Robust Level Coincidences in the Subband Structure of Quasi 2D Systems

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Recently, level crossings in the energy bands of crystals have been identified as a key signature for topological phase transitions. In general, three independent parameters must be tuned appropriately to bring two quantum levels into degeneracy. Using realistic models we show that for Bloch electrons in a crystal the parameter space controlling the occurrence of level coincidences has a much richer structure than anticipated previously. In particular, we identify cases where level coincidences depend on only two independent parameters thus making the level coincidences robust, i.e., they cannot be removed by a small perturbation of the Hamiltonian compatible with the crystal symmetry. We consider HgTe/CdTe quantum wells as a specific example.

Recently level crossings in the energy bands of crystals have become a subject of significant interest as they represent a key signature for topological phase transitions induced, e.g., by tuning the composition of an alloy or the thickness of a quasi two-dimensional (2D) system [1–5]. For example, it was proposed [6] and soon after confirmed experimentally [7, 8] that HgTe/CdTe quantum wells (QWs) show a phase transition from spin Hall insulator to a quantum spin Hall regime when the lowest electron-like and the highest hole-like subbands cross at a critical QW width of $\sim$ 65 Å; see also [2, 9–11]. Here we present a systematic study of level crossings and anticrossings in the subband structure of quasi 2D systems. We show that the parameter space characterizing level crossings has a much richer structure than previously anticipated. In particular, we present examples for robust level coincidences that are preserved while the system parameters are varied within a finite range. We take HgTe/CdTe QWs as a specific example, though many results are relevant also for other quasi 2D systems

Level crossings were studied already in the early days of quantum mechanics [12–15]. They occur, e.g., when atoms are placed in magnetic fields in the transition region between the weak-field Zeeman effect and the high-field Paschen-Back effect. Also, they occur when molecules and solids are formed from isolated atoms. Hund [12] pointed out that adiabatic changes of one-dimensional systems — unlike multi-dimensional systems — cannot give rise to level crossings. Von Neumann and Wigner [13] quantified how many parameters need to be varied for a level crossing. While levels of different symmetries (i.e., levels transforming according to different irreducible representations, IRs) may cross when a single parameter is varied, to achieve a level crossing among two levels of the same symmetry, it is in general necessary to vary three (two) independent parameters if the underlying eigenvalue problem is Hermitian (orthogonal). Subsequently, this problem was revisited by Herring [14, 15] who found that the analysis by von Neumann and Wigner was not easily transferable to the energy bands of Bloch electrons in a crystal due to the symmetry of the crystal potential. Similar to energy levels in finite systems, levels may coincide in periodic crystals if the levels have different symmetries. Of course, unless the crystal is invariant under inversion, this can occur only for high-symmetry lines or planes in the Brillouin zone (BZ), where the group of the wave vector is different from the trivial group C_1. If at one end point $\mathbf{k}_1$ of a line of symmetry a band with symmetry Γ_i is higher in energy than the band with symmetry Γ_j, while at the other end point $\mathbf{k}_2$ the order of Γ_i and Γ_j is reversed, these levels cross somewhere in between $\mathbf{k}_1$ and $\mathbf{k}_2$. Herring classified a level crossing as "vanishingly improbable" if it disappeared upon an infinitesimal perturbation of the crystal potential compatible with all crystal symmetries. In that sense, a level crossing at a high-symmetry point of the BZ such as the Γ point $k = 0$ becomes vanishingly improbable. For energy levels with the same symmetry, Herring derived several theorems characterizing the conditions under which level crossings may occur. In particular, he found that in the absence of inversion symmetry level crossings that are *not* vanishingly improbable may occur for isolated points $\mathbf{k}$ such that these crossings cannot be destroyed by an infinitesimal change in the crystal potential, but they will occur at some point near $\mathbf{k}$. Here we will identify several examples for such robust level coincidences. This illustrates that level coincidences for Bloch electrons can be qualitatively different from level coincidences in other systems [13].

Recently, several studies focusing on topological phase transitions recognized the importance of symmetry for level crossings in energy bands [2, 9–11]. Murakami *et al.* [2] studied the phase transition separating spin Hall insulators from the quantum spin Hall regime, focusing on generic low-symmetry configurations with and without inversion symmetry. They found that without inversion symmetry the phase transition is accompanied by a gap closing at points $\mathbf{k}$ that are not high-symmetry

points. In inversion symmetric systems the gap closes only at points $\mathbf{k} = \mathbf{G}/2$ where $\mathbf{G}$ is a reciprocal lattice vector. Here we show that level crossings in quasi 2D systems can be characterized by a multitude of scenarios, taking HgTe/CdTe quantum wells as a specific example for which it is known that the lowest electron-like and the highest hole-like subbands (anti)cross for a critical QW width of about 65 Å [6–8, 16]. In most semiconductors with a zinc blende structure (point group T_d) the s-antibonding orbitals form the conduction band (IR Γ_6 of T_d), whereas the p-bonding orbitals form the valence band (Γ_8 and Γ_7 of T_d). The curvature of the Γ_6 band is thus positive whereas it is negative for the Γ_8 band. For finite $\mathbf{k}$, the fourfold degenerate Γ_8 states (effective spin $j = 3/2$) split into so-called heavy hole (HH, $m_z = \pm 3/2$) and light hole (LH, $m_z = \pm 1/2$) branches. In HgTe, the order of the Γ_8 and Γ_6 bands is reversed: Γ_6 is located below Γ_8 and it has a negative (hole-like) curvature, whereas Γ_8 splits into an electron ($m_z = \pm 1/2$) and a hole ($m_z = \pm 3/2$) branch [17]. HgTe and CdTe can be combined to form a ternary alloy $\mathrm{Hg}_x\mathrm{Cd}_{1-x}\mathrm{Te}$, where the fundamental gap E_0 between the Γ_6 and Γ_8 bands can be tuned continuously from $E_0 = +1.6$ eV in CdTe to $E_0 = -0.3$ eV in HgTe with a gapless material around $x = 0.16$ [17]. Tuning the material composition x thus allows one to overcome Herring's conclusion [14, 15] that a degeneracy at $k = 0$ between two levels of different symmetries is, in general, vanishingly improbable.

Layers of HgTe and CdTe can also be grown epitaxially on top of each other to form QWs. At the interface the corresponding states need to be matched appropriately. The opposite signs of the effective mass inside and outside the well result in eigenstates localized at the interfaces between these materials [18]. We calculate these eigenstates as well as the corresponding subband dispersion $E_\alpha(\mathbf{k})$ using a realistic 8×8 multiband Hamiltonian $\mathcal{H}$ for the bulk bands Γ_6, Γ_8, and Γ_7, which fully takes into account important details of $E_\alpha(\mathbf{k})$ such as anisotropy, nonparabolicity, HH-LH coupling, and spin-orbit coupling both due to bulk inversion asymmetry (BIA) of the zinc blende structure of HgTe and CdTe as well as structure inversion asymmetry (SIA) if the confining potential $V(z)$ of the QW is asymmetric. For details concerning $\mathcal{H}$ and its numerical solution see Refs. [19, 20]. In the following $\mathbf{k} = (k_x, k_y)$ denotes the 2D wave vector.

The symmetry group $\mathcal{G}$ of a QW and thus the allowed level crossings depend on the crystallographic orientation of the surface used to grow a QW [a (001) surface being the most common in experiments]. It also depends on whether we have a system without or with BIA and/or SIA. The resulting point groups are summarized in Table I. We will show below that these different groups give rise to a rich parameter space for the occurrence of level coincidences. For a proper symmetry classification we project the eigenstates of $\mathcal{H}$ onto the IRs of the respective point group [21]. In the following, all IRs are labeled according to Koster *et al.* [22]. As spin-orbit coupling plays a crucial role for BIA and SIA [19], all IRs referred to in this work are double-group IRs. For comparison, Table I also lists the point groups if the prevalent axial (or spherical) approximation is used for $\mathcal{H}$. In this approximation, BIA is ignored and different surface orientations become indistinguishable.

TABLE I: The point group of a QW for different growth directions starting from a bulk semiconductor with diamond structure (point group O_h) or zinc blende structure (point group T_d) for a system without ("sym.") or with ("asym.") SIA.

		[001]	[111]	[110]	[mmn]	[0mn]	[lmn]	axial appr.
O_h	sym.	D_{4h}	D_{3d}	D_{2h}	C_{2h}	C_{2h}	C_i	$D_{\infty h}$
	asym.	C_{4v}	C_{3v}	C_{2v}	C_s	C_s	C_1	$C_{\infty v}$
T_d	sym.	D_{2d}	C_{3v}	C_{2v}	C_s	C_2	C_1	$D_{\infty h}$
	asym.	C_{2v}	C_{3v}	C_s	C_s	C_1	C_1	$C_{\infty v}$

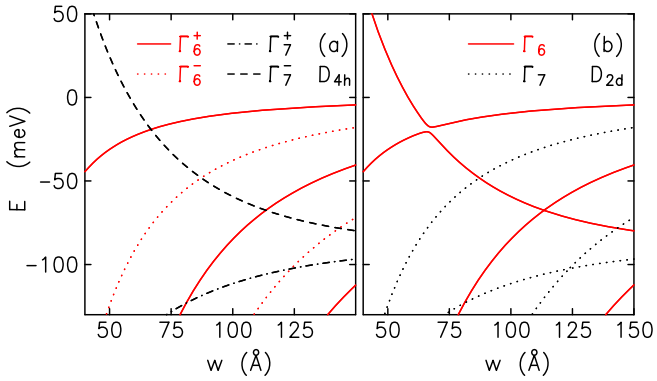

FIG. 1: (Color online) Subband states in a symmetric HgTe/CdTe quantum well (for $k = 0$) as a function of well width w calculated with an 8×8 Hamiltonian (a) neglecting BIA (point group D_{4h}) and (b) with BIA (D_{2d}). States transforming according to $\Gamma_6^\pm$ of D_{4h} (Γ_6 of D_{2d}) are shown in red; states shown in black transform according to $\Gamma_7^\pm$ of D_{4h} (Γ_7 of D_{2d}).

First we neglect the small corrections in $\mathcal{H}$ due to BIA so that the corresponding bulk Hamiltonian has the point group O_h. In the absence of SIA, a quasi 2D system grown on a (001) surface has the point group D_{4h} (which includes inversion) and all electron and hole states throughout the BZ are two-fold degenerate [21]. Subband states in a HgTe/CdTe QW for $k = 0$ as a function of well width w are shown in Fig. 1(a). The HH states (red curves) transform according to $\Gamma_6^\pm$ of D_{4h}. The electron-like and LH-like subbands transform according to $\Gamma_7^\pm$. As expected, the $\Gamma_6^\pm$ and $\Gamma_7^\pm$ subbands may cross as a function of well width.

In the presence of SIA we cannot classify the eigenstates anymore according to their behavior under parity. Without BIA the point group becomes C_{4v}. HH states transform according to Γ_6 of C_{4v} and electron- and LH-

like states transform according to Γ_7. The level crossings depicted in Fig. 1(a) remain allowed in this case [9, 23].

The situation changes when taking into account BIA. Without SIA the point group becomes D_{2d}. In this case all subbands transform alternately according to the IRs Γ_6 and Γ_7 of D_{2d}, irrespective of the dominant spinor components. In particular, both the uppermost HH state and the lowest conduction band state transform according to Γ_6 of D_{2d} so that around $w \simeq 65$ Å we obtain an anticrossing between these levels of about 2.9 meV (for $k = 0$), see Fig. 1(b) [9–11]. With both BIA and SIA the point group becomes C_{2v}. Now we have only one double group IR Γ_5. Thus it follows readily that all subbands anticross as a function of a continuous parameter such as the well width.

While BIA opens a gap at $k = 0$, level crossings remain possible for some $\tilde{\mathbf{k}} \neq 0$ when the well width w is tuned to a critical value $\tilde{w}$, as shown previously by Murakami *et al.* [2]. Considering a (001) surface with BIA, we find, indeed, that *for each direction* ϕ of $\mathbf{k} = (k, \phi)$, critical values $\tilde{w}$ and $\tilde{k}$ exist that give rise to a band crossing. Thus we get a line in $\mathbf{k}$ space where the bands cross when w is varied within some finite range. This result holds for QWs on a (001) surface with BIA, without and with SIA. As an example, Fig. 2(a) shows $\tilde{\mathbf{k}}$ in the presence of a perpendicular electric field $\mathcal{E}_z = 100$ kV/cm.

In general, three independent parameters must be tuned for a level coincidence in a quantum mechanical systems [13] if the underlying eigenvalue problem is Hermitian. While the multiband Hamiltonian $\mathcal{H}$ used here [19] is likewise Hermitian (not orthogonal), only two independent parameters (w and $k = |\mathbf{k}|$) are necessary to achieve a level degeneracy. We have here an example for the robustness of level crossings of energy bands under perturbations that was predicted by Herring [14, 15] to occur in systems without a center of inversion. It demonstrates that level coincidences in energy bands [14, 15] can behave qualitatively different from level coincidences in other quantum mechanical systems [13].

The situation is different for a quasi 2D system grown on a (111) surface. In the absence of BIA and SIA, the point group is D_{3d}. HH states at $k = 0$ transform according to the complex conjugate IRs $\Gamma_5^+ \oplus \Gamma_6^+$ or $\Gamma_5^- \oplus \Gamma_6^-$, where $\oplus$ indicates that these IRs must be combined due to time reversal symmetry. All other subband edges transform according to $\Gamma_4^\pm$. In the presence of BIA and/or SIA the point group becomes C_{3v}. Then HH states transform according to the complex conjugate IRs $\Gamma_5 \oplus \Gamma_6$. Electron-like and LH-like states transform according to Γ_4. Thus it follows that on a (111) surface the HH states always cross the other states at $k = 0$ as a function of a continuous parameter such as the well width [similar to Fig. 1(a)]. The IRs for different geometries starting out from a (001) or (111) surface are summarized in Table II.

Next we consider quasi 2D states on a (110) surface.

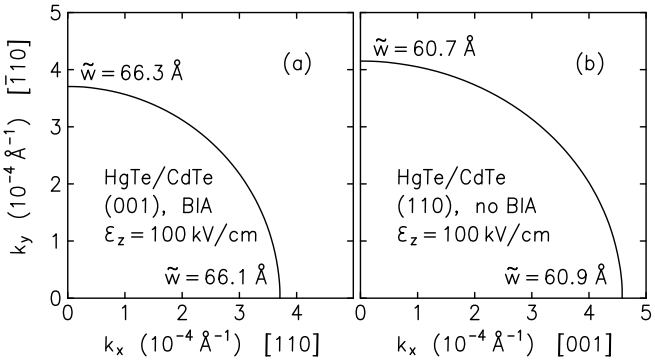

FIG. 2: Critical wave vectors $\tilde{\mathbf{k}}$ that give rise to a level coincidence in a HgTe/CdTe QW (a) on a (001) surface taking into account BIA (b) on a (110) surface neglecting BIA. In both cases a perpendicular field $\mathcal{E}_z = 100$ kV/cm was assumed. In (a) the level coincidence requires a well width $\tilde{w} = 66.1$ Å for $\tilde{\mathbf{k}} \parallel [110]$ and $\tilde{w} = 66.3$ Å for $\tilde{\mathbf{k}} \parallel [\bar{1}10]$. In (b) we have $\tilde{w} = 60.9$ Å for $\tilde{\mathbf{k}} \parallel [001]$ and $\tilde{w} = 60.7$ Å for $\tilde{\mathbf{k}} \parallel [\bar{1}10]$.

TABLE II: Irreducible representations of quasi 2D states on a (001) and (111) surface, starting from a bulk semiconductor with diamond (point group O_h) or zinc blende (point group T_d) structure for a system without ("sym.") or with ("asym.") structure inversion asymmetry.

		(001)			(111)		
bulk		group	c, LH	HH	group	c, LH	HH
O_h	sym.	D_{4h}	$\Gamma_7^\pm$	$\Gamma_6^\pm$	D_{3d}	$\Gamma_4^\pm$	$\Gamma_5^\pm \oplus \Gamma_6^\pm$
	asym.	C_{4v}	Γ_7	Γ_6	C_{3v}	Γ_4	$\Gamma_5 \oplus \Gamma_6$
T_d	sym.	D_{2d}	$\Gamma_{7/6}$	$\Gamma_{6/7}$	C_{3v}	Γ_4	$\Gamma_5 \oplus \Gamma_6$
	asym.	C_{2v}	Γ_5	Γ_5	C_{3v}	Γ_4	$\Gamma_5 \oplus \Gamma_6$

In the absence of BIA and SIA, the point group becomes D_{2h}. Here, all subbands transform alternately according to Γ_5^+ and Γ_5^- with the topmost HH-like subband being Γ_5^+ and the lowest electron-like subband being Γ_5^-. A level crossing as a function of w is thus again allowed at $k = 0$. In the presence of either BIA or SIA the symmetry is reduced to C_{2v}. While the point group in both cases is the same [24], we obtain a remarkable difference between these cases. With SIA the level crossing occurs for a line in $\mathbf{k}$ space, similar to the (001) surface, see Fig. 2(b). With BIA we obtain a level crossing only for $\mathbf{k} \parallel [\bar{1}10]$ with $\tilde{k} \approx 0.0012$ Å^{-1} and $\tilde{w} \approx 62.5$ Å, thus giving an example for the level crossings occurring for isolated points $\tilde{\mathbf{k}} \neq 0$ as discussed by Murakami *et al.* [2]. These examples illustrate that the occurrence of level crossings at either isolated points or along continuous lines in parameter space is not simply related with the system symmetry [24]. In the presence of both BIA and SIA (group C_s) we have the same situation as with BIA only, i.e., adding SIA changes the values of $\tilde{k}$ and $\tilde{w}$, but we keep $\tilde{\mathbf{k}} \parallel [\bar{1}10]$.

Finally, we briefly consider the low-symmetry surfaces

listed in Table I. For all these surfaces with neither BIA nor SIA, we obtain level crossings at $k = 0$, as expected. For (mmn) surfaces with BIA and/or SIA the levels cross for $\tilde{\mathbf{k}} \parallel [\overline{1}10]$. For $(0mn)$ surfaces in the presence of only BIA (only SIA), subbands cross for $\tilde{\mathbf{k}} \parallel [100]$ ($\tilde{\mathbf{k}} \parallel [0\overline{n}m]$). In the presence of both BIA and SIA, the subbands cross for a direction of $\tilde{\mathbf{k}}$ in between these high-symmetry directions that depends on the relative strength of BIA and SIA and can only be calculated numerically. The latter applies also to lowest-symmetry surfaces (lmn) in the presence of BIA and/or SIA (trivial point group C_1).

In conclusion, we have shown that a rich parameter space characterizes the occurrence of level coincidences in the subband structure of quasi 2D systems. In particular, we have identified robust level coincidences that cannot be removed by a small perturbation of the Hamiltonian compatible with the QW symmetry. These level coincidences can be achieved by tuning only two independent parameters such as the thickness of the quasi 2D system and the magnitude (or the direction) of the 2D wave vector. This illustrates that level coincidences in energy bands [14, 15] can behave qualitatively different from level coincidences in other quantum mechanical systems for which it is known that they require the tuning of three independent parameters [13].

As a specific example, we have considered HgTe/CdTe QWs which lately attracted significant interest. While in these systems the range of critical well widths $\tilde{w}$ giving rise to level coincidences is rather small (about 0.1 monolayers), we expect that future research will be able to identify materials showing larger parameter ranges that can be probed more easily in experiments. We emphasize that our symmetry-based classification of level crossings is independent of specific numerical values of the band structure parameters entering the multiband Hamiltonian $\mathcal{H}$ or specific numeric values characterizing the multicomponent eigenfunctions of $\mathcal{H}$. Indeed, our findings are directly applicable also to other quasi 2D systems made of bulk semiconductors with a zinc blende or diamond structure such as hole subbands in GaAs/AlGaAs and SiGe quantum wells. In general, the $\mathbf{k}\cdot\mathbf{p}$ coupling between the LH1 (Γ_7^+ of D_{4h}) and HH2 (Γ_6^-) subbands gives rise to an electron-like dispersion of the LH1 subband for small wave vectors k [25]. If these subbands become (approximately) degenerate at $k = 0$, the coupling between these subbands becomes the dominant effect. This situation is described by the same effective Hamiltonian that characterizes the subspace consisting of the lowest electron and highest HH subband in a HgTe/CdTe QW [6]. It can be exploited if biaxial strain is used to tune the separation between the LH1 and HH2 subbands [26].

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