Theoretical investigation of collective excitations in HgTe/CdTe superlattices. I. Intrasubband excitation

Dan-hong Huang and Shi-xun Zhou
Department of Physics, Fudan University, Shanghai, China
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In this paper, we study in detail the electron collective excitations of HgTe/CdTe superlattices with a simple model superlattice, taking into account the overlap of wave functions at the interfaces for interface states. The linear-response theory has been used with success to calculate the density response of the superlattice to an external perturbation, including many-body effects and electron–heavy-hole coupling in a reasonable way for intrasubband modes. Some attractive features are found compared with those in type-I and -II superlattices, such as localized modulated three-dimensional optical and acoustical plasmons, and so on. Moreover, the coupling of interface states with heavy-hole-like subbands is discussed. Also, a comparison of the collective excitation spectra between the quasi-two-dimensional and purely two-dimensional charge interfaces, along with a discussion on their relevance to experiment, is presented.

I. INTRODUCTION

Superlattices are a new kind of material generally made of multiple alternating layers of two (or more) different binary or pseudobinary compounds. There are two types of superlattices (known as type-I and -II superlattices) whose properties have been extensively studied in the last few years.[1-5] The structures of the subbands and cyclotron resonance have been investigated by both far-infrared-absorption spectroscopy[6-8] and resonant-light-scattering technique.[9-11] Theoretically, one aspect of the physics of these kinds of superlattices that is of most dramatic interest to us is the electron collective-excitation spectrum of a periodic array of equally spaced charge layers.

Recently, great attention has been paid to the type-III superlattices typified by the HgTe/CdTe system,[12-17] which consists of both a semimetal and semiconductor. The computations of the band structure of HgTe/CdTe superlattices given by PWM,[18] linear combination of atomic orbitals (LCAO),[15,17] and envelope-function-approximation (EFA) (Refs. 14 and 19) methods agree well and show that they can be either semiconducting or zero-band-gap semiconductors. Moreover, the electronlike, heavy-hole-like, and light-hole-like states are confined very well in HgTe and CdTe layers[12,13,17] and the interface states are localized near the interfaces.[14,15] It is proved that the thickness of materials HgTe and CdTe will decide the width of the band gap and subbands, respectively. Although superlattice (SL) states include electronlike, light-hole-like, heavy-hole-like, and interface states, in comparison with the situations in type-I and -II superlattices, we still consider that the interface states play the most important role in HgTe/CdTe superlattices. It is evident that the width of band gap strongly depends on the hybridization of interface states with the heavy-hole-like subbands[14] and contributes a great deal to the properties of HgTe/CdTe superlattices in optical absorption, transport, and collective excitation. Besides, the zero-band-gap band structure and the quasi-interface states are consequences of matching up of bulk states belonging to the conduction band in HgTe and the light-hole valence band in CdTe. This matching up is only favorable when the bulk states to be connected are made of atomic orbitals of the same symmetry type and the effective masses on either side of the interface have the opposite sign. To our knowledge no theoretical investigation of plasmons in HgTe/CdTe superlattice has yet been reported.

In this paper we study the collective-excitation spectrum of such superlattices in the simple model, mainly concentrating on the effects of interface states. We assume the layers of HgTe and CdTe have the same thickness $d/2$, and d is small enough so that superlattice will behave exactly like a semiconductor and the self-consistent-field (SCF) method[4,5,20] will be applicable. Furthermore, we consider the motion of electrons in the X-Y plane to be completely free because the EFA method well describes the band structure of HgTe/CdTe superlattices,[19] and that only interface states overlap between adjacent layers. It is expected that the assumption of infinitely thin layers and zero width of localization at interfaces will be reasonably good for low electron densities in HgTe/CdTe superlattices with not too small layer thickness. The approximation of a perfect confinement in the well is usually not very good for the energy levels, but not so bad for the wave function.[21] In view of the attractive characteristics in HgTe/CdTe superlattices, it is interesting to calculate the collective-excitation spectrum of it.

The paper is organized as follows. In Sec. II the SCF treatment of collective excitation of a superlattice is described. In Sec. III we consider the intrasubband modes of interface states with zero width and finite width of localization, and the coupled intrasubband modes of interface and heavy-hole-like states with infinitely thin layer thickness and zero width of localization are studied. We conclude in Sec. IV, presenting some possible future improvements of our theory and some attractive features compared with those in type-I and -II superlattices. Also, the difference between the perfect two-dimensional system and the real system is discussed in this section.

II. SCF TREATMENT OF COLLECTIVE EXCITATION IN HgTe/CdTe SUPERLATTICES

We now proceed to discuss the linear response of a superlattice to an external potential for zero magnetic field. In our approximation mentioned in Sec. I, the single-particle wave function in this model of superlattice can be written as

$$\phi^{(s)}_{\mathbf{k},n,j}(\mathbf{r},z)=\exp(i\mathbf{k}\cdot\mathbf{r})\psi^{(s)}_{n,j}(z-jd/2)/\sqrt{A}\ . \qquad (1)$$

Here $\mathbf{k}$ is a two-dimensional wave vector describing the planar motion in the X-Y plane and A is the two-dimensional area of each layer (needed for normalization of the plane wave), j and n are the layer index and the subband index, respectively; the labels $s=1,2,3,4$ refer to the electronlike, heavy-hole-like, interface, and light-hole-like states, respectively. We choose the SL states to be strictly two dimensional with no overlap between adjacent layers with the exception of the interface states. This approximation is made mainly for the sake of convenience, allowing us to do most of our calculation analytically. We expect it to be reasonable for low electron densities in HgTe/CdTe superlattices with not too small layer thickness. The noninteracting single-particle energy is given by (with $m_j^{(s)}$ as the mass for planar motion)

$$E^{(s)}_{n,j}(\mathbf{k})=E^{(s)}_{n,j}+\hbar^2k^2/2m_j^{(s)}\ . \qquad (2)$$

Here the single-particle wave function $\phi^{(s)}_{\mathbf{k},n,j}(\mathbf{r},z)$ will take the explicit forms

$$\psi^{(1)}_{n,j}(z-jd/2)=\begin{cases}\psi^{e}_{n,j} & \text{for } j \text{ even}\\ 0 & \text{for } j \text{ odd}\ ,\end{cases} \qquad (3)$$

$$\psi^{(2)}_{n,j}(z-jd/2)=\begin{cases}\psi^{\mathrm{hh}}_{n,j} & \text{for } j \text{ even}\\ 0 & \text{for } j \text{ odd}\ ,\end{cases} \qquad (4)$$

$$\psi^{(3)}_{n,j}(z-jd/2)=\psi^{\mathrm{int}}_{n,j},\quad \text{for } j \text{ both even and odd}\ , \qquad (5)$$

$$\psi^{(4)}_{n,j}(z-jd/2)=\begin{cases}0 & \text{for } j \text{ even}\\ \psi^{\mathrm{lh}}_{n,j} & \text{for } j \text{ odd}\ ,\end{cases} \qquad (6)$$

where the layers are labeled by an integer j; even-numbered layers will be taken to be HgTe layers, while odd-numbered layers are CdTe layers.

An external perturbing potential of the form

$$V^{\mathrm{ext}}(\mathbf{r},z,t)=V^{\mathrm{ext}}(\mathbf{q},\omega,z)\exp[i(\omega t-\mathbf{q}\cdot\mathbf{r})] \qquad (7)$$

will lead to an induced electron density, which in turn induces perturbed Hartree and exchange-correlation potentials. Thus

$$V=V^{\mathrm{ext}}+V^{H}+V^{\mathrm{XC}} \qquad (8)$$

is also of the form (7). We use the SCF scheme of Ehrenreich and Cohen to calculate the induced electron density

$$\delta n(\mathbf{q},\omega,z)=\sum_{s,s'}\sum_{n,n',j,j}\Pi^{(s,s')}_{nn',jj'}(\mathbf{q},\omega)\times\langle n,j,s|V(\mathbf{q},\omega)|n',j',s'\rangle\times\psi^{(s')}_{n'j'}(z-j'd/2)\psi^{(s)}_{nj}(z-jd/2)\ , \qquad (9)$$

where the irreducible polarization under the random-phase approximation (RPA) can be expressed as

$$\Pi^{(s,s')}_{nn',jj'}(\mathbf{q},\omega)=\sum_{\mathbf{k}}\frac{f_0(E^{(s')}_{n'j'}(\mathbf{k}+\mathbf{q}))-f_0(E^{(s)}_{nj}(\mathbf{k}))}{E^{(s')}_{n'j'}(\mathbf{k}+\mathbf{q})-E^{(s)}_{nj}(\mathbf{k})-\hbar\omega}\ , \qquad (10)$$

where f_0 is the Fermi distribution function. Although the RPA is a high-density approximation, it has been used with success in the problem of semiconductor superlattices. We let the exchange-correlation potential V^{XC} be zero throughout this paper for convenience. By using the ansatz due to the translational symmetry of the system, that is,

$$\langle n,s|V_j(\mathbf{q},\omega)|0,s'\rangle=\begin{cases}\exp(ik_zjd/2)\langle n,s|V_0|0,s'\rangle\\ \text{for } j \text{ even}\\ \exp[ik_z(j-1)d/2]\langle n,s|V_1|0,s'\rangle\\ \text{for } j \text{ odd}\ ,\end{cases} \qquad (11)$$

we write down straightforwardly a series of basic self-consistent equations under the self-sustaining condition $V^{\mathrm{ext}}=0$ and the electric quantum limit without repeating the computation similar to Refs. 4 and 5,

$$\begin{aligned}\langle n,s|V_0|0,s'\rangle=\Bigg[&\sum_m \Pi^{(3,3)}_{m0}[(A+S_-B+S_+C)\langle m,3|V_0|03\rangle+(S'_-B+S'_+C)\langle m,3|V_1|0,3\rangle\\ &+\sum_{i=1}^{3}\sum_m X^{(i,i)}_{m0}[V^{H}_{mn}(s',s;i,i)+S_-V'^{H}_{mn}(s',s;i,i)+S_+V'^{H}_{nm}(i,i;s,s')]\langle m,i|V_0|0,i\rangle\\ &+\sum_{i=3}^{4}\sum_m X^{(i,i)}_{m0}[S'_-V'^{H}_{mn}(s',s;i,i)+S'_+V'^{H}_{nm}(i,i;s',s)]\langle m,i|V_1|0,i\rangle\\ &+\sum_{i,j=1,2,3}^{i>j}\sum_m X^{(i,j)}_{m0}[V^{H}_{mn}(s',s;j,i)+S_-V'^{H}_{mn}(s',s;j,i)+S_+V'^{H}_{nm}(j,i;s',s)]\langle m,i|V_0|0,j\rangle\\ &+\sum_m X^{(4,3)}_{m0}[S'_-V'^{H}_{mn}(s',s;3,4)+S'_+V'^{H}_{nm}(3,4;s',s)]\langle m,4|V_1|0,3\rangle\Bigg]+\ (m\leftrightarrow 0)\end{aligned} \qquad (12)$$

and

$$\langle n,s|V_1|0,s'\rangle=\Bigg[\sum_m \Pi_{mo}^{(3,3)}[(A+S_-B+S_+C)\langle m,3|V_1|0,3\rangle+(S'_-B+S'_+C)\langle m,3|V_0|0,3\rangle]$$
$$+\sum_{i=3}^{4}\sum_m X_{m0}^{(i,i)}[V_{mn}^H(s',s;i,i)+S_-V_{mn}'^H(s',s;i,i)+S_+V_{nm}'^H(i,i;s,s')]\langle m,i|V_1|0,i\rangle$$
$$+\sum_{i=1}^{3}\sum_m X_{m0}^{(i,i)}[S'_-V_{mn}'^H(s',s;i,i)+S'_+V_{nm}'^H(i,i;s',s)]\langle m,i|V_0|0,i\rangle$$
$$+\sum_{i,j>1,2,3}^{i>j}\sum_m X_{m0}^{(i,j)}[S'_-V_{mn}'^H(s',s;j,i)+S'_+V_{nm}'^H(j,i;s',s)]\langle m,i|V_0|0,j\rangle$$
$$+\sum_m X_{mo}^{(4,3)}[V_{mn}^H(s',s;3,4)+S_-V_{mn}'^H(s',s;3,4)+S_+V_{nm}'^H(3,4;s',s)]\langle m,4|V_1|0,3\rangle\Bigg]+(m\leftrightarrow 0)\ , \tag{13}$$

with the symbols given by

$$V_{m0n}^{H(\pm)}(s',s;p',p)=(2\pi e^2/\epsilon_s q)\int dz\int dz'\,e^{-q|z-z'|}\psi_n^{(s)}(z)\psi_0^{(s')}(z)\psi_0^{(p')}(z'\mp d/2)\psi_m^{(p)}(z')\delta(p'p,33)\ , \tag{14}$$

$$V_{m0n}'^{H(\pm)}(s's,p'p)=(2\pi e^2/\epsilon_s q)\int dz\int dz'\,e^{-q(z-z')}\psi_n^{(s)}(z)\psi_0^{(s')}(z)\psi_0^{(p')}(z'\mp d/2)\psi_m^{(p)}(z')\delta(p'p,33)\ , \tag{15}$$

$$V_{m0n}^{H}(s's,p'p)=(2\pi e^2/\epsilon_s q)\int dz\int dz'\,e^{-q|z-z'|}\psi_n^{(s)}(z)\psi_0^{(s')}(z)\psi_0^{(p')}(z')\psi_m^{(p)}(z')\ , \tag{16}$$

$$V_{m0n}'^{H}(s's,p'p)=(2\pi e^2/\epsilon_s q)\int dz\int dz'\,e^{-q(z-z')}\psi_n^{(s)}(z)\psi_0^{(s')}(z)\psi_0^{(p')}(z')\psi_m^{(p)}(z')\ , \tag{17}$$

and

$$A=V_{m0n}^{H(-)}(s's,33)+V_{m0n}^{H(+)}(s's,33)\ ,$$
$$B=V_{m0n}'^{H(-)}(s's,33)+V_{m0n}'^{H(+)}(s's,33)\ ,$$
$$C=V_{nm0}'^{H(-)}(33,s's)+V_{nm0}'^{H(+)}(33,s's)\ ,$$

where $X_{m0}=\Pi_{m0}+\Pi_{0m}$ and Π_{mn} is given in Eq. (10). "$(m\leftrightarrow 0)$" stands for all the terms in either Eqs. (12) or (13) which are obtained under the interchange of the indices m and 0 of the terms already presented.

Moreover, we have introduced in Eqs. (12) and (13) the symbols $S_\pm$ and $S'_\pm$ defined by

$$S_\pm=\frac{e^{-qd}e^{\pm ik_zd}}{1-e^{-qd}e^{\pm 1k_zd}}\ , \tag{18}$$

$$S'_\pm=\frac{e^{-qd/2}e^{\pm ik_zd/2}}{1-e^{-qd}e^{\pm ik_zd}}\ . \tag{19}$$

It may be proved that both Eqs. (12) and (13) include the contributions of type-I and -II superlattices, excitons in periodic quantum wells, interface states, and the interactions between interface states and the other SL states in HgTe layers and CdTe layers. In fact, we can easily obtain the collective-excitation spectra of type-I $(s,s'=1)$ and type-II $(s,s'=1,4)$ superlattices[4,5] or excitons in multiple quantum wells $(s,s'=1,2)$ separately. Hence the results obtained here are quite general and attractive.

III. INTRASUBBAND MODES

To obtain the intrasubband modes, we set $m=n=0$ in Eqs. (12) and (13). We shall restrict our study to the case of interface states (i.e., $s=s'=3$). For purely two-dimensional charge interfaces, we choose

$$|\psi_{nj}^{(3)}(z-jd/2)|^2=\delta(z-jd/2)\ . \tag{20}$$

By using the well-known long wavelength form[22] for the polarizability of a two-dimensional electron gas (2D EG),

$$\Pi_{00}^{(3,3)}(\mathbf{q},\omega)=\frac{n^{(3)}q^2}{m^{(3)}\omega^2}\ , \tag{21}$$

Eqs. (12) and (13) yield

$$[1-(n^{(3)}q^2/m^{(3)}\omega^2)(2\pi e^2/\epsilon_s q)a(\mathbf{q},k_z)]^2$$
$$=[(2\pi e^2/\epsilon_s q)^2(n^{(3)}q^2/m^{(3)}\omega^2)^2b^2(\mathbf{q},k_z)]\ , \tag{22}$$

with

$$a(\mathbf{q},k_z)=S(\mathbf{q},k_z)[1+\cosh(qd/2)]-\sinh(qd/2)\ , \tag{23}$$

$$b(\mathbf{q},k_z)=S'(\mathbf{q},k_z)[1+\cosh(qd/2)]\ , \tag{24}$$

where $n^{(3)}$ denotes the two-dimensional density of interface states, and the structure factors S and S' are defined by

$$S(\mathbf{q},k_z)=\frac{\sinh(qd)}{\cosh(qd)-\cos(k_zd)}\ , \tag{25}$$

$$S'(\mathbf{q},k_z)=\frac{2\cos(k_zd/2)\sinh(qd/2)}{\cosh(qd)-\cos(k_zd)}\ . \tag{26}$$

For simplicity we have also defined the mass of interface states $m^{(3)}$ by

$$1/m^{(3)}=P/m^{(1)}+(1-P)/m^{(4)} \tag{27}$$

without taking into account different masses of electrons and light holes in computation. P is the integrated probability of finding electrons in the HgTe layer. Solving Eq. (22), we obtain

$$\omega_\pm^2=[\omega_p^{(3)}(q)]^2[a(\mathbf{q},k_z)\pm b(\mathbf{q},k_z)]\ , \tag{28}$$

where

$$[\omega_0^{(3)}(q)]^2=(2\pi e^2 n^{(3)}/\epsilon_s m^{(3)})q \ .$$

In the weak-coupling limit, $qd \gg 1$, Eq. (28) reduces to

$$\omega_+^2=[\omega_p^{(3)}(q)]^2\cos^2(k_z d/4) \ , \qquad (29)$$

$$\omega_-^2=[\omega_p^{(3)}(q)]^2\sin^2(k_z d/4) \ . \qquad (30)$$

The spectrum is then severed in the region $qd \gg 1$ for the reason of overlap of wave functions at the interfaces. Each layer only partly supports its own 2D plasmon, and the excitation in any layer will not remain localized at that layer.

In the strong-coupling limit, $qd \ll 1$, we have three cases to consider as a result of nonanalytic property of the structure factors at the origin of the q-k_z plane in Eqs. (25) and (26). First we consider $k_z=0$. From Eq. (28) we have

$$\omega_+=\Omega_p^{(3)} \ , \qquad (31)$$

$$\omega_-=0 \ , \qquad (32)$$

where

$$(\Omega_p^{(3)})^2=(8\pi e^2 n^{(3)}/\epsilon_s m^{(3)} d) \ .$$

The first mode clearly exhibits the characteristic of 3D optical plasmon, in which the oscillating charge densities are in phase from one supercell to the next, and are out of phase within the supercell. In the second mode, the oscillating charge densities are in phase within the supercell and also between supercells, so that they entirely cancel each other in the whole region for $k_z=0$, due to the localization of interface states at the same interfaces, and the gap of the spectrum between the collective and single-particle intrasubband excitation disappears.

Next, we consider the strong-coupling limit with $k_z \neq 0$. Thus Eq. (28) leads to

$$\omega_0^2=[\omega_p^{(3)}(q)]^2 qd\left[\frac{4\cos^2(k_z d/4)}{1-\cos(k_z d)}-\frac{1}{2}\right] , \qquad (33)$$

$$\omega_-^2=[\omega_p^{(3)}(q)]^2 qd\left[\frac{4\sin^2(k_z d/4)}{1-\cos(k_z d)}-\frac{1}{2}\right] , \qquad (34)$$

so that both branches are acoustical modes, with $\omega \propto q$. The modes, corresponding to in-phase and out-of-phase motion within the unit supercell, are softened. The bandwidth has a maximum for small qd, owing to the strong coupling.

Finally, we consider the strong-coupling limit with $k_z d=(2n+1)\pi$. In this case, Eq. (28) takes the form

$$\omega_+^2=\omega_-^2=[\omega_p^{(3)}(q)]^2 qd/2 \ ; \qquad (35)$$

the modes are degenerate 3D acoustical plasmons. Here the spectrum in the region $qd \ll 1$ shows some analogy to that derived by Tselis and Quinn,[5] and the results above are shown in Fig. 1. Here the single-particle continuum

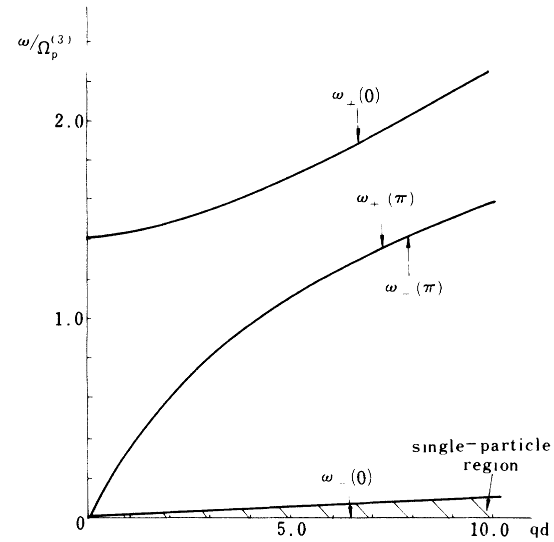

FIG. 1. Collective intrasubband excitation spectrum of interface states with zero-width localization.

region is very close to $\omega=0$ under the normalization, which is shown in all the graphs of this paper.

If we further consider the effect given by different masses and densities of electrons and light holes, the degenerate modes, when $k_z d=\pi$, will be split analogous to the phonon modes in a periodic 1D chain,[23] and the bandwidth is largely reduced (see Fig. 2).

We also present the graphs of ω as a function of $k_z d$ for different values of qd in Fig. 3. From it we can easily see the existence of degenerate modes as $k_z d=\pi$, and the bandwidth is broadened with fixed k_z as qd increases.

In order to gain an insight into the collective-excitation spectrum of the real system with finite width of localiza-

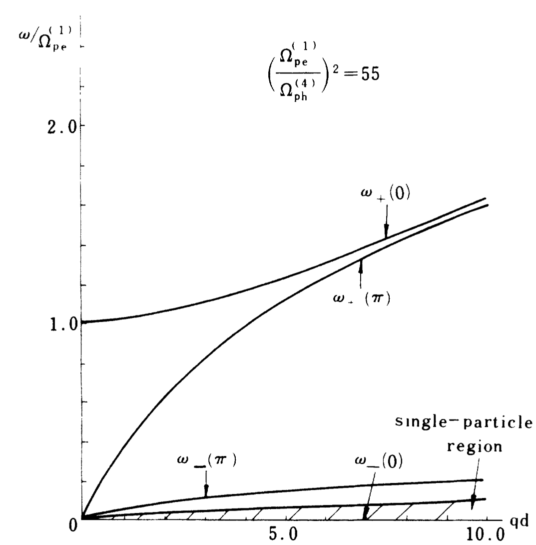

FIG. 2. Collective intrasubband excitation spectrum of interface states in perfect 2D interfaces with different masses and densities of electrons and light holes.

tion at interfaces, the symmetrical ground state can be written as[14]

$$\psi_0^{(3)}(z)=\begin{cases} De^{kd/4}(e^{kz}+e^{-kd}e^{-kz}), & -3d/4\le z\le -d/4 \\ De^{-kd/4}(e^{kz}+e^{-kz}), & -d/4\le z\le d/4 \\ De^{kd/4}(e^{-kz}+e^{-kd}e^{kz}), & d/4\le z\le 3d/4\ , \end{cases} \tag{36}$$

with the normalization factor

$$D=\frac{e^{kd/4}}{[d+2\sinh(kd/2)/k]^{1/2}}\ . \tag{37}$$

Here we set $k_{\rm HgTe}=k_{\rm CdTe}=k$ in the calculation for simplicity. The substitution of Eq. (36) reduces Eqs. (12) and (13) to the form

$$\omega_\pm^2=[\omega_p^{(3)}(q)]^2[(S\pm S')B+(A-B)]\ , \tag{38}$$

with

$$A=\frac{4(2+e^{-kd/2})}{[d+2\sinh(kd/2)/k]^2}\left[\frac{2q}{q^2-4k^2}\left[\frac{\sinh(kd/2)}{k}+\frac{\sinh(kd)}{4k}+\frac{d}{4}\right]+\frac{1}{q}[d+2\sinh(kd/2)/k]\right.$$
$$-\left[\frac{e^{-(2k+q)d/4}}{2k+q}-\frac{e^{-(2k-q)d/4}}{2k-q}+\frac{2e^{-qd/4}}{q}\right]$$
$$\left.\times\left[\frac{\sinh(2k+q)d/4}{2k+q}+\frac{\sinh(2k-q)d/4}{2k-q}+\frac{2\sinh(qd/4)}{q}\right]\right]\ , \tag{39}$$

$$B=\frac{4(2+e^{-kd/2})}{[d+2\sinh(kd/2)/k]^2}\left[\frac{\sinh(2k+q)d/4}{2k+q}+\frac{\sinh(2k-q)d/4}{2k-q}+\frac{2\sinh(qd/4)}{q}\right]^2\ . \tag{40}$$

In the weak-coupling limit, Eq. (38) reduces to

$$\omega_+^2=\omega_-^2=\frac{(2+e^{-kd/2})[\Omega_p^{(3)}]^2}{[1+2\sinh(kd/2)/kd]^2}\times\left[\frac{4\sinh(kd/2)}{kd}+\frac{\sinh(kd)}{2kd}+\frac{3}{2}\right]\ , \tag{41}$$

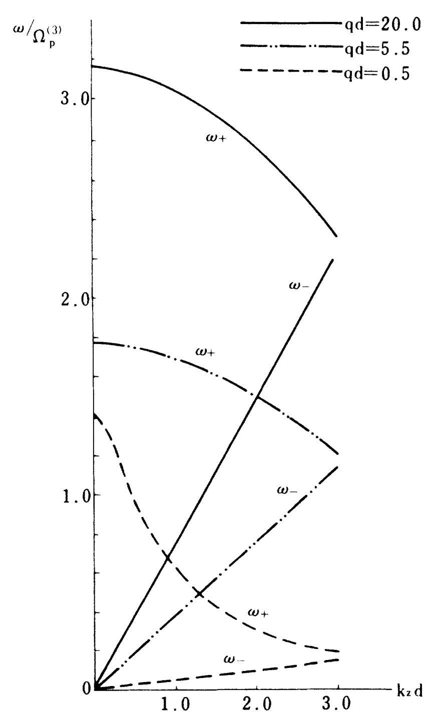

FIG. 3. Collective intrasubband excitation spectra of interface states in purely 2D interfaces as a function of $k_z d$ for different values of qd.

so that they are localized bulklike optical plasmons in which each layer supports a common modulated 3D plasmon, and that is quite different from those in Eqs. (29) and (30) (see Fig. 4).

In the strong-coupling limit we have two cases to study. When $k_z=0$, from Eq. (38) we have

$$\omega_+^2=[\omega_p^{(3)}(q)]^2[4\alpha/qd+(\beta+\alpha d/4+4\gamma/d)q]\ , \tag{42}$$

$$\omega_-^2=[\omega_p^{(3)}(q)]^2(\beta+\alpha d/4)q\ , \tag{43}$$

with the parameters

$$\alpha=2+e^{-kd/2} \tag{44}$$

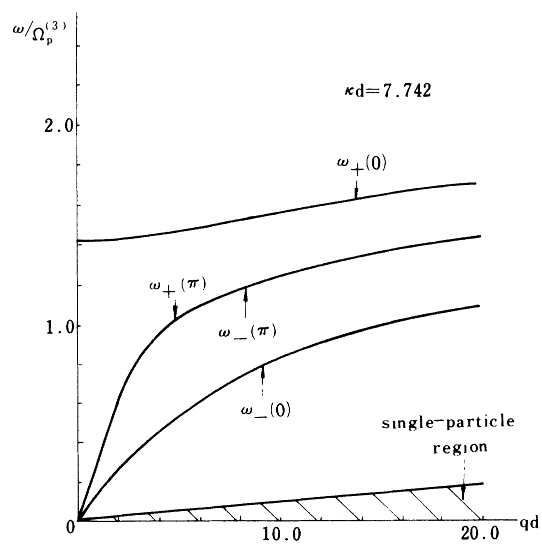

FIG. 4. Collective intrasubband excitation spectrum of interface states with finite width of localization at interfaces.

$$\beta=\frac{-4\alpha d}{[1+2\sinh(kd/2)/kd]^2}\times\left[\frac{1}{24}+\frac{\sinh(kd/2)}{4kd}-\frac{\cosh(kd/2)-\cosh(kd)/4}{2k^2d^2}+\frac{\sinh(kd/2)-\sinh(kd)/8}{k^3d^3}\right], \qquad (45)$$

$$\gamma=\frac{\alpha d^2}{[1+2\sinh(kd/2)/kd]}\times\left[\frac{1}{48}+\frac{\sinh(kd/2)}{8kd}-\frac{\cosh(kd/2)}{k^2d^2}+\frac{\sinh(kd/2)}{k^3d^3}\right]. \qquad (46)$$

The first mode is of the property of 3D optical plasmon and the restoring force is increased due to the out-of-phase motion at the interfaces, while the second mode is acoustical mode, in which the gap of the spectrum is still retained.

Secondly, we study the case with $k_z\neq 0$. Thus Eq. (38) has the solutions

$$\omega_+^2=[\omega_p^{(3)}(q)]^2\left[\frac{2\alpha d\cos^2(k_zd/4)}{1-\cos(k_zd)}+\beta\right]q\ , \qquad (47)$$

$$\omega_-^2=[\omega_p^{(3)}(q)]^2\left[\frac{2\alpha d\sin^2(k_zd/4)}{1-\cos(k_zd)}+\beta\right]q\ , \qquad (48)$$

so that both branches are acoustical modes. Especially, for $k_zd=(2n+1)\pi$, we get the degenerate modes of modulated 3D acoustical plasmons

$$\omega_+^2=\omega_-^2=[\omega_p^{(3)}(q)]^2(\beta+\alpha d/2)q\ , \qquad (49)$$

and the oscillations of electrons and light holes with the opposite phases and the same masses and densities within the adjacent layers can not be distinguished. As it is seen from Figs. 4 and 5 the optical modes will possess more properties of bulklike plasmon in the whole region as kd decreases.

The criterion for the transition behavior from 2D to 3D system can be clearly described as follows: the screening length of Coulomb interaction should be much smaller than the width of localization at the interfaces to ensure the sufficient overlap of wave functions.

In fact, the solution (38) will exactly reduce to Eq. (28) as the condition $kd \gg qd$ is satisfied well.

Moreover, if the effect of different masses and densities of electrons and light holes is taken into account, the degenerate modes for $k_zd=(2n+1)\pi$ will be further split, and the bandwidth becomes much smaller (see Fig. 6).

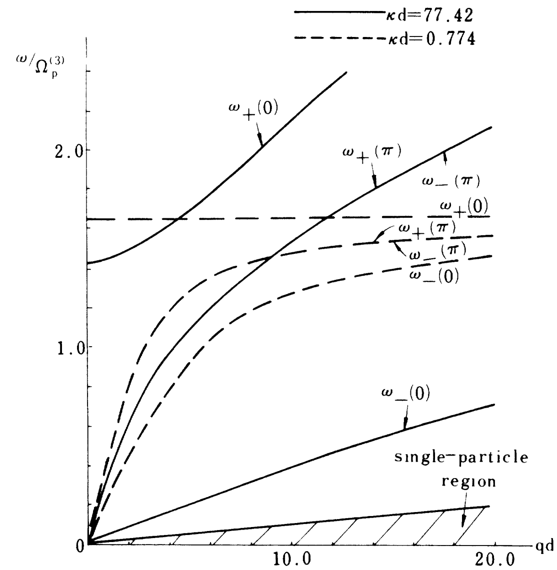

FIG. 5. Collective intrasubband excitation spectrum of interface states with finite width of localization and different values of kd.

The characteristic of bulk material possessed by optical mode seems to be more clear with fixed value of kd.

On the other hand, we are even more interested in the situation in which the interface states are strongly coupled with the heavy-hole-like states with infinitely thin charge layer thickness. In that case, we let $s,s'=2,3$ and $m=n=0$ in Eqs. (12) and (13), and easily get the solutions of intrasubband modes. When $k_z=0$, we have

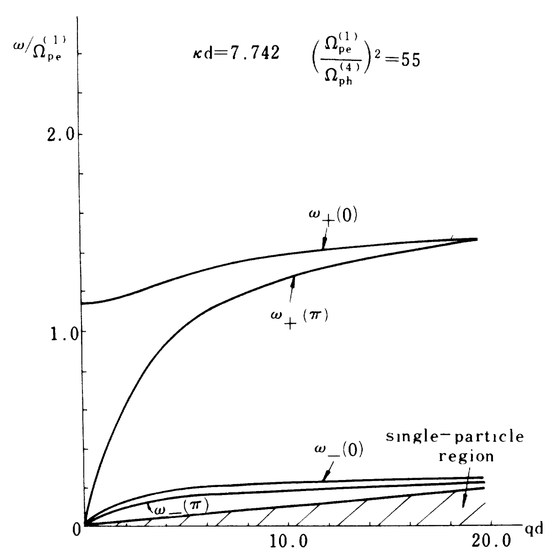

FIG. 6. Collective intrasubband excitation spectrum of interface states in quasi-2D interfaces with different masses and densities of electrons and light holes.

$$\omega_1^2=0\ , \tag{50}$$

$$\omega_{2,3}^2=\{[\omega_p^{(2)}(q)]^2S(\mathbf{q},k_z)+2[\omega_p^{(3)}(q)]^2a(\mathbf{q},k_z)\}/2$$
$$\pm(-\{[\omega_p^{(2)}(q)]^2S(\mathbf{q},k_z)+2[\omega_p^{(3)}(q)]^2a(\mathbf{q},k_z)\}^2-8[\omega_p^{(2)}(q)]^2[\omega_p^{(3)}(q)]^2\{a(\mathbf{q},k_z)S(\mathbf{q},k_z)-2[c(\mathbf{q},k_z)]^2\})^{1/2}/2\ , \tag{51}$$

with

$$c(\mathbf{q},k_z)=S(\mathbf{q},k_z)\cosh(qd/4)-\sinh(qd/4) \tag{52}$$

and $a(\mathbf{q},k_z)$, $S(\mathbf{q},k_z)$ defined above.

For $k_zd=(2n+1)\pi$, Eqs. (12) and (13) have the solutions

$$\omega_1^2=[\omega_p^{(3)}(q)]^2a(\mathbf{q},k_z)\ , \tag{53}$$

$$\omega_{2,3}^2=\{[\omega_p^{(2)}(q)]^2S(\mathbf{q},k_z)+2[\omega_p^{(3)}(q)]^2a(\mathbf{q},k_z)\}/2$$
$$\pm(\{[\omega_p^{(2)}(q)]^2S(\mathbf{q},k_z)+2[\omega_p^{(3)}(q)]^2a(q,k_z)\}^2-8[\omega_p^{(2)}(q)]^2[\omega_p^{(3)}(q)]^2\{a(q,k_z)S(q,k_z)-2[c(q,k_z]^2\})^{1/2}/2\ . \tag{54}$$

In the region $qd \gg 1$, the collective-excitation spectrum of interface states is still sharply severed. The excitation in the layer cannot be localized at that layer. However, each HgTe layer can fully support its own 2D plasmon for heavy-hole-like subbands (see Fig. 7).

In the strong-coupling limit we have one optical mode ($k_zd=0$) and two split acoustical modes ($k_zd=\pi$) for interface states due to the interaction with heavy-hole-like states. It is noted that the optical mode of heavy-hole-like states completely vanishes in the region $qd \ll 1$, and the gap of the spectrum between the collective and single-particle intrasubband excitation for interface states, we think, will remain for the case with finite width of localization. The features in strong-coupling region are fascinating and are quite different from those in type-I and -II superlattices,[5] as sketched in Fig. 8.

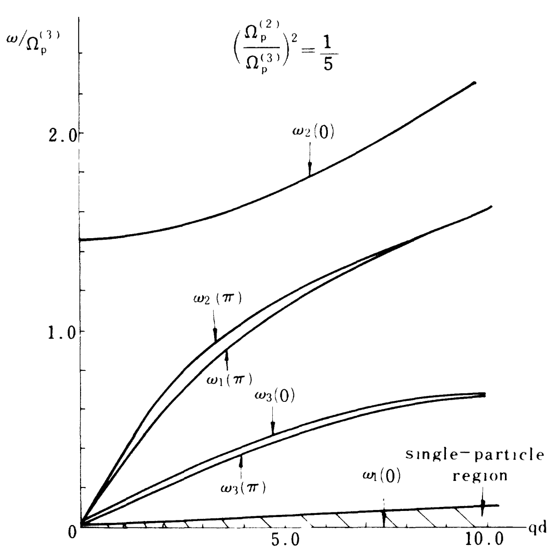

FIG. 7. Coupled collective intrasubband excitation spectra of interface and heavy-hole-like states with infinitely thin layer thickness and zero-width localization.

IV. CONCLUSIONS AND DISCUSSION

In this paper we have presented a survey of the electronic collective excitation in type-III superlattice including the interaction between the interface states and heavy-hole-like subbands. A rich spectrum of excitations is found, such as, localized modulated 3D optical and acoustical plasmons, etc.

We have shown that the intrasubband modes display the evident crossover behavior from 2D to 3D in the whole region as the width of localization increases.

In our work we have not considered the penetrating effect between the adjacent quantum wells, the exchange-correlation potential, and the overlap between the interface states and the other SL states; in that case we should use the Bloch sum of tight-binding functions instead of the sum of plane waves. For systems in which the layers are thin, such overlap is important. When the layer thickness is large enough, on the other hand, HgTe/CdTe superlattices will behave exactly like a semimetal, and the SCF method used here cannot be applicable. In general,

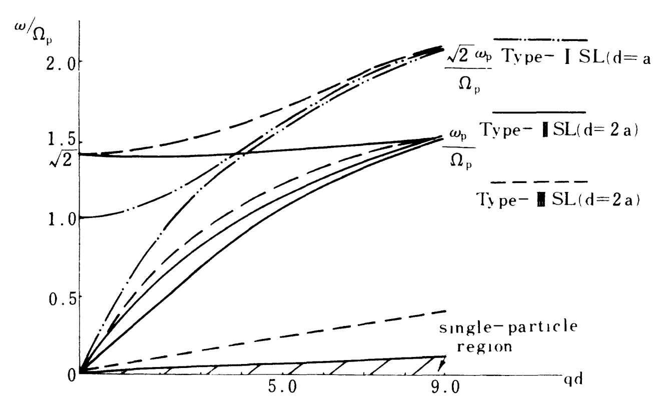

FIG. 8 Collective intrasubband excitation spectra of type-I and -II superlattices in purely 2D charge layers with same masses and densities of electrons and holes.

if we fully count in the contributions of all the SL states in calculation, we will get six spectra for intrasubband excitations, although some of them will be submerged, it is possible to finish the calculations of the spectra by performing a numerical analysis. It would be interesting and important to include the effects of the surface plasmons in a semi-infinite semiconductor superlattice on the linear response of the system. Work in these respects is in progress.

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