Rigorous excitonic theory of field dependent superlattice absorption

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Abstract: We have performed calculations of the field dependent excitonic absorption spectra of semiconductor superlattices in a model which is capable of fully taking into account the Coulomb interaction and both bound and continuum excitonic states. Results are obtained for the complete range of fields from the Franz-Keldysh to the Wannier-Stark regime. The lineshapes of the excitonic spectra are shown to resemble the derivative of the corresponding single particle spectra with respect to the wavelength. In addition characteristic excitonic features have been found, which also have been observed in photocurrent spectra.

Since the first observation of the Wannier-Stark effect in semiconductor superlattices (SL) [1] the electric field dependent properties of such structures have been a matter of continued interest. The crucial point is that the electric field induces a change in the dimensionality of the dynamics of the system. In the zero field limit the electronic states are split into minibands with quasi continuous energy and wavefunctions delocalized in all three dimensions. The states, however, become localized and discrete in energy, if an electric field is applied in SL direction. In the optical properties the latter effect leads to the well known Wannier-Stark (WS) ladder transitions, whereas in the former case M_0 and M_1 critical point behaviour and — for small enough fields — Franz-Keldysh oscillations can be observed [2].

A single particle theory accounts well for a qualitative description of the basic effects [3]. In this approximation the WS ladder is evenly spaced, where $\hbar\omega_n = \hbar\omega_0 + neFd$ is the energy of the n -th transition. $\hbar\omega_0$ is determined by the difference of the center of mass energies of the corresponding electron and hole minibands. The oscillator strengths of the individual transitions undergo characteristic changes as the field decreases and finally reduce to Franz-Keldysh (FK) like oscillations of the absorption [4]. For minibands with bandwidth considerably larger than the exciton binding energy this approach even gives good quantitative results [5], since the excitonic corrections to the shape of the spectra are small except for the miniband edges.

However, detailed understanding of the spectra requires the inclusion of excitonic effects [6]. Here, we treat the full two particle Hamiltonian (neglecting exchange terms)

$$\hat{H} = \hat{H}_{0c} + \hat{H}_{0v} + eF(z_e - z_h) - \frac{e^2}{\kappa_0 |\mathbf{r}_e - \mathbf{r}_h|}, \quad (1)$$

FIG. 1. Comparison of absorption spectra for $F = 20$ kV/cm calculated in the single particle and the excitonic model. The Wannier-Stark transitions are marked by numbers. E_0 and E_1 are the lower and upper combined miniband edges.

where $\hat{H}_{0e}$ and $\hat{H}_{0v}$ are the SL Hamiltonians of electron and hole, respectively. The exciton wavefunction $\Psi^{X,F}(\mathbf{r}_e, \mathbf{r}_h)$ is expanded into coupled electron-hole SL Kane states of field F [7, 3], where we have restricted ourselves to the lowest electron and heavy hole miniband

$$\Psi^{X,F}(\mathbf{r}_e, \mathbf{r}_h) = \sum_{\rho, \mathbf{k}_{\parallel}} \Phi_{\rho}^X(\mathbf{k}_{\parallel}) \cdot \underbrace{\frac{1}{\sqrt{N}} \sum_{\rho'} \phi_{c, \rho'}^F(\mathbf{r}_e) \cdot \phi_{hh, \rho' + \rho}^F(\mathbf{r}_h) \cdot e^{i\mathbf{k}_{\parallel} \mathbf{r}_{\parallel}}}_{\psi_{\rho, \mathbf{k}_{\parallel}}^F(\mathbf{r}_e, \mathbf{r}_h)}, \quad (2)$$

where $\phi_{c, \rho'}^F(\mathbf{r}_e)$ and $\phi_{hh, \rho' + \rho}^F(\mathbf{r}_h)$ denote the electron and hole Kane states of field F centered at the lattice sites ρ' and $\rho' + \rho$, respectively. In the expansion the Bloch theorem for the exciton states has been used and the fact that only excitons with vanishing center of mass quasi momentum contribute to the absorption [8]. $\mathbf{r}_{\parallel}$ is the in-plane separation of electron and hole. The miniband dispersion used in the Kane states [7] is obtained by the Kronig-Penney model, the in-plane dispersion is assumed to be parabolic. By the above approach both bound and continuous exciton states are included implicitly.

The further treatment is analogous to that of Chuang et al [9]. One obtains an integral equation for the amplitudes $\Phi_{\rho}^X(\mathbf{k}_{\parallel})$. The absorption α is proportional to

$$\alpha(\omega) \propto \frac{1}{\omega} \int dE_X \left| \sum_{\rho, \mathbf{k}_{\parallel}} \Phi_{\rho}^X(\mathbf{k}_{\parallel}) \cdot \mu_{\rho}(\mathbf{k}_{\parallel}) \right|^2 \delta_{\Gamma}(\hbar\omega - E_X), \quad (3)$$

where $\mu_{\rho}(\mathbf{k}_{\parallel})$ is the dipole matrix element of the basis state $\psi_{\rho, \mathbf{k}_{\parallel}}^F(\mathbf{r}_e, \mathbf{r}_h)$ and $\delta_{\Gamma}(E)$ a broadened δ -function introducing a phenomenological broadening of the spectra with a parameter Γ .

Fig. 1 shows a typical result of the calculations with and without inclusion of the Coulomb interaction. The single particle spectrum consists of a series of ascending steps corresponding to the WS transitions as it is typical for a quasi two dimensional system. In the excitonic spectra, however, each WS transition contributes with an excitonic peak making the spectra similar in shape to the derivative of the single particle absorption.

In Fig. 2 a set of calculated excitonic absorption spectra for various electric fields is compared with the derivative of the absorption as obtained from the single particle model. The sample under consideration consist of an alternating series of 12 monolayers of GaAs and 6 monolayers of AlAs resulting in a calculated combined electron and heavy hole miniband width of $\Delta E = 23\text{meV}$. The

FIG. 2. Excitonic absorption spectra (a) and single particle spectra of the differentiated absorption (b), for various fields. The transitions are labelled by numbers, the combined miniband edges by E_0 and E_1 . The arrows in the excitonic spectra mark the characteristic shoulders at the onset of the continuum exciton states as described in the text.

parameters have been chosen such that the miniband width is larger than the two and three dimensional exciton Rydberg energies, which are about 16 meV and 4 meV, respectively. This allows to investigate the absorption behaviour related to the delocalized miniband states as well as localization effects due to the electric field.

For high fields the peaks in the single particle spectra mark the exact energetic positions of the WS ladder transitions. The transition energies move equal to $neFd$ (n being the number of the ladder state) as the field decreases. The excitonic spectra are also decoupled into a series of peaks corresponding to the excitonic ground states of the individual electron-hole WS levels. The exciton binding energies (Fig. 3) which are given by the difference between the peak energies of the excitonic and the single particle spectra decrease with the field due to an increasing extension of the wavefunctions in SL direction. The transition strengths for larger $|n|$ decay more rapidly in the excitonic spectra, which is a consequence of the Coulomb attraction tending to localize the electron and hole close to each other. For fields high enough a shoulder in the absorption is found above each exciton peak which moves almost parallel to the excitonic transition immediately below. In Figs. 1 and 2a it is clearly resolved for the $n = 0$ transition for fields above 20 kV/cm and appears as a broadening of the $n = 2$ level on the low energy side for the $n = 1$ transition (marked by arrows in the figures). It consists of both higher bound and continuum states of the exciton, as it lies about 1 meV below the corresponding WS ladder transition energy. Such structure, which is of purely

FIG. 3. Wannier-Stark fan as derived from the calculated spectra. Full lines: Wannier-Stark ladder transitions; circles: excitonic ground state transitions. In the FK regime the peaks can no longer be associated with individual WS transitions.

excitonic origin, has also been observed in experimental spectra [10].

With decreasing field the oscillator strengths of both the single particle and the excitonic transitions become modulated in a characteristic way [5]. These structures result in the miniband FK oscillations, when the separation between the WS transitions becomes smaller than the broadening of the levels. Each maximum of the absorption then consists of a couple of WS peaks rather than one single transition. In the vicinity of the miniband edges the transition strengths are strongly enhanced leading to peaks, which are field independent in position and finally turn into the M_0 and M_1 excitons of the miniband.

In conclusion, we have calculated the excitonic absorption spectra of semiconductor superlattices by diagonalizing the electron-hole Hamiltonian with the Coulomb interaction fully included. The excitonic absorption spectra resemble the derivative of the corresponding single particle spectra with respect to the photon energy. There are important excitonic features resulting in additional structure in the absorption spectra like a shoulder marking the onset of the continuous states of the exciton. Quantitative agreement with the experimental spectra can only be obtained if the Coulomb interaction is taken into account.

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