Resonant states in modulation-doped heterostructures

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Abstract

This thesis deals with the properties of donors placed inside or outside a heterostructure quantum well (QW). The focus of the investigation has been on the formation of resonant states, which are a hybridization of the discrete localized impurity levels and the continuous two-dimensional QW subbands. The impact of such states on the optical properties and the noise spectrum has been studied, and possible applications, in particular related to emission of far-infrared radiation, are considered.

After a summary in Swedish for the general public and an introduction, four original papers are presented. In the first two, the formalism of resonant states is developed, and the two final ones deal with applications.

In Paper 1 the donor is placed outside the quantum well. A model for the resonant coupling of the localized donor state and the QW subbands is developed. Two representations of the impurity potential are considered: a zero-range potential and the Coulomb potential. We calculate the width and position of the resonant state as a function of the distance of the donor to the well, and also investigate the influence of the resonant state on the density of states.

Paper 2 presents a more general method for calculating the energy levels of donors placed both inside and outside quantum wells. From this non-variational method we obtain the binding energies of all localized states and the position and width of the resonant states. We are also able to evaluate the wavefunctions, which are used to calculate the absorption spectrum. The influence on the donor ground state from the central-cell effect, and strain if present, is also considered.

In Paper 3 we perform a self-consistent calculation of the potential profile of a Si/SiGe QW structure which in recent experiments was found to emit intense terahertz radiation. It is shown that the position of the resonant states supports the conclusion that the mechanism behind the generation of the radiation can be similar to that in bulk p-Ge, viz. that the carriers in the heavy-hole QW subband are captured into an excited resonant state attached to the light-hole subband. They may then make a radiative transition to the impurity ground state.

Finally, in Paper 4 we consider a new mechanism (elastic tunneling enabled by the formation of a coupled resonant state) for generation–recombination noise due to shallow donors placed outside a quantum well. The alignment of the QW levels compared to the resonant state energy is found to be of crucial importance.

Key words: Resonant states, impurity levels, quantum well, impurity absorption, central-cell effect, terahertz laser, generation-recombination noise

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Preface

"What does Christopher Robin do in the mornings?" said Eeyore.
"He learns. He becomes Educated. He instigorates
– I *think* that is the word he mentioned (...) –
he instigorates Knowledge. In my small way I also,
if I have the word right, am – am doing what he does."

A. A. Milne, *The House at Pooh Corner*

This thesis completes and summarizes the work I have performed during my, quite exactly, four years as a PhD student at the Division of Solid State Theory, in the Department of Physics of Lund University.

The work deals with the properties of shallow donors placed inside and outside semiconductor heterostructure quantum wells. The key aspect we have been interested in, is the formation of coupled resonant states, which are a hybridization of the discrete localized impurity levels and the continuous two-dimensional subbands. The impact of such states on the electronic and optical properties of the quantum well and the noise spectrum has been investigated. Possible applications, in particular related to emission of far-infrared radiation, are also discussed.

After a summary in Swedish for the general public and an introduction, follow four original articles, on which this thesis is based:

- A. Blom, M. A. Odnoblyudov, I. N. Yassievich, and K.-A. Chao, *Resonant states induced by impurities in heterostructures*, Physical Review B, **65**, 155302 (2002).
- A. Blom, M. A. Odnoblyudov, I. N. Yassievich, and K.-A. Chao, *Donor states in modulation-doped Si/SiGe heterostructures*, submitted to Physical Review B.
- A. Blom, M. A. Odnoblyudov, H. H. Cheng, I. N. Yassievich, and K.-A. Chao, *Mechanism of terahertz lasing in SiGe/Si quantum wells*, Applied Physics Letters, **79**, 713 (2001).
- A. Blom, *A resonant tunneling mechanism for high-frequency generation–recombination noise*, to be submitted to Journal of Applied Physics.

The published articles appear as printed, except that the graphical appearance of some figures has been adjusted to match the overall layout of the thesis. The order of the papers is not entirely chronological. Instead, the first two articles provide the foundation of the theory of resonant states, whereas the two last ones essentially discuss applications of these developed principles.

During my PhD studies I have had the great fortune to attend several conferences. In addition to presenting excellent chances to meet and discuss with world-leading scientists in various areas, this has also provided opportunities to visit many unusual and interesting places. As a testament to these events, I have contributed, more or less, to the following conference proceedings:

- I. V. Altukhov, M. S. Kagan, V. P. Sinis, S. G. Thomas, K. L. Wang, A. Blom, and M. A. Odnoblyudov, *Hole transport due to shallow acceptors along boron doped SiGe quantum wells*, Thin Solid Films, **380**, 218 (2000). (Proceedings of the E-MRS Spring Meeting, Strasbourg, France, 2000.)
- I. V. Altukhov, M. S. Kagan, V. P. Sinis, S. G. Thomas, K. L. Wang, K.-A. Chao, A. Blom, M. A. Odnoblyudov, and I. N. Yassievich, *Terahertz emission of SiGe/Si quantum wells doped with shallow acceptors.* (Proceedings of the 8$^{\text{th}}$ International Symposium on Nanostructures: Physics and Technology, St. Petersburg, Russia, 2000.)
- A. A. Prokof'ev, I. N. Yassievich, A. Blom, M. A. Odnoblyudov, and K.-A. Chao, *Configuration interaction applied to resonant states in semiconductors and semiconductor nanostructures*, Nanotechnology, **12**, 47 (2001). (Proceedings of the 9$^{\text{th}}$ International Symposium on Nanostructures: Physics and Technology, St. Petersburg, Russia, 2001.)
- I. N. Yassievich, A. Blom, A. A. Prokof'ev, M. A. Odnoblyudov, and K.-A. Chao, *Configuration interaction applied to resonant states in semiconductors and semiconductor nanostructures*, Physica B: Condensed Matter, **308**–**310**, 1129 (2001).
  (Proceedings of the 21$^{\text{st}}$ International Conference on Defects in Semiconductors, Giessen, Germany, 2001.)
- M. A. Odnoblyudov, A. Blom, I. N. Yassievich, and K.-A. Chao, *Impurity-induced resonant states in modulation-doped heterostructures.* (Proceedings of the 10$^{\text{th}}$ International Symposium on Nanostructures: Physics and Technology, St. Petersburg, Russia, 2002.)
- A. Blom, M. A. Odnoblyudov, I. N. Yassievich, and K.-A. Chao, *Resonant states in doped quantum wells*, physica status solidi (b), **235**, 85 (2003). (Proceedings of the 10$^{\text{th}}$ International Conference on Shallow-level Centers in Semiconductors, Warsaw, Poland, 2002.)

These papers are however not included in the thesis, since they are basically precursors to the main articles listed earlier, and contain little or no additional information relevant for the thesis. An exception to this is the work by A. A. Prokof'ev *et al.* which also treats the properties of resonant states in the valence band, whereas this thesis work focuses mostly on the conduction band. Furthermore, the last conference paper contains a comparison of two different methods for

determining the width of the resonant state. This point will be instead touched upon in the introduction chapter.

Looking back on the years I have spent working on this thesis, I first of all want to congratulate myself on finishing it! More importantly, I would like to express my deepest gratitude for the wonderful time spent in the company of all the PhD students, post-docs, visitors, and other members of the staff, past and present, at the Division of Solid State Theory. In particular I am indebted to Prof. Koung-An Chao for providing me with a challenging project, with close relationships to interesting applications, and for allowing me to work in a very independent way. Furthermore, I cannot stress enough the importance of the collaboration with Dr. Maxim Odnoblyudov and Prof. Irina Yassievich, and I am most grateful for the knowledge I have derived from our discussions.

My work has been performed within the Nanometer Consortium at Lund University, with the financial support of the Swedish Foundation for Strategic Research and also from NorFA, which has allowed me to travel to the many conferences that I have enjoyed so much participating in. Additional funds from the Royal Physiographic Society in Lund were helpful for arranging the visit to Taiwan in May 2002, during which the friendly and helpful staff (Jenny, Samuel, Julia, Michael, Vanessa, and many others) of the National Chiao Tung University in Hsinchu ensured a most pleasant stay there. The organizing team and the participants of the Kevo Spring School, which took place in the northern-most part of Finland in April 2001, deserve special thanks for making this such a memorable event. The invaluable assistance of Ewa Säwén and Alexei Prokof'ev in many practical matters, and the particular difficulties associated with Russian visa applications, has been very much appreciated.

It must be pointed out that this thesis would never have come into existence, were it not for my family, who is always there for me. Moreover, the quality time spent in the company of friends has meant that life has acquired dimensions which cannot be explained by theoretical physics. Special thoughts go to Mats and Nina, and to Eveliina, Tatu and the children. Finally, Marina, I cannot express in words how much your support and love means to me, and how fortunate I feel to be able to look forward to a bright and happy future together!

Lund, in January 2003
Anders Blom

Contents

Sammanfattning för allmänheten

Titeln på denna avhandling är, översatt till svenska, ”Resonanstillstånd i moduleringsdopade heterostrukturer”, vilket för den oinvigde inte är mycket klarare än på engelska, och inte särskilt annorlunda heller. Vad det handlar om är vissa kvantmekaniska effekter som kan uppstå då man dopar små, eller rättare sagt extremt tunna, halvledarstrukturer och det inflytande detta kan ha på till exempel de optiska egenskaperna hos kvantbrunnar. Avsikten med den här sammanfattningen är att förklara vad detta egentligen betyder, genom att först ge en kort bakgrund och sedan beskriva avhandlingens innehåll med hjälp av enkla analogier.

Mottot för den moderna elektronikindustrin är ”mindre, snabbare och billigare”, och denna drivkraft har de senaste decennierna givit upphov till den explosionsartade utveckling som lett fram till dagens informationssamhälle. De kretsar som bygger upp våra datorer och andra apparater bygger till största delen på klassisk halvledarfysik som, via utvecklingen av den integrerade kretsen i slutet av 1950-talet, går tillbaka ända till 1947 och uppfinningen av transistorn. Naturligtvis har en enorm utveckling skett sedan dess; man kan idag integrera hundratals miljoner transistorer på en yta stor som en tumnagel. Om man fortsätter göra komponenterna mindre och mindre, hamnar man dock snart i den situationen att de element som bygger upp kretsarna blir så små, att de inte längre kan beskrivas i termer av klassisk fysik. Istället är det kvantmekanikens lagar som styr mikrokosmos, och nya teorier måste därför utvecklas. Faktum är, att det redan inom en inte alltför avlägsen framtid kommer att bli nödvändigt för industrin att ta steget in i den kvantmekaniska världen.

Forskningen ligger hela tiden steget före tillämpningarna, och utvecklingen av kvantmekaniska kretsar har pågått i ett par decennier. En nyckelingrediens i dessa är att man numera kan skapa helt nya halvledarmaterial som inte existerar i naturen, och skräddarsy deras egenskaper för just de tillämpningar man är ute efter. Genom att bygga upp materialet atomlager

för atomlager bestående av olika grundämnen eller legeringar, kan man bilda både kvantbrunnar, kvanttrådar och kvantprickar. I dessa så kallade heterostrukturer uppför sig elektronerna effektivt sett som vore de två-, en- eller till och med noll-dimensionella, i motsats till den värld vi vanligen uppfattar som tre-dimensionell. Detta ger upphov till en mängd nya egenskaper som man kan utnyttja för nya intressanta tillämpningar.

Liksom vad gäller klassiska halvledare måste de nya mikroskopiska komponenterna dopas, eftersom halvledare i ren form i stort sett inte alls leder ström. Den mer vardagliga användningen av ordet dopning inom sportens värld ger en ganska bra bild av hur det fungerar. Genom att tillföra en liten mängd främmande atomer kan man förbättra den elektriska ledningsförmågan enormt mycket. Parallellt med denna positiva effekt leder emellertid dopningen också till försämringar. De främmande atomerna (som ofta även kallas föroreningar) bryter den perfekta symmetri som annars råder i materialet, och leder till en rad oönskade egenskaper. Man måste därför hitta en balans, så att man tillför tillräckligt med dopning för att få de elektriska egenskaper man önskar, men inte så mycket att materialet förstörs.

En ny möjlighet som öppnats med heterostrukturer är att man fysiskt kan separera de områden som dopas, från de aktiva områden som leder strömmen. Sådan moduleringsdopning* används i nyskapade material där elektronerna kan uppnå mycket höga hastigheter, tack vare att många av de negativa aspekterna av dopningen försvinner. De oönskade effekterna kan dock aldrig helt elimineras; dopningen måste trots allt placeras så nära det aktiva området att tillräckligt med elektroner kan ta sig dit†. De dopningsatomer som skänker bort sina elektroner blir själva positivt laddade, och därmed påverkar de elektronerna, som ju är negativt laddade, med en elektrostatisk kraft. Det är just de kvantmekaniska aspekterna av denna växelverkan, och effekterna därav, som studerats i denna avhandling.

För att skapa en enkel bild kan man betrakta elektronerna som cyklister som deltar i ett långlopp, medan dopningsatomerna representeras av ganska djupa hål i marken. Om man placerar hålen mitt i vägen kommer en del cyklister förmodligen att trilla ner i dem, och kanske bli fast ett tag innan de kan klättra upp och fortsätta cykla. För att undvika att trilla ner måste andra cyklister köra runt hålen, vilket tar extra tid och sänker deras hastig-

* Det som avses är att koncentrationen av dopningsatomer är modulerad, det vill säga den varierar beroende på var i materialet man befinner sig.

† För att inte komplicera diskussionen i onödan antar vi att varje dopningsatom bär på en extra elektron som kan överföras till det aktiva området, varvid föroreningarna benämns donatorer. Det finns även en annan typ av föroreningar, så kallade acceptorer, som stjäl elektroner vilket förvånansvärt nog också leder till en ökad ledningsförmåga.

het. Den ytterligare aspekt som kvantmekanikens lagar (vilka ofta strider mot vår vardagliga, klassiska bild av verkligheten) tillför är att om nu hålen placeras femtio meter bort från vägen, ute i en åker, så kan cyklisterna fortfarande både trilla ner i hålen och tvingas köra runt dem!

De två första artiklarna i avhandlingen handlar till största delen om hur stor sannolikheten är att elektronerna trillar ner i donatoratomernas hål, och hur stora hålen egentligen är. Båda dessa faktorer visar sig variera kraftigt beroende på elektronernas energi (cyklisternas hastighet), den exakta placeringen av dopningen, samt uppbyggnaden av materialet (vägens allmänna beskaffenhet). Detta påverkar även livstiden (hur lång tid det tar att ta sig tillbaka upp på cykeln) för elektroner som fastnat i ett hål.

Att bedriva professionella cykellopp, alltså dra nytta av elektronernas höga hastighet, är en typisk tillämpning av heterostrukturer, och självklart är det då bäst att placera hålen (dopningen) ute i åkern. Nyligen har det dock visat sig att även gropiga vägar kan utnyttjas på ett positivt sätt. De cyklister som trillar i hålen kan övertalas att plocka med sig ett par värdefulla stenar då de klättrar tillbaka upp. Samlar vi ihop alla bidrag efter cykelturen kan vi bli rika, åtminstone om många cyklister trillat ner.

I den mer korrekta fysikaliska situationen handlar det om att då elektronerna fastnar på dopningsatomerna kan de hoppa mellan olika energinivåer. Samtidigt skickar de ut ljus, och detta kan användas för att konstruera en laser. I den andra artikeln diskuteras hur våglängden på det utsända ljuset kan kontrolleras, genom att ”hålens” egenskaper ganska enkelt kan anpassas då vi bygger upp vår heterostruktur. Särskilt intressant vore det att få fram en laser för terahertz-området*, vilket rymmer en lång rad intressanta tillämpningar inom astronomi, medicin, biologi och fysik, men där man ännu inte har en kompakt och billig strålkälla. En tänkbar kandidat för en terahertz-laser behandlas i den tredje artikeln, även om detaljerna där är lite mer komplicerade då det rör sig om dopning med acceptorer.

Antag nu slutligen att varje cyklist bär på var sin liten del av ett samlat meddelande, som ska nå en person i målfållan. Om vissa cyklister trillar ner i hål, och därför kommer fram för sent, kan man föreställa sig att meddelandet blir mer eller mindre förvrängt. Den här typen av störningar eller brus är ett viktigt problem att studera för elektroniska kretsar, och det är inte svårt att förstå att dopningen bidrar till bruset. Detta är naturligtvis inte ett nytt problem, och det har länge forskats intensivt inom detta område, men våra resultat visar på en ny mekanism för hur brus kan uppstå. Exakt hur mycket detta bidrar till störningarna återstår att studera i detalj, men den fjärde artikeln i avhandlingen är ett första försök att studera denna effekt.

* Terahertz anger frekvensen på ljuset och motsvarar ännu lägre energier än infrarött.

Resonant states: the Wheres, Hows, Whats and Whys

If someone was asked to summarize this thesis in one sentence, that person could say that it delivers an overall picture of the properties of impurity states in modulation-doped quantum wells, while focusing in particular on the formation of hybridized resonant states.

This statement, albeit correct, nevertheless opens up a whole range of new questions, pertaining to the details hiding behind those many fancy words. What is a quantum well? What properties, and how are they found? What is a resonant state, and why is it hybridized (whatever that means)? Why is it interesting to learn more about this topic, and how can we use that knowledge? The answers to all these inquiries can be found in the four articles which follow after this chapter. The information is however unfortunately somewhat hidden behind all the formulas and is scattered between the different papers. Therefore, this introduction is intended to summarize in one place the important key points. The aim is to present the general concepts and consequences, without going into all the technical details. These are, instead, readily found in the articles.

Preceding this chapter is a popular summary (in Swedish) for the general public. For those not closely familiar with the physics of semiconductor heterostructures, it may provide a very basic introduction. Other than that, in order to focus the discussion on the work performed for the thesis, it will be assumed that the reader is familiar with the necessary basic concepts – the theory of semiconductors, in particular. For reference, a list of recommended textbooks and review articles can be found at the end of this chapter. Citations of original articles have however purposely been avoided; these can instead be found in each article, where they are referred to according to the detailed context in which they are relevant.

Before going into all the details of the "resonant states" mentioned in the title of this thesis, it is appropriate to first set the stage by outlining some general features of the systems where such states may appear. The second part of the title in fact already indicates what materials we are interested in. We must of course also have a clear understanding of what resonant states actually are, and in particular how they are formed, before we can study them. Once these preliminaries have been dealt with, we can at last turn to describing the characteristic properties of resonant states and how we calculate them. This will be the main focus of the presentation, as it constitutes the major part of the thesis work. Finally we consider the crucial question, why we are interested in these states. Admittedly, this should perhaps have been the first item on our list. Equipped with a deeper knowledge of the resonant states, we will however be in a better position to deliver a more detailed answer.

It is intended that to a large – although obviously not complete – extent, the following presentation is to be regarded as a direct result of the conclusions arrived at within the thesis work. In this sense, the text will, hopefully, deliver extended knowledge on the topic of impurity states in doped heterostructures, and perhaps even inspire new insights and ideas for novel applications based on them.

Where do they appear?

Modulation-doped semiconductor heterostructures offer an unprecedented freedom of choice for the present-day device designer. This flexibility is achieved by the possibility to fabricate a whole range of novel materials, extremely pure and grown with the utmost precision, atomic layer by atomic layer. Almost every aspect of the final structure can be controlled by changing the material compositions of the layers, varying their widths, and strategically doping suitable areas. This entire process is known as band engineering, and is a key element in the revolutionizing impact that heterostructures have had on semiconductor physics.

At the same time, this huge variety of systems that can be realized, each with its own individual characteristics, may make it difficult to identify the important common physical properties and fundamental mechanisms. One such feature is the fact that electrons confined in thin layers or quantum wells behave as if they were practically two-dimensional, and not three-dimensional like in usual bulk materials. The dimensionality may even be reduced to effectively one- and even zero-dimensional systems, known as quantum wires and dots, respectively.

Like classical semiconductors, heterostructures are in general rather poor conductors, even at room temperature. A further common feature of low-dimensional materials designed for electronic and optoelectronic applications is therefore the need for doping. An important novelty made available with controlled crystal growth is the possibility to use so-called modulation doping. This means that the doping profile can be varied across the structure, in contrast to usual bulk doping where the entire material is doped homogeneously. By spatially separating the doping from the active layers, the impurity scattering can thus be significantly reduced, and the material purity is improved. Modulation-doped devices with extremely high mobilities and low noise figures have indeed been demonstrated, especially at low temperatures.

Still, it is not possible to remove the doping too far away from the active channel, or otherwise the supplied free carriers will never make it into the conducting region. Moreover, one is sometimes interested in exploiting the optical properties of the impurities themselves, and in this case the doping is naturally placed in the active region. The presence of impurities is hence a key ingredient in heterostructure devices, and must always be carefully taken into account when studying such systems.

We have thus identified at least two fundamental common characteristics of heterostructures: the two-dimensional behaviour of electrons confined in a quantum well, and the presence of impurities. As it turns out, these are the two ingredients required, in our case, to form the resonant states we are aiming to study.

Resonant states were certainly not introduced with the advent of semiconductor heterostructures. Localized states degenerate with a continuum – which, in fact, is the very definition of a resonant state – are known from various fields of physics. The initial credit goes to U. Fano, who studied the problem of autoionization in helium, but resonant states can also be formed in e.g. bulk semiconductors, where localized impurity states associated with higher conduction bands may become resonant with the continuum of the lowest conduction band. What is new in the case of heterostructures, and which makes it such an interesting topic to study, is the possibility to manipulate the properties of the resonant states through the band engineering.

The heterostructure resonant states which we will consider in this work are those formed between the localized impurity levels of donors and the continuous quantum well subbands. Therefore, the general properties of the impurity levels is obviously a crucial factor to study. These properties turn out to depend very much on the position of the donor, whether it is placed inside the quantum well or far away in the barrier. Resonant states can be formed in either case, however, as we shall soon see.

The situation is summarized in Figure 1, which visualizes practically all

the key issues that we wish to present in this thesis. The reader is strongly advised to return to this figure as often as needed, in order to relate the complicated and detailed parts of the presentation to a clearer picture of the physical situation. To explain and deliberate on all the various features displayed in Figure 1 is the subject of the remainder of this introduction.

Before that, we shall however first briefly consider some fundamental aspects of the particular two-dimensional heterostructures we will study, namely quantum wells. Also some words on the basic properties of impurities will be offered in the following section. In keeping with our ambition to avoid details, the discussion will however be rather superficial, and instead the reader is referred to the references listed at the end of this chapter for more a thorough presentation. Readers who are well-acquainted with quantum wells, the effective-mass theory and the hydrogenic models may therefore skip the next section altogether.

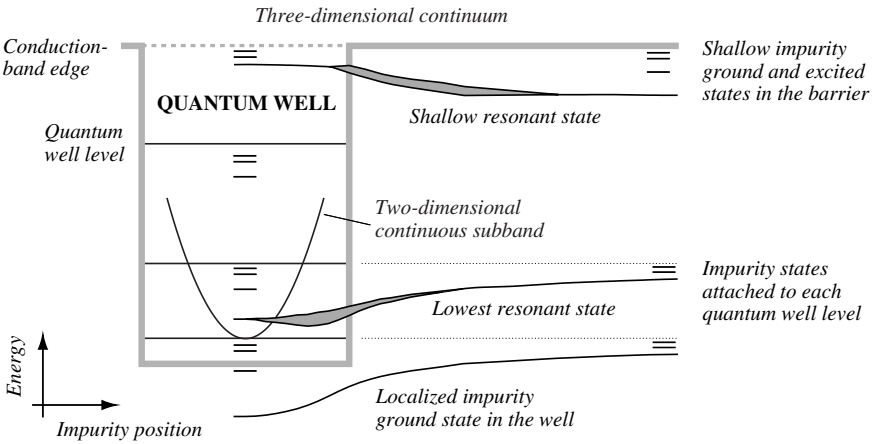

Figure 1: This schematic picture shows the behaviour of all the various heterostructure impurity states as we change the donor position from the center of the quantum well to a remote location in the barrier. The situation when the donor is in the barrier corresponds to the shallow impurity states in the upper-right corner, whereas the left and bottom parts are mostly relevant when the donor is inside or very close to the quantum well. The shaded areas represent the energy width of each coupled resonant states, as defined on page 14. The two-dimensional subband is illustrated with a parabola, which strictly speaking refers to the energy-dependence in the reciprocal space, and not the real space of the figure.

Quantum wells and donors

Put very simply, a heterostructure quantum well is formed from a layer of material that is grown between layers (known as barriers) of another material with a larger band gap. An often used quantum well is GaAs grown between AlGaAs barriers (the content of Al can be varied rather freely). Another example is Si grown between SiGe, which however only is a potential well for electrons; the Si layer is a barrier for holes. It is amusing that the quantum well has been a standard problem in every quantum mechanics textbook for over half a century, but only recently have such systems actually been manufactured. The experimental observations thereby obtained are in reassuring agreement with the theoretical predictions.

The confining potential profile of a quantum well causes the motion along the growth axis to be quantized, and only certain values of the energy are allowed, as is well-known from basic quantum mechanics. Each energy level is the bottom of a two-dimensional continuum, called a subband, corresponding to the free electron motion in the two directions perpendicular to the growth axis. In each subband the density of states does not depend on the energy and vanishes below the subband bottom. These simple facts are, in fact, by themselves responsible for a multitude of effects utilized in heterostructure devices.

As we stated earlier, such devices are generally always doped in order to provide enough free carriers for electronic applications. The dopants, or impurities, are foreign atoms which are introduced substitutionally into the otherwise perfect host material lattice, and they carry an additional carrier* which they can offer as a free carrier to the conduction or valence band. We shall almost exclusively consider shallow donors attached to the conduction band in this work, although resonant states may equally well be formed from acceptors. The complexity of the valence band, however, makes the analysis much more difficult in those cases.

As long as the donor is neutral, which means that it has not yet donated its additional electron to the conduction band, the most often used model to describe the properties of this electron is the so-called hydrogenic model, to which we shall also adhere. In this picture, the electron is considered to be bound to the donor by the attractive Coulomb potential between the negative electron and the remaining positive ion core. However, in contrast to the otherwise very similar case of atomic hydrogen, the electron is now described by an effective mass (see just below) and furthermore does not move in vacuum but in the crystal. The effective mass is generally much smaller than the electron mass and semiconductors have rather large dielec-

* An electron when we have doping by donors, or a hole in the case of acceptors.

tric constants (typically of the order 10). In result, the effective Bohr radius is substantially larger and the binding energy of the electron correspondingly smaller, compared to the energy levels in a hydrogen atom. This small binding energy can easily be overcome by thermal excitation, and this is the reason why doping increases the conductivity of semiconductors.

Like in bulk semiconductors, the properties of the electronic states in heterostructures are usually very well described by the effective-mass approximation. This approximation assumes that the highly complicated influence of the periodic crystal potential can be accounted for by simply replacing the electron mass by an effective mass*. Within this model we furthermore only consider the envelope part of the wave function, and ignore the Bloch part, which describes the detailed behaviour of the electron states very close to the ion cores.

We shall use the effective-mass approximation throughout most of this work. An important exception, where this model fails, is in the description of the central-cell effect, which is introduced to reconcile the difference in the experimentally observed impurity binding energies and those calculated within the effective-mass approximation. In that case one must retain and consider carefully the symmetry properties also of the Bloch functions.

How are they formed?

The basic requirement for the formation of the resonant states we are studying, is that the impurity states must be degenerate with the quantum well subbands. Clearly this is the case when the donor is placed in the barrier, not too close to the quantum well. The binding energy of a shallow donor is typically around 5–50 meV, which is about an order of magnitude smaller than the band offsets (i.e. the depth of the quantum well) of commonly studied heterostructures such as GaAs/AlGaAs and Si/SiGe. The donor ground state† is then resonant with one or several of the quantum well subbands, unless, of course, the quantum well happens to be so narrow that the lowest quantization level is above the donor level.

* This statement is obviously a gross over-simplification; there are many additional important and subtle points of the effective-mass approximation which require careful attention. There is however no particular need to go into such details here.

† The excited states can of course also form resonant states. We shall however exclusively concern ourselves with the ground state when the donor placed in the barrier, since naturally this will be the lowest resonant state, and therefore the most important one for the transport properties of the well.

Things are much less trivial when the donor is placed inside the quantum well. One may be tempted to guess that all impurity states should then appear below the lowest subband bottom, since in the more familiar bulk case the localized donor states lie in the band gap. The situation is however quite different in the quantum well, due to the reduced symmetry of the system. The spherical symmetry of the Coulomb potential is broken by the presence of the well, and instead the systems takes on a cylindrical symmetry around the quantum well growth axis*. This reduction of symmetry is a direct consequence of the lowered dimensionality, but may also occur if we apply for instance a magnetic field to a bulk crystal, as briefly discussed later on in this section.

Instead of a single continuum edge, as formed by the conduction band bottom in the bulk crystal, each quantum well level is associated with a two-dimensional continuous subband. Below each subband, as depicted in Figure 1, will appear a Rydberg-like series of impurity states, which are said to be attached to or associated with that particular subband. The binding energy of an electron in such a state is defined as the minimum energy required to place the electron in the subband to which the state is attached. Once the electron is in the subband, it becomes free to move, in two dimensions, and may escape to infinity, but only along directions perpendicular to the quantum well growth axis.

One can offer many arguments for why there are impurity states attached to each subband like this. First of all, it is clear that these states much somehow be associated with the quantum well levels and not the usual conduction band bottom, since the latter is not a relevant quantity inside the well, due to the confinement. We may then argue that no subband possesses any particular status compared to the others, and hence impurity states can be associated with any level. A less physical, but certainly convincing, argument is that the situation shown in Figure 1 is the result of our (in principle exact) calculations. On the same note, it has been observed in variational calculations that if all impurity states would be bound to the lowest subband, the binding energies for some excited states become negative for certain well parameters, which makes no sense since the binding energy by definition is a positive quantity.

The most powerful arguments in matters like these are often those deduced from considering symmetries, but this is decidedly more challenging in the present case. The reduced symmetry leads to a partial rearrangement of the conventional hydrogenic quantum labels, since the orbital angular mo-

* These symmetries apply when we treat the system within the effective-mass approximation; the symmetry properties of the real crystal are of course much more complicated.

mentum is no longer conserved; only its projection on the growth axis is. In fact, this projection together with a major quantum number to identify states of the same projection are the only available labels for the donor states in the quantum well. To our dissatisfaction, we must however concede that no obvious connection appears to exist between these quantum numbers and the subbands to which the corresponding states are attached.

In light of the facts just outlined, it is clear that resonant states are formed also when the donor is placed inside the quantum well. As soon as the binding energy of an excited impurity state* is smaller than the energy which separates the quantum well level to which the state is attached from any other lower level, that impurity state is resonant with the continuous subband of the lower level. The lowest possible such state is clearly identified in Figure 1. This particular impurity state corresponds in the bulk to the $2p_0$ hydrogenic state, but this labeling is not relevant in the cylindrical quantum well symmetry†. Nevertheless, like the hydrogen $2p$ state, it has a rather large binding energy compared to other excited states. Hence it is only resonant in enough narrow wells; in wide wells its binding energy exceeds the separation of the two lowest subbands, and the state appears below the lowest subband. Higher excited impurity states are resonant under much wider conditions. Still, those states have much lower occupation probabilities; furthermore, unless the concentration of electrons in the well is very high, one usually considers only the lowest subband to be occupied. Thus the lowest resonant state is the most important one, and we shall limit most of the discussion to it, although the results apply quite generally.

It is instructive to study the connection between the quantum well and the bulk cases, by considering very wide or very narrow wells. The number of quantum well subbands depends very much on the width and the depth of the well, but changing these parameters obviously does not affect the symmetry of the system. As the well is made narrower (keeping a constant depth, for simplicity), the well can bind fewer and fewer levels, and the impurity states which are attached to subbands which become unbound, instead become attached to the three-dimensional continuum. In the extreme limit of a vanishingly narrow well, the three-dimensional bulk situation is thus recovered. Note that the binding energies in this limit are determined by the barrier material. In the opposite limit, when the well is made wider and wider, more and more subbands appear, with very small energy spac-

* The ground state always appears below the bottom of the lowest subband, and can never be resonant when the donor is inside the well.

† The correct classification for this state is $1\Sigma_u$; see Paper 2 for details on the labeling of donor states in quantum wells.

ings. The subbands merge into a continuum while all impurity levels finally appear below the lowest subband (i.e. in the band gap), and again the bulk case – in this case of the well material – is obtained.

We have at this point spent a lot of time describing the external circumstances under which a resonant state may be formed from the donor states. An important question now becomes, what actually separates resonant states from usual impurity states? For this purpose it is necessary to clearly define the terminology. We have already defined a resonant state as a discrete, localized energy level which is degenerate with a continuum of states. Now we introduce the concept of a coupled resonant state, which in many respects is the only really interesting kind.

A coupled resonant state may be formed if the impurity state and the continuum have the same symmetry (see below); only in this case can the wave functions of the two initially independent systems interact. The interaction leads – by ways which we shall investigate in more detail in the next section – to a hybridization of the wave functions. This means that a coupled resonant state is described by a wave function which has a partly localized character, originating from the impurity state, and a partly continuous character. In contrast, usual impurity states, such as the ground state of a donor placed inside a quantum well, are completely localized.

In the particular case when all the impurities are placed exactly in the middle of a flat well (like the one in Figure 1), the states can in fact be characterized by yet another quantum number, namely parity with respect to reflections in the plane of the well*. In this case, the resonant impurity states can only couple to subbands of the same parity, which means that the lowest resonant state, which we are focusing on, cannot become hybridized. What we are describing is however a rather unrealistic situation; even with the precise control available with molecular-beam epitaxy, there is always a certain uncertainty in the doping position. The levels are furthermore only characterized by parity if the quantum well profile is exactly symmetric around the center of the well. In reality this also never occurs; there is always some band bending due to charge redistribution within the structure. In a real sample the resonant states can therefore always be considered as more or less coupled. Of course, if the donor is moved away from the middle of the well, or a bias is applied across the quantum well, parity is immediately broken and all resonant states can hybridize.

An important consequence of the hybridization is that the localized part of the wave function no longer is a stationary state. In the words of Fano, the

* One often retains the parity label also when the reflection symmetry is broken. It is then an "approximate quantum number", which still provides a useful characterization, especially for states which are not hybridized.

coupling "dilutes" the discrete impurity level throughout a band of partly continuous states, described by a resonance profile. This statement is by no means trivial, and requires further attention.

The energy of a resonant state is actually complex, but the physical properties we measure are real. It turns out that the imaginary part of the energy manifests itself in two observable ways. First, the effects of a resonant state are felt not only at the resonance energy, but also in a certain energy interval around it. If we measure the strength of this influence as a function of the energy, we obtain exactly Fano's resonance profile. In the simple but typical case when this profile has a Lorentzian shape, the width* coincides with the imaginary part of the resonant state energy. As a second consequence, the quantum-mechanical time evolution of a state with a complex energy predicts an exponential decay of the occupation probability of the state. Thus, if an electron initially resides in a resonant impurity state, it will autoionize with a characteristic lifetime, which is immediately given by the width of the resonance profile, or the energy width of the resonant state as we shall refer to it from now on. Note how the respective widths of the two resonant states singled out in Figure 1 are indicated by the shaded areas.

The continuous part of the hybridized state is also no longer a stationary state on its own, and this will induce scattering between quantum well states. Scattering by ionized impurities is a well-studied process, but in the case of resonant impurity scattering that we are considering, there is an added feature. The electron may be trapped in the localized part of the resonant state, and only after a certain time, of the order of the lifetime, will it be returned to the quantum well. In addition to lowering the mobility as scattering always does, this trapping process gives rise to a high-frequency generation–recombination noise, which we will discuss later on.

As we have seen, coupled resonant states can be formed under quite general conditions in any type of doped quantum wells. The two cases we have discussed, with donors inside the well or far away in the barrier, perhaps appear to be quite different, but they are actually related. Any distinction is more a matter of which numerical approach to use to study the respective resonant states, or what properties one wishes to focus on. We shall return to this in much more detail in the following section. Before that, two other – similar but different – examples of resonant states are worth mentioning for completeness, although we shall not go into any deeper details. A short exposé of these cases will nevertheless hopefully illuminate some of the statements made above.

* The full width at half maximum, to be precise.

The same kind of quantum well resonant states we are discussing here can naturally also be formed by acceptors in heterostructures. There exist however also a slightly different type of valence band resonant states, which may appear even in a bulk material. As in the case of a quantum well, each valence subband (the heavy, light and split-off hole bands) have series of impurity levels attached to them. An externally applied pressure will lift the degeneracy of the heavy and light hole bands, and so localized impurity states belonging to one band will – if the strain-splitting is larger than the binding energy – become resonant with the continuous states of the other band. This effect was proved to be the essential mechanism responsible for the generation of intense light emission, in fact even lasing, in acceptor-doped bulk Ge. We shall return to this in a later section, where we consider applications of resonant states.

Another possibility for the formation of resonant states in doped bulk materials is offered by the application of a magnetic field. If the field is strong enough, the electron motion becomes quantized much like in a quantum well. The "subbands" are in this case denoted Landau levels and each such level will, not surprisingly, have a series of impurity states attached to it. As the magnetic field is increased, the constant separation of the levels becomes larger and the localized impurity states of a certain Landau level may become resonant with the continuum of a lower level. This effect was observed in experiments.

Let us now return to the resonant states under investigation in this thesis, and consider their characteristic properties.

What are their properties?

From what transpired in the preceding section, it is clear that the characterization of the resonant states formed in modulation-doped heterostructures must be based on the properties of the impurity states:

- *The binding energy* – how it depends on the quantum well parameters and the donor position, for both ground and excited impurity states, inside and outside the well; how to define the binding energy of a coupled resonant state is an important point.

- *The resonant state wave function* – what part of the wave function is localized and what part is continuous.

- *The energy width of a resonant state* – how to calculate it, and how it depends on the same parameters which influence the binding energy.

- *The central-cell effect* – in order to compare the calculations with experimental results, the deficiency of effective-mass theory to describe the region very close to the impurity has to be remedied.

Before we go into the details of these properties, we will first spend some time to discuss various ways how to calculate them. In earlier works, the two situations where the doping is placed inside or outside the quantum well have been treated as separate problems. If the donor is in the barrier, far away from the quantum well, the energy levels should resemble those of the isolated impurity. The binding energies and envelope wave function can then be obtained by bulk variational calculations, perhaps with some perturbation from the presence of the well. More or less sophisticated variational approaches can also be used if the donor is placed inside the well, as long as the reduced symmetry due to the confinement is accounted for.

Although the so-obtained results for the binding energy of both the ground and excited (even resonant) states are in good agreement with experimental observations, the variational method has a number of disadvantages. First of all, a suitable form of the wave function must be supplied as an initial guess. While this is straightforward for the ground state, it is a virtually impossible task for anything but a few of the lowest excited states. It is also known that variational functions may produce an accurate estimate of the binding energy without encompassing the precise details of the correct wave function. Thus one cannot expect to use the variational function for the evaluation of e.g. optical matrix elements. The application to non-isotropic materials such as Si is even more cumbersome, which is reflected in the fact that only III–V quantum wells have been considered in this way. For our purposes, however, the most severe deficiency of the variational method is the fact that it is completely incapable of delivering the energy width of the coupled resonant state.

We have resolved all the issues listed above by employing a different, non-variational method for calculating the impurity states in modulation-doped heterostructures. The approach is based on expanding the wave functions of the combined quantum well/donor system in a complete basis. This turns the Schrödinger equation into a matrix problem, which is diagonalized to yield both the energies and wave functions of all localized impurity states, the continuous quantum well states and also the (possibly hybridized) resonant states. The mathematical details are described in Paper 2 of this thesis, and will not be repeated here.

The developed method also allows for the evaluation of the energy width of the resonant states, by ways which will be described later on. Moreover, since the approach is non-variational, the obtained wave functions can be used to calculate various matrix elements. The consideration of non-isotropic materials such as Si or Ge presents no additional problems. It is even

possible to include the discontinuity of the effective mass in the directions parallel to the quantum well interfaces, caused by the fact that the barriers and well consist of different materials*. The effect of this discontinuity, which is almost always ignored otherwise, is to introduce non-parabolicity of the quantum well subbands. This is not to be confused with the non-parabolicity which arises due to the coupling to the valence band; this latter effect can in fact also easily be included in the method. With some additional effort it is furthermore possible to take into account the difference between the respective dielectric constants in the well and barrier.

A different method may be used if the donor is placed far away in the barrier, when the coupling to the well is rather weak. The relevant resonant state is then formed from the more or less bulk-like donor states bound to the three-dimensional continuum. We shall in what follows often refer to this state as the shallow resonant state, and its properties can be calculated using the so-called resonant coupling method, presented in Paper 1 of this thesis. This method, in the spirit of Fano, initially treats the quantum well and the impurity as two separated and uncoupled systems, and their respective Hamiltonians are easily diagonalized. Coupling is then added, following Dirac, by considering the combined quantum well/donor system as a scattering problem. The total wave function is written as a linear combination of, on the one hand, the localized impurity wave function, weighted by a so-defined trapping coefficient, and on the other hand the unperturbed quantum well states, weighted by scattering coefficients and a resonant energy denominator. Proceeding essentially within the Born approximation, we are able to diagonalize the total Hamiltonian using this form of the wave function, and calculate the trapping and scattering coefficients. We shall see later how these can be used to determine the energy position and width of the resonant state.

The basis expansion works irrespectively of the impurity being located in the well or in the barrier, and so it enables a unified treatment of donor states in modulation-doped heterostructures. The method is exact in the sense that it contains no approximations beyond those inherent in effective-mass theory. In order to obtain accurate results, however, a very large basis which also includes the three-dimensional continuum must be used. In result, the numerical work becomes very heavy, but not insurmountable. The resonant coupling method is numerically more efficient†, but only able

* The discontinuity of the effective mass in the growth direction must of course also be considered, but this is standard.

† In its original form, the resonant coupling method is strictly speaking less efficient; it is however vastly improved by the use of inventive interpolation schemes. This is however not the place to discuss such technicalities.

to treat the case when the donor is far away from the well, due to the approximations made within it. The figure on page 8 is based on results obtained from calculations using both methods. A final thing to point out is that both the two approaches consider only the effects of a single donor. It is therefore necessary that the doping concentration is small enough that the donors do not interact.

Binding energy

The most fundamental property of an impurity state is its binding energy. For purely localized states the definition of the binding energy is straightforward, as the energy distance from the state itself to the subband to which it is attached. It can however be impossible to judge to which subband a certain impurity state is attached, by only looking at the energies, since its binding energy may be larger than the subband separation. Instead a detailed study of the wave functions is often necessary, a topic to which we will dedicate a separate section below. If the well is made narrower, thereby increasing the distances between the subbands, the situation becomes clearer, and one can then follow each state as the well is again made wider. How to properly define the binding energy (or, more precisely, the energy position) of a coupled resonant state is an even more delicate question, which will be deferred to the section about the resonant state energy width. For now we will just assume that the binding energies of all states have, somehow, been determined, and discuss how they depend on the quantum well parameters and the donor position.

The first thing to note is that the binding energy of the ground state is quite much larger when the donor is placed in a narrow quantum well, compared to in the bulk well material. The reason is of course the additional confinement due to the well potential profile. In the limits of very narrow or wide wells, the bulk situations corresponding to the bulk barrier and well materials, respectively, are regained, as already noted earlier. As also mentioned before, the ground state always appears below the lowest quantum well subband, and hence it is completely localized. Rydberg-like series of excited impurity levels are attached to each subband, as well as to the three-dimensional continuum. As the donor is moved out from the center of the well, the binding energies – which are still measured relative to the corresponding quantum well levels – of all impurity states slowly decrease towards zero, with exception for the states attached to the three-dimensional continuum, which behave in a more complicated manner. These behaviours are qualitatively sketched in Figure 1 on page 8.

As a result of the position-dependence of the binding energy, we conclude that for continuously doped quantum wells one must consider each impurity

state to form a band, and not a single well-defined level. The energy width of this band may very well be comparable to the distance between the subbands, at least for the donor ground state, and it is further increased by the central-cell effect, as will be discussed later on.

When the donor has been moved far away from the well, each impurity state still remains bound to its initial quantum well level, with a vanishingly small binding energy. This situation appears to be incorrect, as it would mean that the donor ground state is determined by the quantum well levels, even when the donor is placed infinitely far away from the well. However, if we study the electron density, we find to our relief that these "impurity states" are in fact localized in the well, and not on the impurity.

Instead, the relevant impurity states in the barrier, far away from the well, are indeed the familiar shallow states, bound to the three-dimensional continuum, which have the electron density located on the donor. We may now consider what happens if we start with the donor infinitely far away, and move it towards the quantum well. Rydberg-like series of impurity states – localized in the well – are then pushed down from each quantum well level. The donor ground state (and of course also the excited states), which is discrete at infinite distance, broadens due to the coupling (indicated by the shaded area in Figure 1), and a hybridized state is formed. The binding energy of this state is typically smaller than for the uncoupled donor state. Thus the resonant state is generally pushed up towards the continuum, although a more complicated behaviour can be observed if the resonance is very close to a quantum well level.

As the donor is moved even closer to and inside the well, the shallow resonant state remains bound to the three-dimensional continuum. Meanwhile, there is a continuous transfer of electron density at the donor position into the deepest impurity state attached to the lowest subband, and at some point – which is not really well-defined – this state assumes the role of the impurity ground state.

Wave function

Within the basis expansion method briefly outlined above, the wave functions of each eigenstate of the matrix problem are readily obtained from the eigenvectors, along with the eigenenergies. What is not immediately obvious is how to determine which eigenstate is a localized state, a quantum well state or a resonant state. The key to this problem turns out to lie precisely in the wave functions. Again we refer to Paper 2 for the details, but the observations which enable us to classify each eigenstate will be repeated here.

In principle any complete basis can be used in an expansion method, but

in our case it is clearly most convenient to use the unperturbed quantum well eigenstates, obtained without any impurity present. This means that each basis state belongs to a particular subband or quantum well energy level. The eigenstates are constructed as specific linear combinations of these basis states, and from the results of our calculations we now observe the following:

- *Localized impurity states* are constructed exclusively from basis states belonging to quantum well levels with higher energy than the impurity state itself.
- *Continuous quantum well subband states* contain only basis states belonging to levels with lower energy than the state in question.
- *Hybridized (coupled) resonant states* have contributions from basis states associated with both higher and lower quantum well levels.

The quantum well states are naturally modified in the presence of the donor. However, unless any hybridization takes place, the only noticeable effect is that the two-dimensional wave vector, which is a good quantum number for the isolated well, no longer is conserved. Instead, states arise that contain a mix of various wave vectors, and this is exactly what brings about the resonant scattering. These states are often referred to as scattering states, which shows the connection to the resonant coupling method, where we in fact assume all eigenstates to be scattering states.

Things are much more interesting under conditions when a coupled resonant state can be formed. In this case the continuous subbands are strongly affected in the energy region close to the resonance, and they acquire, through the hybridization, a partly localized character. At the same time the impurity state becomes partly delocalized. In fact, one can no longer clearly separate impurity states and quantum well states at these energies. Instead we obtain a sequence of hybridized eigenstates which all contain both a localized part and a continuous part, constructed out of the basis states of higher and lower levels, respectively.

In addition to providing these useful insights into the very mechanism of the formation of the hybridized state, the resonant state wave functions also enable the evaluation of the energy width of a coupled resonant state, which we turn to next. We shall return to some further deliberations on the properties of the impurity state wave functions in the section on the central-cell effect later on.

Width

The most important property of a hybridized state, next to the energy position, is its width*. If an electron is initially placed in the shallow resonant state in the barrier it will – due to the hybridization – eventually tunnel into the quantum well and find a lower state. The tunneling time is immediately given by the width of the resonant state. When the donor instead is placed inside the well, the widths of the resonant states largely determine the optical spectrum. Furthermore, the width is closely related to the cross-section of resonant scattering, irrespective of where the donor is situated.

Clearly it is therefore imperative to determine this width in order to clarify the impact of a resonant state on the electronic transport and optical properties of modulation-doped quantum wells. How to calculate it, is however not immediately an easy problem to solve. Simple variational calculations are certainly inadequate, since they assume a completely localized form of the wave function. Instead, we have discovered how the information contained in the hybridized wave function can be used to determine the width.

By plotting, as a function of the energy in an interval around the resonance, the part of the norm of the wave function associated with the localized part of the hybridized state, we obtain exactly the resonance profile mentioned by Fano. Examples of resonance profiles are given in both Paper 1 and Paper 2. More specifically, in the resonant coupling method it is the capture coefficients which are plotted against the energy, whereas in the expansion method we use the basis expansion coefficients. In either case, the resonance profile directly corresponds to the relative norm of the localized part. The profile often, but certainly not always, has a Lorentzian shape, and its width is inversely proportional to the lifetime of the resonant state. The resonance profile is also used to determine the energy of the resonance, defined as the peak position.

The resonant coupling method actually allows for a separate way to determine the width and position of the shallow resonant state, as described in Paper 1, without explicitly using the hybridized wave functions. The values obtained using the two different methods usually agree reasonably well if the donor is not too close to the well. An essentially equivalent method has been attempted for treating also impurities placed inside the well. However, as we have shown†, this approach fails to produce quantitatively correct results,

* We shall in what follows by the width of a state exclusively mean the energy width. The spatial extension of a state, or rather its wave function, is also a relevant quantity in many contexts, and will be referred to as the radius of the state.

† The relevant reference is the last conference paper listed in the Preface on page vi.

as a direct consequence of the neglect of higher-order terms; the Coulomb interaction is simply too strong, compared to the quantum well potential. Only if the coupling is weak, as when the donor is relatively far away from the well, can the resonant coupling method be expected to yield accurate results for the width. The energy position of the lowest resonant state is however reproduced correctly by the coupling method also with the donor inside the well.

The widths of the resonant states differ widely between different materials and quantum well configurations, and naturally depend strongly on which resonant state we actually consider. In any case, when the donor is inside or close to the well, the widths are usually not extremely much smaller than the binding energies. Detailed numerical results are presented in Papers 1 and 2 (and in the conference paper referred to in the footnote on page 21) for both GaAs/AlGaAs and Si/SiGe systems. To summarize, the typical width of the lowest resonant state in a Si well is 1–10 meV, and smaller by about an order of magnitude in GaAs quantum wells, in which the impurity binding energies are also quite much smaller.

It is interesting to consider how the width of the lowest resonant state depends on the impurity position and the quantum well parameters. If the donor is inside a perfectly flat quantum well, as the one shown in Figure 1, the lowest resonant state cannot hybridize unless the parity symmetry is broken, either by not placing the impurity exactly in the middle of the well, or by e.g. applying an electric field across the well. Hence the width of this particular resonant state is zero in the middle of well. As the donor is moved away from the center of the well, the energy width grows quite rapidly, reaching a maximum at a relative offset from the center of approximately 30–35% of the well width. It then decreases to zero, slower than exponentially, as the donor is moved towards the edge and outside of the well. For the shallow resonant states in the barrier, the width decays exponentially with the distance to the well. Very far from the well the shallow impurity states are thus practically completely localized; the width tends to zero and the lifetime becomes infinitely long.

Many factors contribute to the width; the radius (or equivalently the binding energy) of the impurity state is one, in particular when the donor is in the barrier. This is expected, since the radius largely determines the overlap between the impurity state and the quantum well states. For donors inside the well a less obvious influence on the width is observed from the kinetic energy of the continuous states participating in the hybridization. The closer to the bottom of the subband the resonance appears, the broader the resonant state becomes. At the same time, the amplitude of the resonance, as measured by the part of the norm contained in the localized part, decreases if the width increases. Furthermore, or rather as a consequence,

the resonance is wider for wider wells than in narrower ones. It can sometimes be difficult to separate the influence of the kinetic energy from the changes in the overlap matrix elements between the impurity wave function and the quantum well states, due to e.g. the varying of the binding energy or the impurity position. The results obtained in Paper 2 when applying an electric field across the well nevertheless seem to support the conclusion that the influence from the kinetic energy is the dominant one.

When the donor is placed outside the well it often happens that the shallow impurity state is resonant with more than one subband. One then obtains separate values for the width and resonance position for each subband, but they are almost always in agreement with each other. The strong influence of the kinetic energy on the width that we commented on above, when we discussed the resonant states attached to the quantum well subbands, is thus not observed in this case.

Finally, and still for the shallow resonant state in the barrier, the resonance width depends crucially on the alignment of the quantum well levels with the donor energy. This can easily be understood from the formulas derived in Paper 1, since the width is essentially proportional to the density of states at the resonance, which changes abruptly when a subband bottom is crossed. In Paper 4 this effect is demonstrated explicitly, and there we also discuss the influence this may have on the noise spectrum.

Central-cell effect

It is well-known that the binding energies calculated within the effective-mass approximation do not agree with experimentally obtained values. The simple hydrogenic model furthermore predicts, contrary to observations, that the binding energies are the same for all impurity species, and only depend on the host material. These effects primarily apply to the ground state and to lesser extent the excited state of even parity, whereas the energies of odd-parity states are often accurately reproduced. In this section we shall therefore be discussing only the impurity ground state.

The physical reasons for the observed discrepancies are well understood. Effective-mass theory is simply incapable of correctly describing the details of the donor state in the spatial region very close to the impurity atom. Inside the outer electron shells, screening by the valence electrons is absent, and thus the very parameters which determine the effective-mass binding energy, the dielectric constant and the effective mass, are no longer relevant quantities. It is obviously therefore, in principle, impossible to consider these effects within the effective-mass approximation, and one must resort to much more elaborate methods such as first-principles calculations.

The chemical shift – defined as the difference between the hydrogenic

binding energy and the correct value – is often so large that it cannot be ignored. Therefore, attempts have been made to nevertheless obtain a phenomenological model based on effective-mass theory. In these approaches one usually adds to the impurity Coulomb potential a strong attractive short-range potential, with a few adjustable parameters which are chosen such that the calculated ground state binding energy agrees with the experimental observations. This potential is known as the central-cell potential, and its influence is dubbed the central-cell effect. The physical foundation of this approach is precisely the lack of screening close to the nucleus, which increases the strength of the impurity potential substantially.

The central-cell method works reasonably well in bulk materials, but for impurities in quantum wells things are more complicated. The adjustable parameters in the central-cell potential will in the quantum well case depend on the width and depth of the well, and also on the impurity position. Hence the situation becomes quite intractable, since the parameters furthermore must be determined from comparisons with experiments, which then have to be performed for all possible quantum well configurations.

Instead, a different approach, which has also been employed in the bulk case, is to relate the quantum well chemical shift to the amplitude of the envelope (i.e. effective-mass) wave function of the impurity state, at the position of the donor. This can be formally justified (the details are given in Paper 2), but is also intuitively reasonable; the more time the electron spends close to the nucleus, the larger the shift becomes. A simple expression can then be derived, where the chemical shift is found to be proportional to the ratio of two wave function amplitudes, viz. those of the quantum well and bulk impurity states, respectively, both evaluated at the impurity position. The constant of proportionality can be evaluated from the experimental binding energies of the bulk material. For a Si quantum well between SiGe barrier the lattice constant mismatch of these materials adds some further complications, due to the strain splitting of the conduction band, which is also discussed in detail in Paper 2.

A point to carefully consider is what wave function to use for the bulk impurity state. As we have already pointed out, while variational functions may produce accurate binding energies, they need not resemble very closely the true envelope wave function. An important exception, to which we shall return shortly, is that the long-range exponential tail, which is the part which actually determines the binding energy, typically has the correct decay length. But in the region close to the impurity, which is what we need in order to determine the chemical shift, the variational function fails miserably. Instead, we propose to use the amplitude of the wave function obtained within the basis expansion method – which in principle is exact for the envelope function – for very wide wells.

Having expressed the chemical shift through a few parameters, some taken from bulk experiments and other obtained within the basis expansion calculations, it is possible to calculate the ground state shift for any impurity position and for arbitrary quantum well configurations. Numerical results for Si wells are given in Paper 2 and are discussed there. A few key observations deserve to be repeated here, as a sort of summary. On the one hand, it is expected that the central-cell effect is stronger in quantum wells than in the bulk material, in the same way the binding energy itself is larger, due to the additional confinement. This is indeed observed to be the case, and the enhancement can be substantial for narrow wells. On the other hand, the wave function ratio approaches unity rather quickly as the well width is increased, in which case the effect from the strain splitting instead leads to the quantum well chemical shift in Si becoming smaller than the bulk shift. The same actually applies to strained bulk Si, whereas for an unstrained well (such as GaAs) the shift will always be larger than in the corresponding bulk.

The considerations of the previous paragraph apply to the donor being placed in the middle of the quantum well. If it instead is moved towards the edge of the well, the wave function amplitude at the donor position decreases rapidly. This indicates that the electron density of the impurity state is actually not located around the impurity position. We touched upon this while discussing the behaviour of the quantum well impurity states as the donor is moved far into the barrier, but the effect is quite pronounced even while the donor is still inside the well. Hence the chemical shift almost vanishes for donors placed close to the edge of the well. In result, since at the same time the shift is enhanced at central positions, the spreading of the impurity energies in a continuously doped quantum well is further increased by the central-cell effect.

The exponential tail of the donor envelope function is reasonably reproduced by the simple variational hydrogenic function. This is the part which controls the effective-mass binding energy, and at the same time it is also the part which overlaps with the quantum well states and thus determines the degree of hybridization. Furthermore, as we have pointed out, the alignment of the donor energy level relative to the quantum well subbands is a crucial factor, when the donor is placed in the barrier. It is therefore necessary to use not the effective-mass binding energy, but also to account for the chemical shift when calculating the resonance position and the width of the shallow resonant state. Taken together, this leads to the conclusion that we must relinquish the well-established relationship between the donor energy and the radius of its wave function. It might then appear that also the impurity potential must be modified, to include the central-cell potential which then would serve to reproduce the desired binding energy. This is however

not necessary, since that potential has a completely negligible overlap with the quantum well states, and so it can be ignored for the coupling calculations. Hence it is possible to keep the simple hydrogenic wave function, and at the same time use the binding energy taken from experiments.

Why are we interested in them?

As we are nearing the end of this introduction, it is due time to answer the all-important question why resonant states are important – or even interesting. A few hints have already been given, and in this concluding section we shall delve into some of the possible implications and applications of the presence of hybridized impurity states in heterostructures.

One of the corner-stones of practically all scientific work is of course the desire to learn more about everything. To explore the fundamental properties of things – in our case impurity states in modulation-doped quantum wells – is therefore, perhaps somewhat arrogantly, often stated as motivation enough. To this aim, it is hoped that this thesis has brought about a more complete understanding of the behaviour of the impurity states, as the parameters of the donor and the well are changed. By considering different methods for calculating these properties, we have also been able to study the mechanisms of the formation of hybridized resonant states.

The principles we have considered are quite general, although the quantitative results obviously vary between different materials and structures, depending on factors such as the impurity binding energy and the quantum well width and depth. Nevertheless, the developed methods can be used for further investigations in other kinds of potential barriers. One may e.g. be interested in studying impurity-phenomena in resonant tunneling systems.

The importance of resonant states is however far from limited to a mere fundamental theoretical interest. Instead, as was pointed out earlier, hybridized states appear in practically any doped heterostructure, and must be seriously considered in relation to all applications based on these.

One of the most useful aspects of heterostructure devices is the possibility to separate the doping from the active region. By placing the donors at some distance into the barriers, the ionized impurity scattering is strongly reduced. However, we also have to take into account the hybridization of the current-carrying quantum well states with the impurity states. The resulting formation of a resonant state induces resonant scattering in a certain energy interval around the resonance. Scattering is a purely detrimental effect which degrades the performance of the heterostructure by lowering the mobility. A detailed knowledge of all possible scattering mechanisms

is therefore essential for the optimization of high-speed modulation-doped devices.

As we have shown in Paper 1, the width of the resonant state depends strongly (exponentially) on the doping distance. At the same time, the strength of the resonance varies over several orders of magnitude within this energy interval. In result, the resonant scattering mechanism has a very sensitive energy-dependence, and the scattering cross-section furthermore depends crucially on the relative alignment of the quantum well levels and the donor energy.

Scattering is however in many, if not most, respects a dynamic process. It is therefore not possible to properly assess the impact of resonant states on e.g. the mobility by using only the static models considered here so far. The influence on the distribution function and other transport properties must instead be investigated with truly dynamic models like Monte Carlo simulations. The input for such calculations is, among other things, "static" quantities such as the scattering cross-sections, which nevertheless can be calculated by the methods developed in this thesis.

Another process intimately related to both impurities and to the performance of high-speed devices is noise. It is unfortunately impossible to do justice to this enormously important and equally vast field in just a few words, although the concept of noise is intuitively quite easy to understand. Let us just state the obvious fact, that all possible noise mechanisms must be investigated carefully, if one is aiming at a complete understanding and characterization of any electronic device. Noise is also inherently dynamic, and therefore the contribution our results can make is somewhat limited, but certainly not without relevance.

A well-studied type of noise, known as generation–recombination noise, arises from the capture (recombination) of electrons by ionized impurities, and the reverse ionization (generation) process. In bulk materials the capture is often considered as an inelastic process, mediated by phonons, since the impurity states lie in the band gap. The phonons – and also the generation process which is thermal – gives rise to a strong temperature dependence of the noise frequency and amplitude.

With modulation-doping it becomes possible to have elastic capture, by allowing the electron to tunnel into the localized part of the hybridized impurity state. It is then reasonable to assume that the characteristic noise frequency is associated with the lifetime of the shallow barrier resonant state. In this case there is no explicit temperature dependence, and also the noise frequencies are quite different from those otherwise considered for generation–recombination noise. The resonant state lifetime is often of the order picoseconds, which means that the noise lies in the gigahertz range. A detailed knowledge of the properties of the resonant state may there-

fore provide valuable insight into the noise spectrum and its temperature dependence, as we illustrate with a simple example in Paper 4. As with scattering, much further work is however needed to clarify the influence of resonant states on the noise properties of modulation-doped structures.

Noise is most often associated with negative aspects, but noise spectroscopy is also a useful tool for investigating e.g. the properties of impurity states. Most of the results presented in this thesis are only based on theoretical calculations, and it would be most valuable to compare them against experimental results. While the binding energies of the impurity levels are rather simple to measure, it is a challenging task to determine the width of a resonant state. An indirect method, using the noise frequencies to obtain the lifetime, could therefore be of interest.

A more direct way to measure the width of a resonant state would be to use optical absorption, and simply deduce the width from the spectral shape. Although there are some practical difficulties*, coupled resonant states have indeed been observed in such experiments. Now, where there is absorption one can also have emission. If one furthermore can arrange for this emission to be stimulated, the possibility to create a laser opens up.

As a final, but perhaps the most interesting, point we shall now discuss the possibilities of using coupled resonant states in doped quantum wells for optical emitters (and detectors) in the far infrared frequency range. In order to employ the impurity states for optical applications, it is clear that the doping should be placed in the active region, inside the quantum well. In this case the relevant resonant states are those appearing below each subband. We will consider only the lowest resonant state (see Figure 1 on page 8), for two reasons. First, most of the free electrons in the well usually occupy the lowest subband, which is the one resonant with this state. Second, in the limit of an infinitely wide quantum well this impurity level corresponds to the hydrogenic $2p_0$ state, and obviously the impurity ground state corresponds to the hydrogenic $1s$ state. The optical transition between these two states can therefore be expected to be particularly strong – in fact it is known as the resonance line in atomic hydrogen, but the name refers to something different in that case.

As pointed out already, the resonant state we are considering has opposite parity to the lowest subband, and hence they are unable to hybridize if the donor is centered in a flat quantum well. Coupling can however easily be introduced by either moving the impurity position slightly away from the center, or by applying an electric field across the quantum well. In either

* One of the specific hurdles to overcome pertains to the polarization selection rules, as discussed in Paper 2.

case, a coupled resonant state is formed, and the electrons traveling in the subband, under the influence of a bias applied perpendicular to the well growth axis, can be captured into the localized part of the hybridized state. Note that this is exactly the kind of process we try to avoid for high-speed applications, but in those cases nobody would of course think of placing the doping inside the well.

Once the electrons are trapped in the resonant state, they may make an optical transition to the impurity ground state (or for that matter any other lower donor level). The optical matrix element for this transition is quite large and obeys strong polarization selection rules; the calculated spectrum can be found in Paper 2. If it were possible to arrange an inverted population between the ground and the resonant state, one would be able to design a laser based on the mechanism just outlined. The opposite process, absorption from the ground state and ionization of the resonant state into the subband, could furthermore perhaps be used to create a detector.

It should be pointed out that the proposed scheme has already been shown to work, but in a slightly different system. If bulk acceptor-doped Ge is subjected to an external pressure, the heavy and light hole valence bands split and resonant states, of essentially the same character as in the quantum well case, appear. An inverted population can be achieved by impact ionization of the impurity ground state, and a working laser was recently realized on these principles. The need for external pressure is however impractical, and the idea appeared to replace it by the built-in strain due to the lattice mismatch of a SiGe quantum well between Si barriers (still in the valence band). Indeed intense radiation has been observed from such structures, and we present some theoretical and also experimental results on this subject in Paper 3. Unfortunately the complexity of the band structure of the valence band makes it rather difficult to analyze all the relevant details, and this is why we here suggest to use the conduction band instead.

One of the most appealing points of a quantum well resonant state laser is the possibility to control the wavelength of the emitted radiation. The energy distance between the impurity states participating in the lasing transition can be varied over a very wide range, simply because the states are attached to the subbands and these move quite much when the well width changes. As illustrated in Paper 2, the transition energy can be tuned between 25–125 meV (this is in the far infrared) using well widths between 2 and 8 nanometers*. In principle a transverse electric field can also provide some additional fine-tuning, but more importantly such a bias can be used

* Actually, the tuning range is even larger, because the central-cell effect was not accounted for.

to turn on and off the coupling (or at least control the strength of it), in particular if the impurities are placed near the middle of the well.

Naturally a great deal of design work and engineering is always required to develop applications such as the ones discussed there, and all sorts of complications may arise on the rocky road from idea to product. In particular it may be interesting to discuss what material system that would be most suitable to use. Si/SiGe has a number of advantages related with far-infrared optical applications, also from the point of view of possible integration with existing device fabrication technology. The large impurity binding energy gives rise to wide and deep resonant states, which can be populated without having to supply very large kinetic energy to the electrons in the subband. At the same time, however, the large binding energy may make it difficult to devise a mechanism for depopulating the ground state. In this respect GaAs would be more suitable, but in this material other problems soon become apparent, such as the large intrinsic absorption in the relevant wavelength region.

Clearly much work still has to be devoted to the matter, before a quantum well resonant state laser will see the light of day. We shall however not speculate further on these details here; this is a theoretical work, and we are, for now, content with having presented the underlying physical properties which, hopefully, will allow the realization of the envisioned devices. Instead it is appropriate to conclude this introduction on this note, hinting at promising future applications of the results developed in this thesis. Those readers who have been enticed by this summary to inquire further into more specific details of resonant states, are now recommended to proceed with the four articles which follow. We have referred to them now and then in the foregoing discussion, and in particular it should be pointed out that many of the results discussed in words here are illustrated both qualitatively and quantitatively by the various figures in the papers.

General references

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Contains a rich flora of experimental data and theoretical details on modern low-dimensional semiconductor devices.