

Adaptive design of excitonic absorption in broken-symmetry quantum wells

Jason Thalken, Weifei Li, and Stephan Haas^{a)}

Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089

A. F. J. Levi

Department of Electrical Engineering and Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089

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Adaptive quantum design is used to identify broken-symmetry quantum-well potential profiles with optical response properties superior to previous *ad hoc* solutions. This technique performs an unbiased stochastic search of configuration space. It allows us to engineer many-body excitonic wave functions and thus provides a new methodology to efficiently develop optimized quantum-confined Stark effect device structures. © 2004 American Institute of Physics. [DOI: 10.1063/1.1768311]

Excitonic optical absorption at near-band-gap photon energies in III–V compound semiconductor quantum-well structures is of great interest for device applications. By applying an electric field perpendicular to the plane of the quantum well, the excitonic optical absorption strength and energy can be manipulated. This “quantum-confined Stark effect” (QCSE)¹ requires that electron confinement by the quantum well potential influences electric field dependent absorption. Compared to bulk semiconductors, the excitonic absorption strength in QCSE structures is greater, even in the presence of large externally applied electric field. This performance advantage is the reason why the QCSE has been used to design optical modulators and detectors.^{1–3} Typically, such designs make use of simple rectangular potential wells in the AlGaAs/GaAs or InP/InGaAsP material system. However, conventional *ad hoc* approaches to device design do not fully exploit the ability of modern crystal growth techniques to vary the quantum well potential profile on an atomic monolayer scale in the growth direction.

In this letter, we introduce an adaptive quantum design methodology that can be used to find a desired target response that is best suited for a QCSE device. In contrast to the conventional approach, we perform an unbiased search of design space to find the quantum well potential profile $V(x)$ that most closely approaches the target response. Because the model of exciton absorption is a many-body effect, the adaptive quantum design algorithm may be thought of as manipulating a many-body wave function to achieve a desired behavior by varying the potential profile, $V(x)$.

Here, we model the QCSE using a two band tight-binding Hamiltonian of the semiconductor single electron states and a variational method to find the exciton binding energy.⁴ The effective masses of the electron ($m_e^* = 0.067m_0$) and the heavy hole ($m_h^* = 0.34m_0$) determine the tight-binding hopping parameters $t_e = 1.787$ eV and $t_h = 0.35$ eV. The confining potentials are calculated using a band gap of $E_g = 1.43$ eV and an offset ratio of $\Delta E_c/\Delta E_v = 67/33$ between the conduction and the valence band. This model, evaluated on a discretized lattice with 100 sites, re-

produces the single particle energies and wave functions $\Psi_e(x_e)$ and $\Psi_h(x_h)$ of Ref. 4 to an accuracy of 1%. Following Refs. 4 and 5, a variational ansatz for the $1s$ exciton wave functions, $\Psi_{ex}(x_e, x_h, \rho) = \sqrt{2/\pi} \Psi_e(x_e) \Psi_h(x_h) \exp(-\rho/\lambda)/\lambda$, is used to minimize their binding energies. Here, ρ denotes the separation between the electron and the hole in the plane of the quantum well and perpendicular to the applied field F , x_e , and x_h are the coordinates of the electron and the hole perpendicular to the plane of the quantum well, and λ is the variational parameter. This wave function is optimized by minimization of the exciton energy. The exciton contribution to the photon absorption spectrum, governed by the spatial overlap of the electron and hole wave functions, is then calculated.⁵ The contribution of the particle-hole continuum is included to account for the complete absorption spectrum.

Our approach reproduces the main field-dependent spectral features of other, more detailed models^{4,6} of the QCSE in a simple rectangular potential well profile. In Fig. 1, we show the calculated absorption spectra, α , as a function of photon energy E for different electric fields, F , applied along the x direction. As seen on the left-hand side, an increase of the field strength leads to a tilt of the confining potential. Consequently, the electron wave function is shifted towards the right, whereas the hole wave function moves to the left, resulting in a reduced spatial overlap. This in turn causes (i) a shift towards lower energy, and (ii) a strong reduction in spectral weight of the dominant excitonic contributions to the photon absorption spectrum. On the lower-right-hand side, the calculated peak exciton absorption is shown as a function of photon energy for applied electric fields in the range $0 \text{ kV/cm} < F < 140 \text{ kV/cm}$. The arrow indicates the direction of increasing applied electric field. Shown as light gray curves are individual spectra for 10 kV/cm field increments used to calculate the exciton peak absorption curve. This exciton absorption curve captures the essential *functionality* of the QCSE. Maximum exciton absorption decreases and shifts to lower photon energy with increasing applied electric field. This rapid loss of resonant behavior in the presence of a bias voltage dramatically limits the tunability of quantum well based optical devices.

What we wish to show here is that it is possible to use an adaptive design methodology to create new types of

^{a)}Electronic mail: shaas@usc.edu

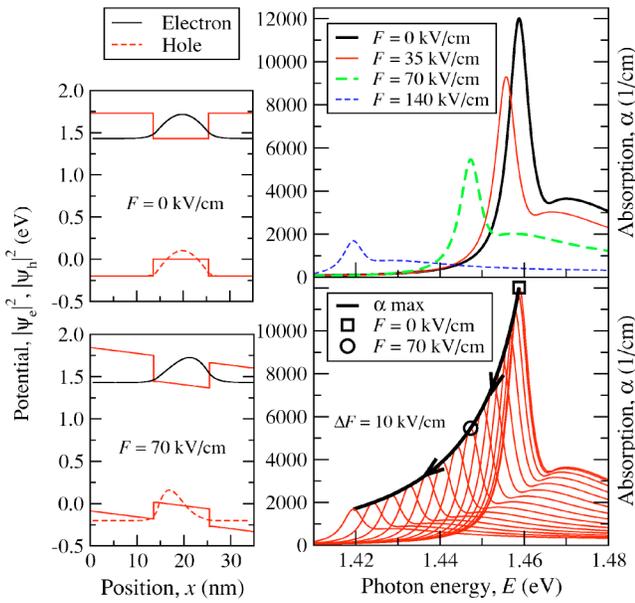


FIG. 1. Absorption spectrum of a rectangular quantum well of width 10 nm. In the left panel, the electron (solid curve) and hole (broken curve) wave functions are shown along with the profile of the well potential. At finite electric field, F , applied in the x direction the confining potential is tilted, shifting the wave functions and reducing their spatial overlap. In the right panel, the zero-temperature absorption spectrum is shown for various electric fields. The QCSE leads to a shift of the dominant exciton peak toward lower energies, and to a strong reduction of the maximum absorption with incremental increase in field, ΔF .

functionality. For example, consider the situation where we wish to design a device in which the excitonic absorption peak at $F=0$ kV/cm and $F=70$ kV/cm is the same, only shifted in photon energy by at least 10 meV. This particular functionality would allow us to rapidly switch the frequency of a quantum well exciton absorption resonance without loss of its absorption strength. Let us initially constrain the search for an enabling broken-symmetry structure to double wells with variable depths and widths. Our numerical optimization uses a genetic algorithm⁷ with a fitness function that simultaneously optimizes the strength and separation of the exciton absorption peak at zero and finite (70 kV/cm) electric field.⁸ The best solution found by our adaptive quantum design method for this restricted search is shown in Fig 2.⁹ It is reminiscent of structures investigated previously.^{10,11} The optimized double well causes the ground state wave function of the hole (broken curve) to develop two maxima whose relative weight is shifted from left to right as the electric field is increased. Simultaneously, the center of the electron wave function (solid curve) moves from left to right, having a maximum spatial overlap with the right peak of the hole wave function at $F=0$ kV/cm and with the left peak at $F=70$ kV/cm. The resulting exciton peaks in the absorption spectrum, shown on the right, have the desired strength and separation. They are located on two sides of a maximum resonance that is reached at $F=20$ kV/cm. In this broken symmetry structure, the maximum of the excitonic absorption peak (α max) initially increases with applied field, and then drops. The corresponding shift of the resonant energy is also nonmonotonic.

However, there are other, even better solutions if the arbitrarily imposed initial constraints on the numerical search are relaxed. Figure 3 shows the result of a numerical optimization of the quantum well in which the positions of the

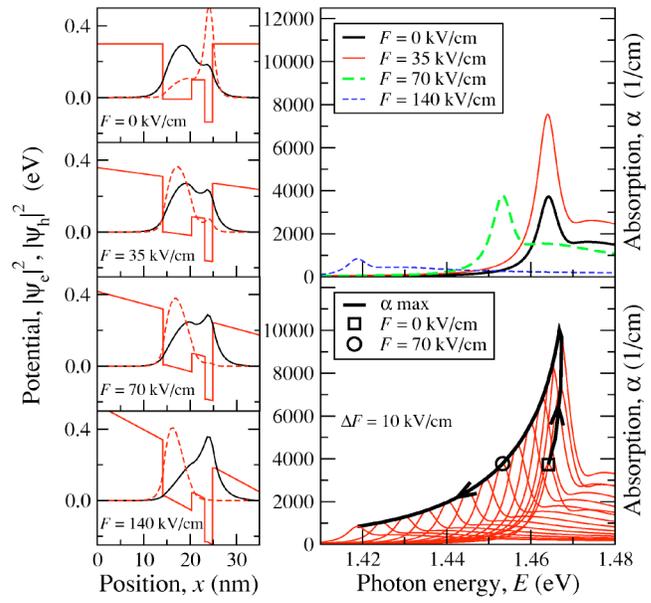


FIG. 2. Broken-symmetry double quantum well obtained from numerical optimization of well width and depth parameters. The target response is an absorption spectrum with maximized, equal-height excitonic peaks at electric fields $F=0$ kV/cm and $F=70$ kV/cm which are separated in energy by 10 meV.

corners of the double wells are allowed to overlap. The obtained potential profile is surprisingly simple. The steep drop of $V(x)$ close to the right boundary of the well pins the hole wave function (broken curve), whereas the electron wave function (solid curve) is still able to shift its weight with increasing applied electric field. The resulting exciton resonances in $\alpha(E)$ at $F=0$ kV/cm and 70 kV/cm are more pronounced than in the solution of Fig. 2. Furthermore, in this design the exciton absorption curve peak (α max) exhibits a functionality that is different from that of Fig. 2. It first shifts towards higher energies with increasing applied electric field

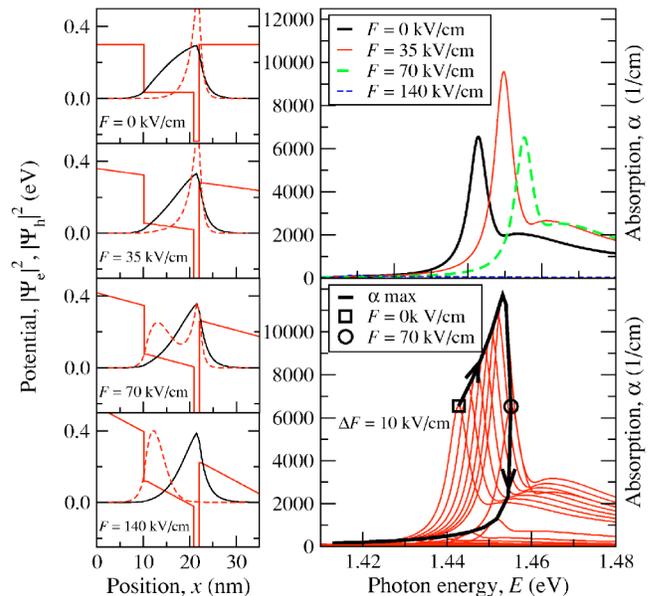


FIG. 3. Broken-symmetry quantum well structure obtained from numerical optimization with additional search parameters compared to Fig. 2. The target response is an absorption spectrum with maximized, equal-height excitonic peaks at electric fields $F=0$ kV/cm and $F=70$ kV/cm which are separated in energy by 10 meV.

before it drops rapidly and eventually shifts back towards lower photon frequencies. Note, that this almost vertical drop of $\alpha(E)$ in a very narrow range of electric fields indicates an exponential sensitivity that is highly desirable for the design of quantum well based modulators.

In summary, the adaptive quantum design methodology used in this work reveals design options that have not been explored using conventional *ad hoc* approaches. The large number of possible solutions along with their exponential sensitivity to small parameter changes render the problem prohibitive to searches by hand.^{11,12} Instead, numerical searches identify optimized broken-symmetry structures which enable desired target functionalities that are useful in the design of quantum-well based photonic switches and modulators. This new approach allows us to engineer many-body excitonic wave functions and thus illustrates a new paradigm in nanoscale design.

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