# Motionally Dependent Bound States in Semiconductor Quantum Wells

R. E. Doezema[(a)] and H. D. Drew

*Department of Physics and Astronomy, Joint Program for Advanced Electronic Materials, and Laboratory for Physical Sciences, University of Maryland, College Park, Maryland 20740*

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With a simple model it is demonstrated that semiconductor quantum wells can exhibit motionally dependent binding. The dependence of binding on transverse motion results from mass mismatch at the quantum-well interfaces and can occur in both parabolic and nonparabolic systems. Accumulation layers on degenerate semiconductors such as $n$-InAs are shown to provide observational evidence for the effect. Implications for quantum-well experiments and applications are discussed.

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With the advent of the technology for creating high-quality quantum wells and superlattices has come a remarkably broad and promising vista of future new semiconductor physics and device applications.[1] Therefore, the nature of the electronic states in such structures is of great current interest. In this Letter we focus on a particular aspect of one-dimensional quantum wells. We find that effective-mass discontinuities at the well-barrier interface can lead to carrier confinement that depends on the transverse motion. Consequently the subband dispersion relations terminate either above or below a critical transverse momentum depending on the mass mismatch. Such a mismatch occurs naturally in quantum wells based on narrow-gap semiconductors and we frame our discussion in terms of nonparabolic systems, but, as we shall see, the characteristic dependence of quantum-well binding on transverse motion occurs whenever a quantum well is formed by materials with differing effective masses. These ideas are used to interpret data on $n$-InAs accumulation layers. In addition we explore some consequences and possible applications of this new effect.

To illustrate the effect we discuss a rectangular potential well in the framework of the two-band model. The results can be generalized to more complicated nonparabolic models and to other potential wells. Figure 1 shows the model: a material with energy gap $E_g = E_1$ and thickness $2a$, sandwiched between material with $E_g = E_2 \geqslant E_1$. The two-band dispersion relations for each material are given by[2]

$$E^2 = (E_1/2)^2 + \beta_{l1} k_{l1}^2 + \beta_{t1} k_t^2,$$
$$(E - V)^2 = (E_2/2)^2 + \beta_{l2} k_{l2}^2 + \beta_{t2} k_t^2, \tag{1}$$

where the wave-vector components along the normal to the layer plane and transverse to it are given by $k_l$ and $k_t$, respectively. Any potential difference is denoted by $V$ (determining the band offset), and $\beta_{l,t} = E_g \hbar^2 / 2m_{l,t}^*$, where $m_{l,t}^*$ are the band-edge mass components.[3] The same $k_t$ appears in each dispersion relation, reflecting translational invariance in the layer plane. For simplicity we have assumed ellipsoidal constant-energy surfaces with rotation axes oriented normal to the interfaces.

At the interfaces, the assumption of continuous two-band envelope wave functions[4-6] gives the bound-state eigenvalue equation:

$$(r\beta_{l1} k_{l1} \tan k_{l1} a - i\beta_{l2} k_{l2})(r\beta_{l1} k_{l1} \cot k_{l1} a + i\beta_{l2} k_{l2}) + k_t^2 (r\beta_{t1} - \beta_{t2})^2 = 0,$$
$$r = (E - V + E_2/2)/(E + E_1/2), \tag{2}$$

containing both even- and odd-parity solutions. For $k_t = 0$, i.e., no motion in the layer plane, bound-state solutions for electrons occur only for $\frac{1}{2}E_1 < E < \frac{1}{2}E_2 + V$ and hole bound-state solutions only for $-\frac{1}{2}E_1 > E > -\frac{1}{2}E_2 + V$. To investigate the effect of a finite $k_t$ on the bound-state solutions, we have numerically solved the eigenvalue equation (2) together with the dispersion relations (1) with the realistic narrow-gap–semiconductor parameters, $E_1 = 200$ meV, $E_2 = 300$ meV, $V + 25$ meV, $2a = 80$ Å, $m_{t1}^* = 0.22 m_0$, and $m_{l1}^* = 0.022 m_0$, where $m_0$ is the free electron mass. While the chosen mass anisotropy is particularly appropriate for the lead salts, for example, it is not critical as we show below by using a second example with an isotropic mass. Additionally, in the spirit of the two-band model, we have assumed that the effective masses scale with the gap energy, i.e., $\beta_{l1} = \beta_{l2}$ and $\beta_{t1} = \beta_{t2}$. The resulting subband dispersion relations are shown in Fig. 1.

At $k_t = 0$ we find two bound-electron solutions and two bound-hole solutions. As $k_t$ increases the hole subbands vanish, whereas additional electron subbands are found (infinitely many). If the sign of $V$ is reversed, electrons can become motionally unbound and holes motionally bound. For $V = 0$ there is no motionally dependent binding in the model with $\beta_{t1} = \beta_{t2}$.

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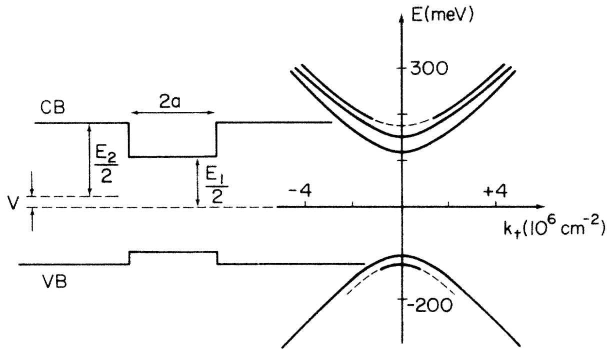


FIG. 1. Model quantum well and subband dispersion. Dashed dispersion curves denote unbound resonant states. For positive $V$, conduction-band (CB) states are motionally bound and valence-band (VB) states are motionally unbound.

Motional binding is not limited to quantum wells in narrow-gap materials. Examination of the dispersion relations (1) in the parabolic limit shows that the longitudinal motion is constrained by an energy barrier given by[7]

$$V_{\rm eff}=V_0+\tfrac{1}{2}\hbar^2k_t^2(1/m_{t2}^*-1/m_{t1}^*), \tag{3}$$

where $V_0=\frac{1}{2}E_2-\frac{1}{2}E_1+V$ is the band offset. Quantum wells composed of materials which have differing effective masses (such as those proposed for effective-mass superlattices[8]) will therefore exhibit motionally dependent binding. Whether the binding is enhanced or reduced with $k_t$ depends on the sign of the mass discontinuity.

We turn now to a related system, an accumulation layer, to demonstrate the observability of motional binding. Accumulation layers at semiconductor surfaces are bound in potential wells formed by the surface barrier, which can often be assumed infinitely high, and a self-consistent screening potential. If the semiconductor is degenerate, and for illustration $n$ type, the Fermi level lies in the conduction band as shown in Fig. 2. Accumulation layers are therefore potential-well systems with finite barrier heights and thus, for nonparabolic semiconductors, will exhibit motionally induced binding. In degenerate systems, as in Fig. 2, a motionally bound subband may be occupied if the energy $E_c$, corresponding to the wave number $k_t=k_c$ at which motional binding begins, lies below the Fermi level $E_{\rm F}$. The occupancy for such a subband $i$ is given by $N_{si}=(k_{\rm F}^2-k_c^2)/2\pi$ for spin degeneracy 2, where $k_{\rm F}$ is the Fermi wave vector for subband $i$ as indicated in the figure. In tunable accumulation layers, where $N_{si}$ is controlled by a gate voltage $V_g$, the occupancy can be varied smoothly from $N_{si}=0$ through the value $k_{\rm F}^2/2\pi$ which occurs when $k_c$ has vanished. This is in sharp contrast to the parabolic case of no motional binding where the occupancy

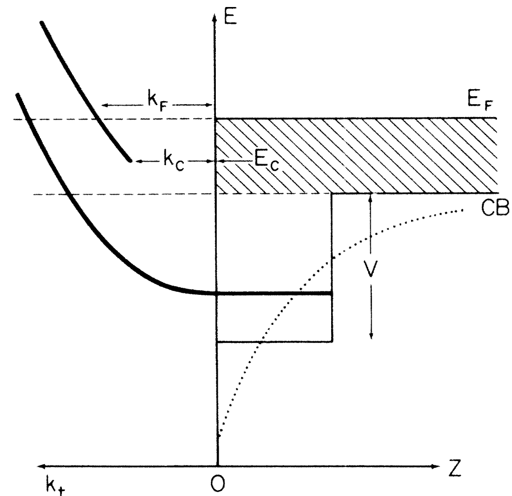


FIG. 2. Accumulation-layer potential and subband dispersion for a degenerate semiconductor. Our calculation models the self-consistent potential (dotted curve) by a half square well with infinite potential step at $z=0$.

would jump discontinuously from 0 to $k_{\rm F}^2/2\pi$ upon binding.[9]

The frequency, $B_f$, of Shubnikov–de Haas (SdH) oscillations for a given subband is given by $B_f=\hbar ck_{\rm F}^2/2e$ (for spin degeneracy 2 and valley degeneracy 1), i.e., it is always determined by a Fermi "surface" area. Thus for $k_c=0$, the SdH frequency is a direct measure of subband occupancy.[10] When $k_c\neq 0$ and a subband is motionally bound, however, the SdH frequency does *not* measure the subband occupancy but is "pinned" to $k_{\rm F}^2$. Such pinning of the SdH frequency has been observed for accumulation layers on $n$-InAs[9] and on $\rm Hg_{1-x}Cd_xTe$,[11,12] but was interpreted in terms of discontinuities in subband occupancies valid only for strictly parabolic systems.

To illustrate the SdH pinning quantitatively, yet avoid the necessary self-consistency of real accumulation layers, we model the potential by a step of depth $V$ and width $a$ in the semiconductor and assume an infinite barrier at the interface. The energy eigenvalues for this well are the odd-parity solutions of the square-well problem discussed above with $E_g=E_1=E_2$. We choose $E_g=400$ meV, $a=200$ Å, and $E_{\rm F}=30$ meV above the conduction-band edge to correspond roughly to the $n$-InAs accumulation layers.[9] For $V$ in the range 70 to 77 meV, the ground-state ($i=0$) solution is bound for all $k_t$, the first excited state is only motionally bound (not bound for $k_t=0$) yet occupied. Figure 3 shows $k_{\rm F}^2$ (proportional to $B_f$) plotted against the subband occupancy together with an inset of the observed behavior[9] for the $i=1$ subband. (The dependence of $N_{s1}$ on gate voltage $V_g$ depends on the details of the screening, of course, but the dependence is one to one.) We believe that

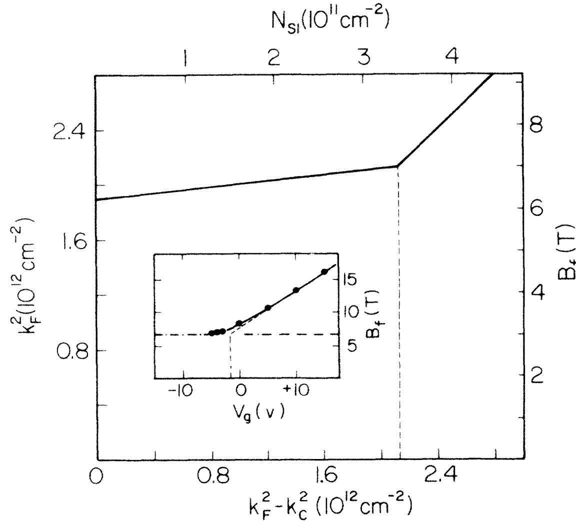


FIG. 3. Calculation SdH frequency vs carrier density in the first excited subband for the model InAs accumulation layer. Parameters are $a = 200$ Å, $E_g = 400$ meV, $E_F = 30$ meV above the conduction-band minimum. Dashed line indicates $N_{s1}$ discontinuity which would occur in a strictly parabolic system. Inset: Observed (Ref. 7) SdH frequency vs gate voltage $V_g$ for the first excited subband for an $n$-InAs sample with $E_F = 30$ meV.

motional binding nicely accounts for the experimental observations.

The existence of motionally bound subbands will also be reflected in a variety of other experiments. The most obvious of these are those which can involve the motionally bound states as initial or final states in electronic transitions. Thus intersubband resonance, intersubband photoemission, and interband photoluminescence will all exhibit effects due to the motional binding. For example, in the accumulation layer we have just discussed, a $0 \to 1$ intersubband resonance will be observable at gate voltages not only below the onset voltage predicted by a $k_t = 0$ calculation, but below the gate voltage at which the $i = 1$ SdH oscillations vanish.

It is instructive to apply the effective potential of Eq. (3) to the InAs case. The nonparabolicity can be approximately included by incorporation of energy-dependent terms in the effective masses: $m_{t1}^* = m_{t1}(0)[1+2E/E_g]$ and $m_{t2}^*(0)[1+2(E-V)/E_g]$. The mass discontinuity, $m_{t2}^* - m_{t1}^*$, is therefore negative and thus $V_{\rm eff} - V$ is positive, leading to enhanced binding with increasing $k_t$ as our model calculation showed. When $V=0$, we also note that $m_{t1}^* = m_{t2}^*$ and there is no motional dependence of the binding as we observed above for the quantum well of Fig. 1. For strictly two-band systems, therefore, the motional binding (or debinding) for finite $V$ is due to the mass discontinuity which results from the nonparabolicity.

Effects of motionally dependent binding are also found in the presence of a magnetic field, as suggested by our use of SdH data in the discussion of the InAs accumulation layer. When the magnetic field is aligned along the normal to the quantum-well interfaces, the energy-level structure may be easily found by replacement of $k_t^2$ in Eq. (1) with $2n/\lambda^2$, where $\lambda$ is the magnetic length $\lambda = (\hbar c/eH)^{1/2}$, and $n$ is the Landau index. Just as the binding energy depends on $k_t$ for the zero-field case, the binding energy depends on the value of $n$ when $H$ has some fixed value. In the case of motionally enhanced binding, it is possible, therefore, to have a situation in which Landau levels for $n$ below some critical index are unbound while those for higher $n$ are bound and compose the Landau ladder corresponding to a given, motionally bound subband. If any such Landau levels lie below the Fermi level, cyclotron resonance corresponding to motionally induced binding can be observed.

When a subband becomes unbound it merges into a set of virtually bound or resonant states as indicated in Fig. 1 with dashed "subbands." In the case of motionally enhanced binding, this leads to the interesting and surprising result that electrons in motionally bound states can escape from the well by losing energy (through acoustic phonon emission for example) and scattering into the lower-lying resonant states. This process may have important applications in the development of infrared detectors[13] or lasers based on quantum wells of mass-mismatched materials. A key feature of such quantum wells is the coupling between the transverse and longitudinal motion. It is intriguing to consider, therefore, the possible utility of this mechanism in the quest for ultrahigh-speed submicron transistors. In a system with motionally enhanced binding, for example, ballistic electrons injected into a quantum-well channel with momentum $k_t$ could pass current in the perpendicular direction only if $k_t$ were below the critical value $k_c$ at which motional binding is induced. Thus the transverse ballistic current would control the perpendicular current.

As a final note we recall the formal analogy[2] between the Dirac equation and the two-band model in semiconductors which was recently exploited, for example, in discussing cyclotron resonance of inversion-layer electrons in InSb for crossed electric and magnetic fields.[14] A quantum well as in Fig. 1 with $E_1 = E_2$ corresponds formally to the one-dimensional square-well case for a Dirac electron capable of three-dimensional motion.

Our purpose in this paper has been to point out that existing[4–6] theories describing the electronic states in quantum wells within the envelope-function approximation predict a dependence of the confinement on the transverse motion whose consequences are observable, and we have used the InAs accumulation layer to demonstrate the observability. Detailed proposals for

device applications will be published elsewhere. In addition, the sensitivity of the motional binding or debinding to the potential $V$ could be exploited to give a measure of the band offset in certain materials. Furthermore, the dependence of the effect on the mass mismatch at the interfaces may allow an experimental study of the validity of the envelope-function approximation.

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[a]Permanent address: Department of Physics and Astronomy, University of Oklahoma, Norman, OK 73019.

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