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Conversion of hole states by acoustic solitons

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The hole states in the valence band of a large class of semiconductors are degenerate in the projections of angular momentum. Here we show that the switching of a hole between the states can efficiently be realized by acoustic solitons. The microscopic mechanism of such a state conversion is related to the valence-band splitting by local elastic strain. The conversion is studied here for heavy holes localized at shallow and deep acceptors in silicon quantum wells.

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I. INTRODUCTION

The strain-induced effects have been proved to be an efficient tool to study basic properties of semiconductor structures yielding information on their point-group symmetry, band parameters, spin-orbit coupling, etc.[1,2] During the last decade the possibility emerged to study such effects in nanostructures on the extremely short time scale of picosecond range. This could be done employing acoustic solitary waves (solitons).[3–6] The acoustic soliton is a pulse of strong nonlinear elastic strain propagating along the crystal with the velocity larger than the sound speed.[7] Due to rather high values of deformation-potential constants in semiconductors, such a local strain efficiently modifies the band structure and thereby interacts with charge carriers. The important point is that, unlike linear acoustic waves, the soliton-type strain does not change its sign within the pulse.[3,7] Therefore, after the soliton has passed through the sample, the electron state of a system may differ from the initial one.

In this paper we show that, in semiconductor structures where the electron or hole states are degenerate in the absence of strain, acoustic solitons can cause a transition of carriers between these quantum-mechanical states. We study such a state conversion for heavy holes localized at acceptors in quantum wells (QWs). The ground state of localized holes in most of the cubic semiconductors is degenerate in the projection of the angular momentum because of the complex structure of the valence band. We show that the propagation of the acoustic soliton of a certain amplitude through the area of hole localization changes the projection of the hole angular momentum. The effect of state conversion, particularly between two easily distinguished states, is of interest not only from fundamental point of view but can also be utilized for the information processing and storage.

The acoustic soliton represents a perturbation of purely mechanical origin, therefore, in the first approximation it does not interact with the carrier spin. Accordingly, it is convenient to consider the effect of state conversion for semiconductor structures with negligible spin-orbit interaction (such as Si, SiC, etc). Below we focus on silicon-based quantum wells although the main conclusions can be generalized to other systems. The paper is organized as follows. Section II is devoted to the calculation of ground hole states in QWs with weak spin-orbit coupling. In Sec. III, we consider the effect of an acoustic soliton on the hole states and show that it leads to switching the hole between different quantum-mechanical states. In Sec. IV, we demonstrate that such a state conversion can be fruitfully considered as a precession of hole pseudospin.

II. TWO-DIMENSIONAL HOLE STATES IN Γ_{25}' BAND

We neglect spin-orbit coupling and, therefore, assume that in bulk material the valence-band states at the center of the Brillouin zone belong to the representations Γ_{25}' or Γ_{15} and denote the basis functions as X, Y, and Z. Due to quantum confinement, the heavy-hole states in a structure grown along the z axis are formed from the Bloch amplitudes X and Y,[8] while the light-hole states are formed from the Z amplitude. The corresponding wave functions of heavy holes have the form

$$\Psi(\boldsymbol{r}) = \alpha(\boldsymbol{\rho})u(z)X + \beta(\boldsymbol{\rho})u(z)Y, \tag{1}$$

where $\alpha(\boldsymbol{\rho})$ and $\beta(\boldsymbol{\rho})$ are smooth envelopes in the QW plane, which can be combined into a two-component column $\psi(\boldsymbol{\rho})=[\alpha(\boldsymbol{\rho}),\beta(\boldsymbol{\rho})]^T$, $\boldsymbol{\rho}=(x,y)$ is the in-plane coordinate, $u(z)$ is the function of size quantization, x, y, and z are the cubic axes. We note that each state [Eq. (1)] is degenerate in spin and the spin index is omitted for simplicity. Such a description of hole states in QWs is valid for structures where the energy separation between the heavy-hole and light-hole subbands exceeds the energy of spin-orbit coupling.

The envelope functions $\psi(\boldsymbol{\rho})$ of a hole localized at an acceptor in a narrow quantum well can be found by solving the matrix Schrödinger equation $\hat{H}\psi(\boldsymbol{\rho})=E\psi(\boldsymbol{\rho})$, where $\hat{H}$ is the effective Hamiltonian assuming in the spherical approximation the form

$$\hat{H} = \gamma\begin{bmatrix} \boldsymbol{k}^2 & 0 \\ 0 & \boldsymbol{k}^2 \end{bmatrix} + \gamma'\begin{bmatrix} k_x^2 - k_y^2 & 2k_xk_y \\ 2k_xk_y & k_y^2 - k_x^2 \end{bmatrix} + U(\boldsymbol{\rho})\hat{I}. \tag{2}$$

Here $\boldsymbol{k}=(k_x,k_y)$ is the momentum operator divided by the reduced Planck constant $\hbar$, γ and γ' are the band parameters which are expressed in terms of the parameters L and M (see Ref. 1) via $\gamma=(L+M)/2$ and $\gamma'=(L-M)/2$, $U(\boldsymbol{\rho})$ is the attractive potential of the acceptor, and $\hat{I}$ is the unit matrix 2×2. We assume the acceptor potential $U(\boldsymbol{\rho})$ to be isotropic.

Then, the hole states are described by the quantum number $n(n=0,1,2,\ldots)$ and the projection of the orbital angular momentum onto the z axis $j(j=0,\pm1,\pm2,\ldots)$. The state with the projection j can be presented as a superposition of the Bloch amplitudes $(X+iY)/\sqrt{2}$ and $(X-iY)/\sqrt{2}$ multiplied by the envelope functions $\eta_{nj}(\rho)e^{i(j-1)\varphi}$ and $\xi_{nj}(\rho)e^{i(j+1)\varphi}$, respectively, where $\boldsymbol{\rho}=(\rho,\varphi)$ are the polar coordinates in the QW plane. The corresponding two-column envelope functions $\psi_{nj}(\boldsymbol{\rho})$ are given by

$$\psi_{nj}(\boldsymbol{\rho}) = \frac{e^{i(j-1)\varphi}}{\sqrt{2}}\begin{bmatrix} \eta_{nj}(\rho) + \xi_{nj}(\rho)e^{2i\varphi} \\ i\eta_{nj}(\rho) - i\xi_{nj}(\rho)e^{2i\varphi}\end{bmatrix}, \tag{3}$$

where $\eta_{nj}(\rho)$ and $\xi_{nj}(\rho)$ satisfy the equation set

$$\gamma\left[\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{(j+1)^2}{\rho^2}\right]\xi_{nj}(\rho)+\gamma'\left[\frac{d^2}{d\rho^2}+\frac{1-2j}{\rho}\frac{d}{d\rho} + \frac{j^2-1}{\rho^2}\right]\eta_{nj}(\rho)=[U(\rho)-E_{nj}]\xi_{nj}(\rho),$$

$$\gamma'\left[\frac{d^2}{d\rho^2}+\frac{1+2j}{\rho}\frac{d}{d\rho}+\frac{j^2-1}{\rho^2}\right]\xi_{nj}(\rho)+\gamma\left[\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho} - \frac{(j-1)^2}{\rho^2}\right]\eta_{nj}(\rho)=[U(\rho)-E_{nj}]\eta_{nj}(\rho). \tag{4}$$

E_{nj} is the energy of the state $\psi_{nj}(\boldsymbol{\rho})$ measured from the subband edge. We note that the states (n,j) and $(n,-j)$ have the same energy and their envelope functions are related by $\psi_{n,-j}(\boldsymbol{\rho})=\psi^*_{n,j}(\boldsymbol{\rho})$. From Eq. (3) it follows that only the states with $j=\pm1$ contain envelope functions of s type which are nonzero at the acceptor and efficiently overlap with the acceptor attractive potential. Therefore, the ground state of localized holes is degenerate in the projection of orbital angular momentum and described by the functions

$$\psi_{0,\pm1}(\boldsymbol{\rho}) = \frac{1}{\sqrt{2}}\begin{bmatrix} \eta_{0,1}(\rho)+\xi_{0,1}(\rho)e^{\pm2i\varphi} \\ \pm i\eta_{0,1}(\rho) \mp i\xi_{0,1}(\rho)e^{\pm2i\varphi}\end{bmatrix}. \tag{5}$$

Below we denote them as $\psi_{\pm}(\boldsymbol{\rho})$, respectively.

To elaborate the effect of state switching by an acoustic soliton we consider two models of the acceptor: (i) Coulomb potential $U(\rho)=-e^2/(\epsilon\rho)$, where e is the elementary charge and ϵ is the dielectric constant and (ii) zero-radius potential.[9,10] In the first case, the ground hole states and the localization energy $E_0>0$ are calculated numerically by solving Eq. (4). The latter approach allows us to find the states analytically for a given E_0 assuming that the range of attractive potential is much shorter than the hole localization length. Within this approach, solution of Eq. (4) for the ground state has the form

$$\eta_{0,1}(\rho)=\frac{\rho_1\rho_2}{\sqrt{2\pi(\rho_1^2+\rho_2^2)}}\left[\frac{K_0(\rho/\rho_1)}{\rho_1^2}+\frac{K_0(\rho/\rho_2)}{\rho_2^2}\right],$$

$$\xi_{0,1}(\rho)=\frac{\rho_1\rho_2}{\sqrt{2\pi(\rho_1^2+\rho_2^2)}}\left[\frac{K_2(\rho/\rho_1)}{\rho_1^2}-\frac{K_2(\rho/\rho_2)}{\rho_2^2}\right], \tag{6}$$

where $K_0(x)$ and $K_2(x)$ are the modified Bessel functions of the second kind (Macdonald functions), the radii ρ_1 and ρ_2 are given by $\rho_1=\sqrt{-(\gamma+\gamma')/E_0}$, $\rho_2=\sqrt{-(\gamma-\gamma')/E_0}$, and it is assumed that $\gamma+\gamma',\gamma-\gamma'<0$. The functions Eq. (6) can be obtained from Eq. (4) by the Fourier transformation method.

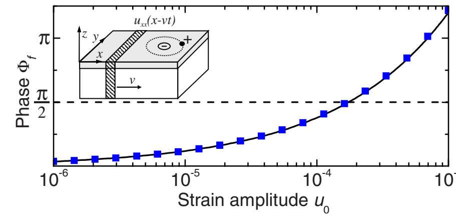

FIG. 1. (Color online) Dependence of the phase shift Φ_f on the strain amplitude u_0 calculated numerically for the Coulomb potential (squares) and plotted after Eq. (15) for the zero-radius potential (solid curve). Dashed line corresponds to $\Phi_f=\pi/2$ which is optimal for the state conversion. Inset sketches the propagation of strain soliton along the quantum well.

III. STATE CONVERSION BY ACOUSTIC SOLITON

In the absence of strain, the ground state is degenerate in the projection of angular momentum and the hole wave function represents a superposition of $\psi_+(\boldsymbol{\rho})$ and $\psi_-(\boldsymbol{\rho})$. The acoustic soliton lifts the degeneracy causing the transition of a hole between the above states.

The strain effect on the heavy-hole subband is described by the effective Hamiltonian[1]

$$\hat{V}=\begin{bmatrix} lu_{xx}+mu_{yy} & nu_{xy} \\ nu_{xy} & mu_{xx}+lu_{yy}\end{bmatrix}, \tag{7}$$

where l, m, and n are the deformation potential constants, $u_{\alpha\beta}$ are the strain tensor components. We consider that the bulk acoustic soliton propagates in the x direction along the quantum-well plane inducing time-dependent component $u_{xx}(x,t)$ of the strain tensor, see inset to Fig. 1. The strain pulse is assumed weak enough not to cause ionization of the localized hole or its transition to excited states. Then, according to the perturbation theory, the hole wave function $\psi(\boldsymbol{\rho},t)$ can be expanded over the nondisturbed states $\psi_{\pm}(\boldsymbol{\rho})$ as follows:

$$\psi(\boldsymbol{\rho},t)=c_+(t)\psi_+(\boldsymbol{\rho})+c_-(t)\psi_-(\boldsymbol{\rho}), \tag{8}$$

where the coefficients $c_j(t)(j=\pm)$ satisfy the coupled equations

$$i\hbar\frac{dc_+(t)}{dt}=V_{++}(t)c_+(t)+V_{+-}(t)c_-(t),$$

$$i\hbar\frac{dc_-(t)}{dt}=V_{-+}(t)c_+(t)+V_{--}(t)c_-(t), \tag{9}$$

and $V_{jj'}(t)=\int\psi_j^\dagger(\boldsymbol{\rho})\hat{V}\psi_{j'}(\boldsymbol{\rho})d\boldsymbol{\rho}$ are the matrix elements of the perturbation Eq. (7). The specific form of the functions Eq. (5) and the perturbation $V\propto u_{xx}(x,t)$ leads to the relations $V_{++}(t)=V_{--}(t)$ and $V_{+-}(t)=V_{-+}(t)$, which makes Eq. (9) easily solvable.

The solution of Eq. (9) assumes the form

$$c_+(t) = [a_+ \cos \Phi(t) - ia_- \sin \Phi(t)]e^{-i\Theta(t)},$$

$$c_-(t) = [a_- \cos \Phi(t) - ia_+ \sin \Phi(t)]e^{-i\Theta(t)}, \quad (10)$$

where $a_+=c_+(-\infty)$ and $a_-=c_-(-\infty)$ are coefficients of the initial state at $t=-\infty$, $\Phi(t)$ and $\Theta(t)$ are phases given by

$$\Phi(t) = \frac{1}{\hbar}\int_{-\infty}^{t} V_{+-}(t')dt', \quad \Theta(t) = \frac{1}{\hbar}\int_{-\infty}^{t} V_{++}(t')dt'. \quad (11)$$

It follows from Eq. (10) that it is the phase $\Phi(t)$ that describes the hole state evolution while $\Theta(t)$ constitutes the common phase factor. In the final state, i.e., at $t=+\infty$ when the soliton has completely passed through the area of hole localization, the phase shift has the form

$$\Phi_f = \frac{l-m}{2\hbar}\int \eta_{0,1}^2(\rho)d\boldsymbol{\rho}\int_{-\infty}^{+\infty} u_{xx}(x,t)dt. \quad (12)$$

Since the average value of the strain u_{xx} is nonzero within the soliton, $\Phi_f \neq 0$, and the final hole state differs from the initial one. The most efficient conversion of the hole state occurs if the soliton amplitude is so that

$$|\Phi_f| = \pi(n+1/2), \quad n=0,1,2,\ldots \quad (13)$$

In this particular case, the soliton-hole interaction results in the complete switching of the hole angular momentum: The initial state $\psi_+(\boldsymbol{\rho})$ is converted into the state $\psi_-(\boldsymbol{\rho})$ and vice versa, see Eq. (10).

Acoustic solitons in crystals are typically approximated by solutions of the Korteweg-de Vries (KdV) wave equation[3] or the doubly dispersive equation.[11] Since the particular soliton shape is not crucial for our results, we consider the KdV soliton so that u_{xx} has the form

$$u_{xx}(x,t) = u_0 \cosh^{-2}\left(\frac{x-vt}{L}\right), \quad (14)$$

where u_0 is the strain amplitude, v and $L=d/\sqrt{u_0}$ are the soliton velocity and size, respectively, and d is a material constant. In this case $\int_{-\infty}^{+\infty}u_{xx}(x,t)dt=2d\sqrt{u_0}/v$.

Figure 1 shows dependence of the phase shift Φ_f on the strain amplitude u_0. Squares correspond to the numerical calculation of Φ_f given by Eq. (12) for the Coulomb localizing potential, solid curve represents the analytical dependence

$$\Phi_f = \frac{l-m}{2\hbar}\frac{d\sqrt{u_0}}{v}\left[1 + \frac{\gamma^2-\gamma'^2}{2\gamma\gamma'}\ln\left(\frac{\gamma+\gamma'}{\gamma-\gamma'}\right)\right] \quad (15)$$

derived in the zero-radius-potential approach by integrating the wave function [Eq. (6)]. The band parameters of silicon used in the calculation are as follows: $\gamma=-4.65\hbar/(2m_0)$, $\gamma'=-1.13\hbar/(2m_0)$,[12] where m_0 is free-electron mass, the deformation-potential constants $l=-4.9$ eV and $m=-1.5$ eV.[1] The soliton parameters $d=1.5$ Å, $v=0.9\times10^6$ cm/s, and the strain amplitude u_0 in the range $10^{-6}-10^{-3}$ are chosen, which corresponds to experimental data on acoustic phonon pulses in silicon.[13]

From Fig. 1 it follows that the phase shift $\Phi_f=\pi/2$ optimal for the state conversion is achieved in Si-based structures at a moderate strain amplitude $u_0\approx1.8\times10^{-4}$. It proves that the hole states can be efficiently manipulated by acoustic solitons. Moreover, both Coulomb and zero-radius potentials lead to the same quantitative result indicating that Φ_f weakly depends on the form of localizing potential for silicon band parameters. This can be attributed to the fact that the envelope function of the ground heavy-hole state is mainly of s type even at $\gamma'/\gamma\approx0.24$. Therefore, the integral $\int\eta_{0,1}^2(\rho)d\boldsymbol{\rho}$ determining the conversion efficiency [see Eq. (12)] is approximately equal to 1 in accordance with the wave-function normalization and independent of the explicit form of $\eta_{0,1}(\rho)$.

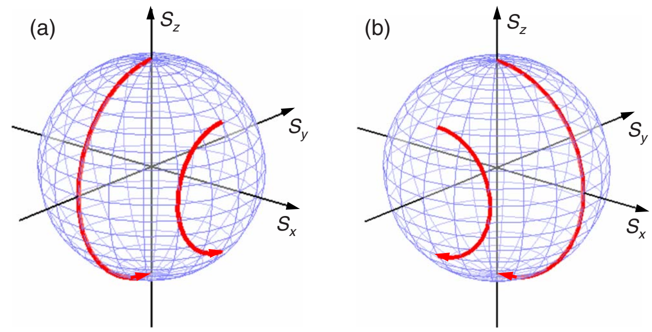

FIG. 2. (Color online) Trajectories on the Bloch sphere representing the time evolution of the hole state caused by acoustic soliton propagating along (a) x and (b) y axes. Different curves on each sphere correspond to different initial states. The trajectories connecting two poles depict the complete conversion of the hole state from $\psi_+(\boldsymbol{\rho})$ into $\psi_-(\boldsymbol{\rho})$.

For the strain amplitude $u_0=1.8\times10^{-4}$ optimal for the state conversion, the soliton length L is estimated as 110 Å that is approximately seven times larger than the radius of hole localization $a_0=e^2/(\epsilon E_0)\approx16$ Å in silicon quantum wells. In the approximation of $L\gg a_0$, the time evolution of the phase $\Phi(t)$ for the soliton shape [Eq. (14)] has the form

$$\Phi(t) = \Phi_f\frac{\tanh(vt/L)+1}{2}. \quad (16)$$

IV. PSEUDOSPIN REPRESENTATION

The soliton-induced evolution of a hole state can fruitfully be considered as a precession of pseudospin or a trajectory on the Bloch sphere. In this approach,[14] any superposition [Eq. (8)] of two states, $\psi_+(\boldsymbol{\rho})$ and $\psi_-(\boldsymbol{\rho})$, is attributed to a unit vector $\boldsymbol{S}$ or a point (S_x,S_y,S_z) on the sphere, see Fig. 2. The components of $\boldsymbol{S}$ are given by

$$\boldsymbol{S} = \chi^\dagger\boldsymbol{\sigma}\chi, \quad (17)$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices and χ is the spinor composed of the coefficients $c_+(t)$ and $c_-(t)$, $\chi=[c_+(t),c_-(t)]^T$. In particular, the pure states $\psi_+(\boldsymbol{\rho})$ and $\psi_-(\boldsymbol{\rho})$ correspond to the polar points (0,0,1) and (0,0,−1), respectively, while the states $[\psi_+(\boldsymbol{\rho})+e^{i\alpha}\psi_-(\boldsymbol{\rho})]/\sqrt{2}$ with arbitrary phase α are mapped onto the Bloch sphere equator.

During the soliton-hole interaction the coefficients $c_\pm$ vary in time, see Eq. (10), which corresponds to motion of the point (S_x, S_y, S_z) on the Bloch sphere. Equation describing the time evolution of $\boldsymbol{S}$ can be derived from Eq. (9). It gives

$$\frac{d\boldsymbol{S}}{dt} = [\boldsymbol{\Omega}(t) \times \boldsymbol{S}], \tag{18}$$

where $\boldsymbol{\Omega}(t) = (1/\hbar)\Sigma_{jj'} V_{jj'}(t)\boldsymbol{\sigma}_{j'j}$. For a given initial state $\boldsymbol{S}_0$ and $\boldsymbol{\Omega}(t)$, Eq. (18) allows one to calculate the trajectory $\boldsymbol{S}(t)$ and restore the wave function. Shown in Fig. 2 are examples of such trajectories under a soliton-induced uniaxial strain. The strain $u_{xx}(x,t)$ produced by soliton propagating along the x axis corresponds to $\boldsymbol{\Omega}(t) \| x$ and, therefore, causes $\boldsymbol{S}$ to rotate around the x axis [Fig. 2(a)] while the strain $u_{yy}(y,t)$ corresponds to $\boldsymbol{\Omega}(t) \| y$ leading to the rotation of $\boldsymbol{S}$ around the y axis [Fig. 2(b)]. In the case of complete conversion of the hole state from $\psi_+(\boldsymbol{\rho})$ into $\psi_-(\boldsymbol{\rho})$, the trajectories pass from one pole of the Bloch sphere to the other.

The time of switching the hole states is given by $\tau = 2(L + a_0)/v$. It is of picosecond scale and much less than the lifetime of localized holes at low temperatures as well as the soliton lifetime. It suggests that the effect can be studied experimentally by means of time- and space-resolved optical spectroscopy. Indeed, the states $\psi_+(\boldsymbol{\rho})$ and $\psi_-(\boldsymbol{\rho})$ are characterized by projections +1 and −1 of the orbital angular momentum, therefore, optical pumping by circularly polarized light leads to a predominant population of one of the states. The hole angular momentum can be registered in turn by analyzing the polarization of recombination radiation or the polarization change of a probe pulse (see, e.g., Ref. 15). The soliton propagation through the area of hole localization reverses the projection of hole angular momentum leading to a change in optical response. We note that ultrashort strain pulses in experiments consist typically of a few acoustic solitons ("soliton train") followed by bipolar oscillations[5] which can further modify the hole wave function. The detailed time-resolved study of the hole state evolution can provide information about the energy spectrum and relaxation times of localized holes as well as the strain pulse parameters.

To summarize, we have demonstrated the possibility of switching the quantum-mechanical state of a localized hole by an acoustic soliton. The amplitude of the strain soliton required for switching the hole states in silicon-based quantum wells is found to be $\approx 2 \times 10^{-4}$ which corresponds to strain pulses studied experimentally.

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