2 D(E)} . \tag{4}$$

Here q is the asymmetry parameter of the Fano line shape, $D(E)$ is the density of continuum states, and $R(E)$ is its Hilbert transform, i.e.,

$$R(E)=\mathrm{P}\int D(E')(E-E')^{-1}dE' , \tag{5}$$

where P stands for the principal value.

In the problem we discuss, which is somewhat different from Ref. 11, T_e is not the electronic Raman matrix element but the direct transition matrix element of the electron, and T_p is not the phonon Raman matrix element but the resonant absorption matrix element of the phonon. Such an adaptation is based on the fact that the Fano theory is independent of the transition mechanisms.[1]

The broadening Γ and the frequency shift $\Delta\omega_p$ are related to the reduced-energy expression (3) as follows:

$$\hbar\Gamma=\pi V^2 D(E) \tag{6}$$

and

$$\hbar\Delta\omega_p=V^2R(E) . \tag{7}$$

As shown in Fig. 2, we consider the case that only one bound state exists in the quantum well with a barrier height V_b. Let the energy (E_0) of the bound (ground) state be zero ($E_0=0$), the energy of the bottom of the well be $-E_1$ ($E_1>0$), and hence the energy for the barrier height be $E_b=V_b-E_1$. In order to obtain Fano interference, the quantum-well structure is so designed that the energy of the discrete one-phonon excited state falls within the extended continuum of electronic states. This means $\hbar\omega_p \geq E_b$. When an optical beam irradiates the quantum well, an electron in the ground state can absorb a photon and be excited to the extended state which has the same energy as the photon. The corresponding transition matrix element is

$$T_e=\langle N,\phi_e|H_{\mathrm{el}}(\hbar\omega_l)|\phi_0,N\rangle , \tag{8}$$

where ϕ_0 and ϕ_e are, respectively, the electronic wave functions of the ground and extended states in the conduction band, N is the phonon number in the system, and $H_{\mathrm{el}}(\hbar\omega_l)$ is the electron-photon interaction Hamiltonian with $\hbar\omega_l$ being the energy of the absorbed photon.

At the same time, if the energy of the incident photon is equal to the energy of the LO phonon in the well material (e.g., GaAs), i.e., $\hbar\omega_l=\hbar\omega_p$, a resonant absorption phenomenon occurs. In the resonant process, an electron absorbs the photon and makes a transition to an excited state and immediately emits an optical phonon with the same frequency of the photon, and then returns to the ground state. According to perturbation theory,[12] for the second-order transition we can obtain the resonant transition matrix element as

$$T_p=\sum_e \frac{\langle N+1,\phi_0|H_{ep}|\phi_e,N\rangle\langle N,\phi_e|H_{\mathrm{el}}(\omega_l)|\phi_0,N\rangle}{\hbar\omega_l-E_e}$$
$$=\sum_e \frac{VT_e}{E_p-E_e} , \tag{9}$$

where H_{ep} is the electron–LO-phonon interaction Hamiltonian, and N and $N+1$ are, respectively, the numbers of phonons in the quantum well before and after absorption.

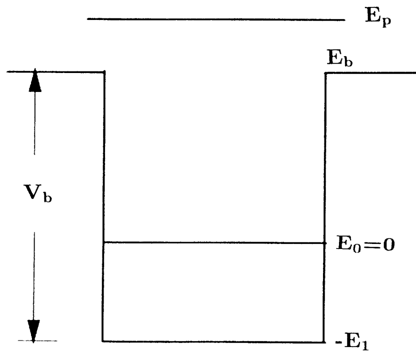

FIG. 2. Energy-level structure of a quantum well with barrier height V_b. $E_0=0$ denotes the bound (ground) state, $-E_1$ is the energy at the bottom of the well, $E_b=V_b-E_1$, and E_p denotes the one-phonon excited energy.

III. CALCULATION OF Γ, q, AND $\Delta\omega_p$

In the quantum well, the Fermi energy E_F depends on the doping density n, the temperature T, and the quantum well width a through the relation[13]

$$n=\frac{m_w k_B T}{a\pi\hbar^2}\ln[1+\exp(E_F/k_BT)] , \tag{10}$$

where m_w is the electron effective mass in the well, and k_B is the Boltzmann constant. In Eq. (10) we have assumed approximately that the electrons are all populated in the ground state with energy $E_0(=0)$. The density of the electronic continuum in extended states is given by the expression[10]

$$D(E_e)=\frac{a^*}{2\pi}\frac{\sqrt{2m_w}}{2\hbar\sqrt{E_e-E_b}} , \tag{11}$$

where a^* is the effective well width.

The electron–LO-phonon Hamiltonian for the polarization potential (Fröhlich term) is[14]

$$H_{ep}=i\left[\frac{e^2\omega_p\hbar}{2V_A}\left[\frac{1}{\epsilon(\infty)}-\frac{1}{\epsilon(0)}\right]\right]^{1/2}\times\sum_{\mathbf{q}}\frac{1}{q}\exp(i\mathbf{q}\cdot\mathbf{r})[a^\dagger(-\mathbf{q})+a(\mathbf{q})]\ , \tag{12}$$

where V_A is the volume of the sample, $a(\mathbf{q})$ is the annihilation operator for a photon with wave vector $\mathbf{q}(q_x,q_y,q_z)$, and $\epsilon(\infty)$ and $\epsilon(0)$ are, respectively, the high-frequency and static relative permittivities. The initial and final electronic states for the phonon emission process can be written, respectively, as

$$\phi_e(\mathbf{k}',\mathbf{r})=\frac{1}{\sqrt{S}}\exp(i\mathbf{k}_t'\cdot\rho)F'(x) \tag{13}$$

and

$$\phi_0(\mathbf{k},\mathbf{r})=\frac{1}{\sqrt{S}}\exp(i\mathbf{k}_t\cdot\rho)F(x)\ , \tag{14}$$

where $F'(x)$ and $F(x)$ are the electronic envelope wave functions, x is along the growth direction of the quantum well, S is the quantum-well area, and $\rho=(y,z)$ and $\mathbf{k}_t'=(k_y,k_z)$ are the in-plane components of the electron position vector and electron wave vector. We can derive the modulus square of the electron–LO-phonon interaction matrix element for phonon emission as follows:

$$V^2=|\langle N+1,\phi_0|H_{ep}|N,\phi_e\rangle|^2=\frac{e^2\hbar\omega_p}{2(2\pi)^3\epsilon_p}(N+1)\int\int\int_{-\infty}^{+\infty}\frac{|I(q_x)|^2}{Q^2+q_x^2}dq_x d\mathbf{Q}\ , \tag{15}$$

where

$$Q^2=|\mathbf{k}_t'-\mathbf{k}_t|^2\ , \tag{16}$$

$$I(q_x)=\int dx\, F'(x)F^*(x)\exp(iq_x x)\ , \tag{17}$$

$$\epsilon_p^{-1}=\epsilon^{-1}(\infty)-\epsilon^{-1}(0)\ , \tag{18}$$

and N is the thermal population of optical phonons:

$$N=[\exp(\hbar\omega_p/k_BT)-1]^{-1}\ . \tag{19}$$

In Eq. (15) we have assumed that photons in the well are bulklike modes. Calculating the integral for q_x in Eq. (15), we obtain

$$\int_{-\infty}^{+\infty}\frac{\exp[iq_x(x_1-x_2)]}{Q^2+q_x^2}dq_x=\frac{\pi}{Q}\exp[-Q|x_1-x_2|]\ . \tag{20}$$

Since the transition process for the phonon is induced by the light-excited electron and the wave vector of the absorbed photon is very small, the corresponding change $Q\,(=|\mathbf{k}_t'-\mathbf{k}_t|)$ of the in-plane wave vector of the phonon is also very small. Thus we have

$$\exp(-Q|x_1-x_2|)\approx 1-Q|x_1-x_2|\ . \tag{21}$$

Substituting Eq. (21) into (20) and its result into (15), and using (17), we obtain

$$\int_{-\infty}^{+\infty}\frac{|I(q_x)|^2}{Q^2+q_x^2}dq_x=-\pi\int\int dx_1dx_2[F'^*(x_1)F(x_1)\times F'(x_2)F^*(x_2)\times|x_1-x_2|]\ . \tag{22}$$

The envelope wave functions for the bound and extended states $F(x)$ and $F'(x)$ can be expressed as[15]

$$F(x)=\begin{cases}B\exp(k_1x)\ , & x<-a/2\\ C\cos(kx)\ , & -a/2\le x\le a/2\\ B\exp(-k_1x)\ , & x>a/2\end{cases} \tag{23}$$

and

$$F'(x)=\begin{cases}B'\cos(k_2x-\xi)\ , & x<-a/2\\ C'\sin(k'x)\ , & -a/2\le x\le a/2\\ B'\cos(k_2x+\xi)\ , & x>a/2\ ,\end{cases} \tag{24}$$

where B (B') and C (C') are the normalization coefficients, and the phase ξ makes the wave function of the extended state to match at the interface. The wave vectors k, k', k_1, and k_2 are

$$k=\frac{\sqrt{2m_wE_1}}{\hbar}\ , \tag{25}$$

$$k'=\frac{\sqrt{2m_wE_e}}{\hbar}\ , \tag{26}$$

$$k_1=\frac{\sqrt{2m_bE_b}}{\hbar}\ , \tag{27}$$

$$k_2=\frac{\sqrt{2m_b(E_e-E_b)}}{\hbar}\ , \tag{28}$$

where m_b is the electron effective mass in the barrier. As mentioned in the above section, the resonant condition $\hbar\omega_l=\hbar\omega_p$ for the phonon emission is satisfied by the energy $\hbar\omega_p$ of the LO phonon of the well material. The contribution of the Fano interference comes mainly from the well region, because the energy of the phonons of the barrier material is off-resonance. Thus Eq. (22) can be simplified as

$$\int_{-\infty}^{+\infty}\frac{|I(q_x)|^2}{Q^2+q_x^2}dq_x=-\pi C^2C'^2\int_{-a/2}^{a/2}dx_2[\cos(kx_2)\sin(k'x_2)P(x_2)] \tag{29}$$

with

$$P(x_2)=\int_{-a/2}^{a/2}dx_1[\cos(kx_1)\sin(k'x_1)|x_1-x_2|]=-\frac{\sin[(k'+k)x_2]}{(k'+k)^2}-\frac{\sin[(k'-k)x_2]}{(k'-k)^2}+\frac{x_2\cos[(k'+k)a/2]}{k'+k}+\frac{x_2\cos[(k'-k)a/2]}{k'-k}\ . \tag{30}$$

Substituting the calculated result of Eq. (29) into (15) and then integrating for Q in the range of the photon wave vector (i.e., $|Q| \leq \omega_l / c$), after some mathematical manipulation, we obtain

$$V^2 = \frac{e^2 \hbar \omega_p}{2(2\pi)^3 \epsilon_p}(N+1)\frac{\pi E_e}{c\hbar} C^2 C'^2 \pi f(k') , \tag{31}$$

where

$$f(k') = -\frac{\sin[(k'+k)a]}{4(k'+k)^3} - \frac{\sin[(k'-k)a]}{4(k'-k)^3} + \frac{a}{4(k'+k)^2} + \frac{a}{4(k'-k)^2} - \frac{\sin(k'a)}{4k'(k'+k)^2} - \frac{\sin(k'a)}{4k'(k'-k)^2} + \frac{\sin(ka)}{4k(k'+k)^2} + \frac{\sin(ka)}{4k(k'-k)^2} + G\left[\frac{a\cos[(k'+k)a/2]}{2(k'+k)} - \frac{\sin[(k'+k)a/2]}{(k'+k)^2} + \frac{a\cos[(k'-k)a/2]}{2(k'-k)} - \frac{\sin[(k'-k)a/2]}{(k'-k)^2}\right] \tag{32}$$

with

$$G = \frac{\cos[(k'+k)a/2]}{k'+k} + \frac{\cos[(k'-k)a/2]}{k'-k} . \tag{33}$$

The largest contribution from the density of states to the Fano profile parameters (q, Γ, and $\Delta\omega_p$) is made at the phonon frequency. Hence we obtain the broadening

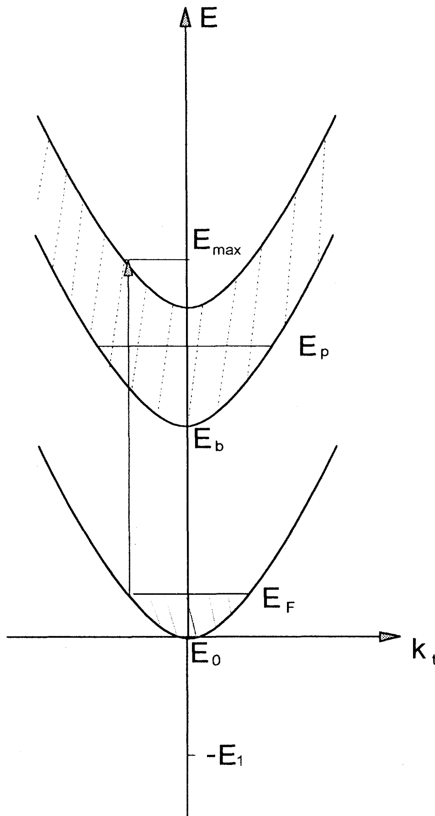

FIG. 3. In-plane component k_t of electron wave vector and the corresponding energy-level structure. E_F denotes the Fermi energy and $E_{\max}$ corresponds to the higher limit in the electronic continuum associated with the direct transition. The other notations are the same as in Fig. 2.

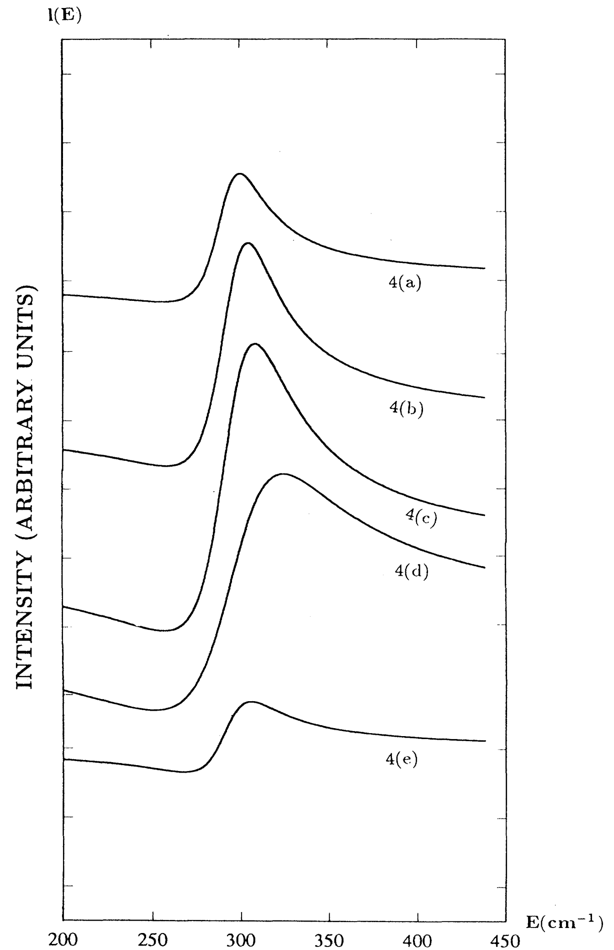

FIG. 4. Asymmetric Fano profiles in absorption spectra corresponding to quantum-well structures with (a) well width $a = 30$ Å, barrier height $V_b = 71.06$ meV, and doping density $n = 1.71\times10^{18}$ cm^{-3}; (b) $a = 40$ Å, $V_b = 71.06$ meV, and $n = 1.29\times10^{18}$ cm^{-3}; (c) $a = 50$ Å, $V_b = 71.06$ meV, and $n = 1.03\times10^{18}$ cm^{-3}; (d) $a = 60$ Å, $V_b = 71.06$ meV, and $n = 0.86\times10^{18}$ cm^{-3}; (e) $a = 30$ Å, $V_b = 107.66$ meV, and $n = 1.71\times10^{18}$ cm^{-3}.

TABLE I. The quantum-well parameters and Fano-profile characteristic quantities.

Corresponding Fano profile	Fig. 4(a)	Fig. 4(b)		Fig. 4(c)	Fig. 4(d)	Fig. 4(e)
Aluminum composition x			0.1			0.15
Well width a (Å)	30	40		50	60	30
Barrier height V_b (meV)			71.06			107.66
Ground-state energy E_1 (meV)	55.6	48.8		42.4	36.0	77.0
Doping density n (10^{18} cm^{-3})	1.71	1.29		1.03	0.86	1.71
Asymmetry parameter q_r	1.78	1.49		1.13	0.58	0.70
Frequency shift $\Delta\omega_p$ (cm^{-1})	0.144	0.300		0.511	0.719	0.106
Broadening Γ (cm^{-1})	0.161	0.400		0.905	2.458	0.302

$$\hbar\Gamma=\frac{a^*}{2}\frac{\sqrt{2m_w}}{2\hbar\sqrt{E_p-E_b}}\frac{e^2\hbar\omega_p}{2(2\pi)^3\epsilon_p}(N+1)\frac{\pi E_p}{c\hbar}\times C^2C'^2\pi f(k_p)\ , \quad (34)$$

with

$$k_p=\sqrt{2m_wE_p/\hbar^2}\ . \quad (35)$$

Figure 3 shows the in-plane component k_t of the electron wave vector and the corresponding energy level structure. The parabola represents the total electronic energy E_t given by $E_t=E_z+m_w\hbar^2k_t^2/2$, where E_z is the electronic energy along the growth direction of the quantum well, and $E_z=E_0$ for the bound (ground) state and $E_z=E$ for the extended excited state. E_F denotes the Fermi level and $E_{\max}$ corresponds to the higher limit in the electronic continuum associated with the direct transition. Considering the conservation of electronic wave vector in the optical transition and estimating the range[10] of wave vectors by using the uncertainty principle, we can derive from Eq. (11) the Hilbert transform of the density of continuum states as follows:

$$R(E_p)=\frac{a^*}{4\pi\hbar}\sqrt{2m_w}\,\mathrm{P}\int_{E_b}^{E_{\max}}\frac{dE'}{\sqrt{E'-E_b}(E_p-E')}$$
$$=\frac{a^*}{2\pi\hbar}\frac{\sqrt{2m_w}}{\sqrt{E_p-E_b}}\ln\left|\frac{\sqrt{E_{\max}-E_B}+\sqrt{E_p-E_b}}{\sqrt{E_{\max}-E_b}-\sqrt{E_p-E_b}}\right| \quad (36)$$

with

$$E_{\max}=E_1+E_F+E_b\ . \quad (37)$$

Substituting Eqs. (8), (9), (11), and (36) into (4), and making an algebraic replacement,[10] we can get the asymmetric parameter as follows:

$$q=\frac{V^2\left[\mathrm{P}\int D(E')(E_p-E')^{-1}dE'+i\pi\sum_e\delta(E_e-E_p)\right]+V^2R(E_p)}{\pi V^2D(E_p)}$$
$$=\frac{2}{\pi}\frac{R(E_p)}{D(E_p)}+i=\frac{4}{\pi}\ln\left|\frac{\sqrt{E_1+E_F}+\sqrt{E_p-E_b}}{\sqrt{E_1+E_F}-\sqrt{E_p-E_b}}\right|+i\ . \quad (38)$$

Putting Eqs. (31) and (36) into (7), we can obtain the frequency shift caused by the Fano effect as follows:

$$\hbar\Delta\omega_p=\frac{e^2\hbar\omega_p}{2(2\pi)^3\epsilon_p}(N+1)\frac{\pi E_p}{c\hbar}C^2C'^2\pi f(k_p)\times\frac{a^*}{2\pi\hbar}\frac{\sqrt{2m_w}}{\sqrt{E_p-E_b}}\ln\left|\frac{\sqrt{E_1+E_F}+\sqrt{E_p-E_b}}{\sqrt{E_1+E_F}-\sqrt{E_p-E_b}}\right|. \quad (39)$$

In order to get the correct line shape, the Fano line shape [Eq. (2)] is convoluted with a Lorentzian corresponding to pure resonant absorption by an LO phonon in the quantum well. The convoluted line shape is also Fano-like,[9] in the form

$$I(q,\epsilon')=\frac{\Gamma}{\Gamma+\gamma}\frac{|q+\epsilon'|^2}{1+\epsilon'^2}+\frac{\gamma}{\Gamma+\gamma}\ , \quad (40)$$

where

$$\epsilon'=\frac{E-E_p-\hbar\Delta\omega_p}{\hbar(\Gamma+\gamma)} . \qquad (41)$$

Here γ is the linewidth of the LO phonon in the absence of interaction with the electronic continuum. This linewidth γ is usually determined by anharmonic decay into two acoustic phonons.[11] The dependence of γ on the temperature T is given by[16]

$$\gamma(T)=\gamma(0)\left[1+\frac{2}{\exp(\hbar\omega_p/2k_BT)-1}\right] . \qquad (42)$$

We take GaAs/$Al_xGa_{1-x}As$ quantum-well structures as an example. For a given Al composition x, the barrier height V_b of the quantum well can be written as[17]

$$V_b=Q(1266x+260x^2) , \qquad (43)$$

where $Q=0.55$ is the band-offset factor. To obtain a stronger Fano effect in the absorption spectra we optimize the structure parameters (x and a) and doping density n of the quantum well. Table I shows some numerical examples, where we also show the corresponding calculated results for the ground state energy E_1, the real part (q_r) of the asymmetry parameter q [from Eq. (38)], the broadening Γ [from (34)], and the frequency shift $\Delta\omega_p$ [from (39)]. In the calculation we have used the following parameters: LO-phonon energy in GaAs, $\hbar\omega_p=36.2$ meV,[18] the phonon decay constant $\hbar\gamma(0)=0.58$ meV,[19] and $T=300$ K. Substituting the values in Table I into Eqs. (40) and (41), we can obtain the corresponding Fano profiles for absorption spectra, as illustrated in Figs. 4(a)–4(f).

In summary, the Fano interference between a discrete phonon and an electron continuum will occur in the intersubband absorption in an appropriately designed quantum-well structure. Hence, in the absorption spectrum there will be an absorption minimum at a particular frequency.

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