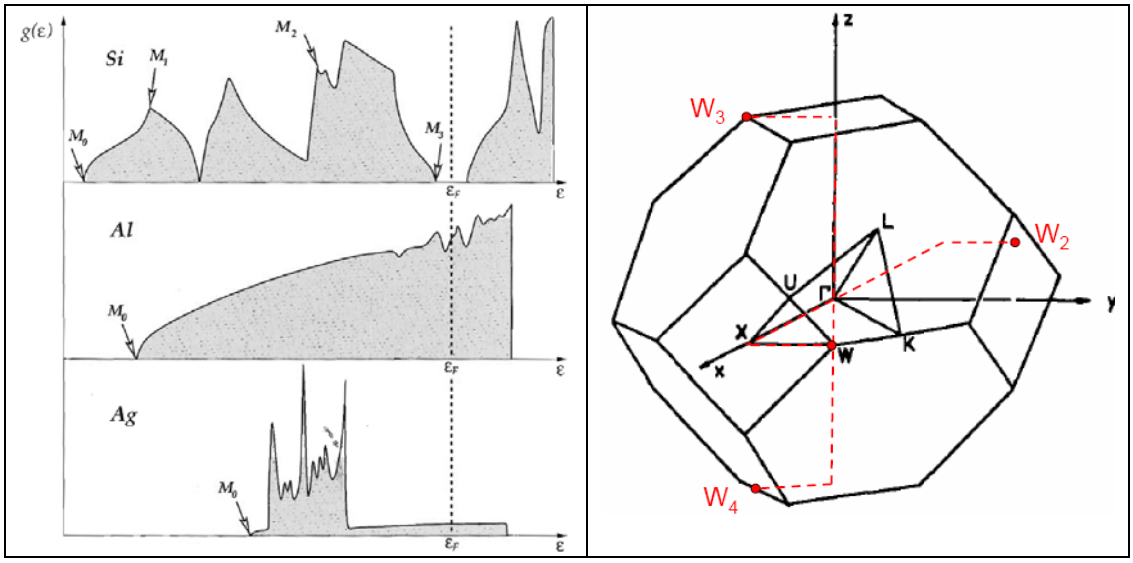
Lines of accidental degeneracies (lines of Dirac points) and Berry phases in electron energy bands: aluminum as an example.



Aluminum is a "free electron metal. The electron density of states, from E. Kaxiras, *Atomic and Electronic Structure of Solids* (Cambridge, 2003), is shown above, and compared with those of Si and Ag. There are three valence electrons, enough to fill the *fcc* Brillouin zone 1.5 times. Thus, a little below the Fermi energy, the bands start to intersect the Brillouin zone boundary. At this point, gaps of order 1 eV or less, open, pushing the lower bands to lower energy and the higher bands to higher energy, but not far enough to open a full gap. In an applied dc magnetic field, oscillations at low T (de Haas-van Alphen effect, and other related effects) can be measured, and show that the geometrical shapes of the Fermi surface are quite complicated. Nevertheless, they can be understood as the consequence of a weak crystal potential. The Brillouin zone is shown in the adjacent figure. The "W" points (at wavevector W=(2π/a)(1,.5,0), one of 24 rotationally similar points) are farthest from the zone center. The corresponding free electron energy (using Rydberg atomic units where Planck's constant is 1 and the mass of the electron is ½) is $\varepsilon_0 = 1.25(2\pi/a)^2$=0.855 Ry, using the lattice constant a=4.02 Angstrom. This lies only 2% below the free electron Fermi energy, $\varepsilon_{F0} = (9/2\pi)^{2/3}(2\pi/a)^2$=0.869 Ry=11.8 eV, using 3 free electrons, per unit cell of one atom. Of the 24 W points, groups of 4 are translationally equivalent, differing by reciprocal lattice vectors. Consider the quartet

$$\begin{aligned}
\vec{W}_1 &= (2\pi/a)(1,.5,0) \\
\vec{W}_2 &= (2\pi/a)(-1,.5,0) = \vec{W}_1 - (2\pi/a)(2,0,0) = \vec{W}_1 - \vec{G}_{200} \\
\vec{W}_3 &= (2\pi/a)(0,-.5,1) = \vec{W}_1 - (2\pi/a)(1,1,-1) = \vec{W}_1 - \vec{G}_{11\bar{1}} \\
\vec{W}_4 &= (2\pi/a)(0,-.5,-1) = \vec{W}_1 - (2\pi/a)(1,1,1) = \vec{W}_1 - \vec{G}_{111}
\end{aligned} \tag{1}$$

These are all translationally "the same" k-vector. If we want to find the energy of the nearly free electron state at the W point, we must solve the 4 x 4 matrix formed by coupling these 4 plane-wave states. It was realized around 1960 by Harrison, Heine, and Ashcroft, that the important region of $\vec{k}$ -space where the Fermi surface is close to zone

boundaries, is mostly quite close to a W point. For a *k*-vector $\vec{k}_1$ close to the W_1 point, the crystal potential will couple the plane wave $|1\rangle = \exp\left(i\vec{k}_1 \cdot \vec{r}\right)$ to three other plane waves $|2\rangle = \exp\left(i\vec{k}_2 \cdot \vec{r}\right)$, $|3\rangle = \exp\left(i\vec{k}_3 \cdot \vec{r}\right)$, and $|4\rangle = \exp\left(i\vec{k}_4 \cdot \vec{r}\right)$, where $\vec{k}_1 = \vec{W}_1 + \vec{\delta}$, $\vec{k}_2 = \vec{W}_2 + \vec{\delta}$, $\vec{k}_3 = \vec{W}_3 + \vec{\delta}$, and $\vec{k}_4 = \vec{W}_4 + \vec{\delta}$. The vector $\vec{\delta}$ is the small increment of wavevector that separates $\vec{k}_1$ from $\vec{W}_1$.

The Hamiltonian matrix for this state is

$$H\left(\vec{k}_1\right) = \begin{pmatrix} \varepsilon_1 & V_4 & V_3 & V_3 \\ V_4 & \varepsilon_2 & V_3 & V_3 \\ V_3 & V_3 & \varepsilon_3 & V_4 \\ V_3 & V_3 & V_4 & \varepsilon_4 \end{pmatrix} \tag{2}$$

where ε_i is the free electron energy $\vec{k}_i^2 = \left(\vec{K}_i + \vec{\delta}\right)^2$, V_3 (often written as V_{111}) is $\langle 3|V|1\rangle = V\left(\vec{G}_{111}\right)$, a Fourier component of the crystal potential, and V_4 (often written as V_{200}) is $\langle 2|V|1\rangle = V\left(\vec{G}_{200}\right)$. Right at the W point, the matrix is particularly simple,

$$H\left(\vec{W}\right) = \begin{pmatrix} \varepsilon_0 & V_4 & V_3 & V_3 \\ V_4 & \varepsilon_0 & V_3 & V_3 \\ V_3 & V_3 & \varepsilon_0 & V_4 \\ V_3 & V_3 & V_4 & \varepsilon_0 \end{pmatrix}, \tag{3}$$

and can be diagonalized easily with the help of group theory. The 48 symmetry operations of the crystal point group O_h generate only 6 translationally distinct W points, so the "little group" of the wavevector W has 8 elements and is D_{2d}. The character table

D_{2d}	E	$2S_4$	C_2	$2C'_2$	$2\sigma_d$	linear functions, rotations	quadratic functions	cubic functions	Plane waves
A_1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2	xyz	$(W_1+W_2+W_3+W_4)/2$
A_2	+1	+1	+1	-1	-1	R_z	-	$z(x^2-y^2)$	
B_1	+1	-1	+1	+1	-1	-	x^2-y^2	-	
B_2	+1	-1	+1	-1	+1	z	xy	z^3, $z(x^2+y^2)$	$(W_1+W_2-W_3-W_4)/2$
E	+2	0	-2	0	0	(x, y) (R_x, R_y)	(xz, yz)	(xz^2, yz^2) (xy^2, x^2y) (x^3, y^3)	$(W_1 - W_2)/\sqrt{2}$ $(W_3 - W_4)/\sqrt{2}$
W	4	0	0	0	2				A_1+B_2+E

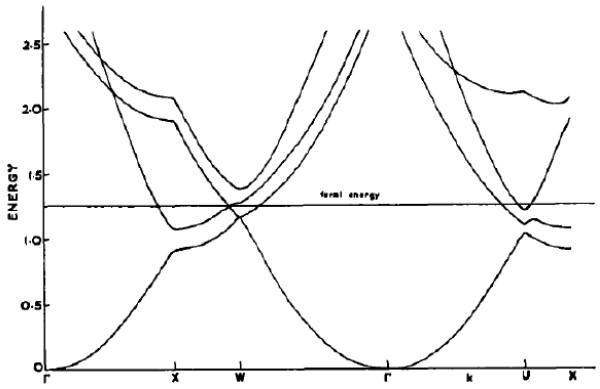
is given above. The z axis is the C_2 axis; the x axis coincides with the C'_2 axis. The four equivalent W points correspond to four different plane waves which generate a 4-dimensional reducible representation, which reduces to A_1+B_2+E. The eigenvectors are columns of the unitary matrix

$$U^{+}=\begin{pmatrix} 1/2 & 1/2 & 1/\sqrt{2} & 0 \\ 1/2 & 1/2 & -1/\sqrt{2} & 0 \\ 1/2 & -1/2 & 0 & 1/\sqrt{2} \\ 1/2 & -1/2 & 0 & -1/\sqrt{2} \end{pmatrix}, \tag{4}$$

and the corresponding eigenvalues are the diagonal elements of $\widetilde{H}=UHU^{+}$,

$$H_0=\widetilde{H}\left(\vec{K}\right)=\begin{pmatrix} \varepsilon_0+2V_3+V_4 & 0 & 0 & 0 \\ 0 & \varepsilon_0-2V_3+V_4 & 0 & 0 \\ 0 & 0 & \varepsilon_0-V_4 & 0 \\ 0 & 0 & 0 & \varepsilon_0-V_4 \end{pmatrix}. \tag{5}$$

Ashcroft found that the Fermi surface data were best fitted by the choices V_3=0.0179 Ry V_4=0.0562 Ry. Thus the doubly degenerate level of E symmetry is lowest, below the Fermi energy, the B_2 level is next, just above the Fermi energy, and the A_1 level is highest. The bands are shown in the picture below, taken from Ashcroft's thesis (N. W. Ashcroft, Phil. Mag. **8**, 2055 (1962).



Notice that this figure shows not only the predicted degeneracy of the lowest band at W, but also a nearby degeneracy, almost (but not exactly) at the Fermi energy, between the band that evolves downward from the B_2 level in the direction W to X, and the upper of the two bands that evolves from the E level at W. The wavevector along this line has the form $\vec{k}=\left(2\pi/a,\pi/a+\delta_y,0\right)$ where δ_y, the y-component of $\vec{\delta}$, is a negative number. The little group of the wavevector is C_{2v}, whose character table is shown below. We see that the E doublet splits into B_1 and B_2, while the A_1 and B_2 singlets have both become A_1 representations. Thus the symmetry labels of the two bands which cross at a small negative δ_y are A_1 and B_1. Since they are different, the crossing is not forbidden by symmetry. In the first set of notes, conditions for having a degeneracy are discussed. For

C_{2v}	E	C_2 (y)	σ_v(zy)	σ_v(xy)	linear functions, rotations	quadratic functions	cubic functions	Plane waves
A_1	+1	+1	+1	+1	y	x^2, y^2, z^2	y^3, x^2y, z^2y	$(W_1+W_2)/\sqrt{2}$ $(W_3+W_4)/\sqrt{2}$
A_2	+1	+1	-1	-1	R_y	xz	xyz	
B_1	+1	-1	+1	-1	z, R_x	zy	zx^2, zy^2, zz^2	$(W_3-W_4)/\sqrt{2}$
B_2	+1	-1	-1	+1	x, R_z	xy	xx^2, xy^2, xz^2	$(W_1-W_2)/\sqrt{2}$
W	4	0	2	2				$2A_1+B_1+B_2$

matrices like this which can be written as real matrices, two equations must be satisfied. In the 2 x 2 case, the conditions are equality of diagonal elements and vanishing of off-diagonal. At the W point, symmetry guarantees both. For the band crossing we see between W and X, symmetry guarantees only the vanishing of the off-diagonal element, and equality of the diagonal elements happens at an accidental point along the line.

Our aim is now to ask how the *k*-points of double degeneracy evolve in *k*-space as we go away from the symmetry line connecting W and X. In the absence of spin-orbit interaction, the Hamiltonian matrix is real and the two conditions can be satisfied along lines in *k*-space where the degeneracy is "accidentally" preserved. To find these, we need to investigate in detail the bands near the K-point. To do this, it is convenient to represent the Hamiltonian as $\widetilde{H}$, that is, not in the original plane-wave basis, but in the basis of eigenstates of H at K. The result is $\widetilde{H} = \widetilde{H}_0 + \widetilde{H}_1$ where $\widetilde{H}_0$ was already constructed, and $\widetilde{H}_1$ is

$$\widetilde{H}_1 = \begin{pmatrix} \frac{\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4}{4} - \varepsilon_0 & \frac{\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4}{4} & \frac{\sqrt{2}(\varepsilon_1-\varepsilon_2)}{4} & \frac{\sqrt{2}(\varepsilon_3-\varepsilon_4)}{4} \\ \frac{\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4}{4} & \frac{\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4}{4} - \varepsilon_0 & \frac{\sqrt{2}(\varepsilon_1-\varepsilon_2)}{4} & -\frac{\sqrt{2}(\varepsilon_3-\varepsilon_4)}{4} \\ \frac{\sqrt{2}(\varepsilon_1-\varepsilon_2)}{4} & \frac{\sqrt{2}(\varepsilon_1-\varepsilon_2)}{4} & \frac{\varepsilon_1+\varepsilon_2}{2} - \varepsilon_0 & 0 \\ \frac{\sqrt{2}(\varepsilon_3-\varepsilon_4)}{4} & -\frac{\sqrt{2}(\varepsilon_3-\varepsilon_4)}{4} & 0 & \frac{\varepsilon_3+\varepsilon_4}{2} - \varepsilon_0 \end{pmatrix}. \quad (6)$$

When the free electron form of the kinetic energies is used, the matrix simplifies. For example, the term $(\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4)/4 - \varepsilon_0$ becomes δ^2. The terms linear in $\vec{\delta}$ cancel because of the symmetric pattern of the four vectors $\vec{K}_i$, shown in the first figure. Similarly, $(\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4)/4$ becomes $(2\pi/a)\delta_y \equiv \Delta_y$. Then the Hamiltonian $\widetilde{H}$, without approximation, is

$$\widetilde{H}(\vec{K}+\vec{\delta}) = (\varepsilon_0 + \delta^2)\hat{1} + \begin{pmatrix} 2V_3+V_4 & \Delta_y & \sqrt{2}\Delta_x & \sqrt{2}\Delta_z \\ \Delta_y & -2V_3+V_4 & \sqrt{2}\Delta_x & -\sqrt{2}\Delta_z \\ \sqrt{2}\Delta_x & \sqrt{2}\Delta_x & -V_4+\Delta_y & 0 \\ \sqrt{2}\Delta_z & -\sqrt{2}\Delta_z & 0 & -V_4-\Delta_y \end{pmatrix}. \quad (7)$$

We are using the upper case delta ($\vec{\Delta} = (2\pi/a)\vec{\delta}$) to denote a scaled wavevector that has units of energy in Rydberg units. The transformed matrix (7) is fully equivalent to Eq.(2). We now use this to study how degeneracies evolve in $\vec{k}$ -space.

The first question is this. According to matrix (7), what is the nature of the degenerate levels (3rd and 4th eigenstates) as the $\vec{k}$ -vector $\vec{\Delta}$ evolves away from the K point $\Delta=0$? To answer this requires degenerate perturbation theory. The Schroedinger equation in matrix form is

$$(\widetilde{H} - E)\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = 0 = \begin{pmatrix} A-E & C \\ C^+ & B-E \end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}, \text{ where } A = \begin{pmatrix} 2V_3+V_4 & \Delta_y \\ \Delta_y & -2V_3+V_4 \end{pmatrix}, \text{ etc.}$$

The symbols α, β denote 2-component column vectors, the first two entries and the last two in the 4-vector eigenstates. We want to solve this to order Δ^2, that is, for energies close to

the unperturbed energy $-V_4$ of the E doublet at k=K. Therefore we can replace A-E by A_0-B_0, and write an effective 2 x 2 matrix,

$$(\tilde{H}_{eff}-E)\beta=0\,,\ \text{with}\ \tilde{H}_{eff}=B-C^{+}(A_0-B_0)^{-1}C\ \text{and}\ (A_0-B_0)^{-1}=\frac{1}{2}\begin{pmatrix}\dfrac{1}{V_4+V_3} & 0\\ 0 & \dfrac{1}{V_4-V_3}\end{pmatrix}.$$

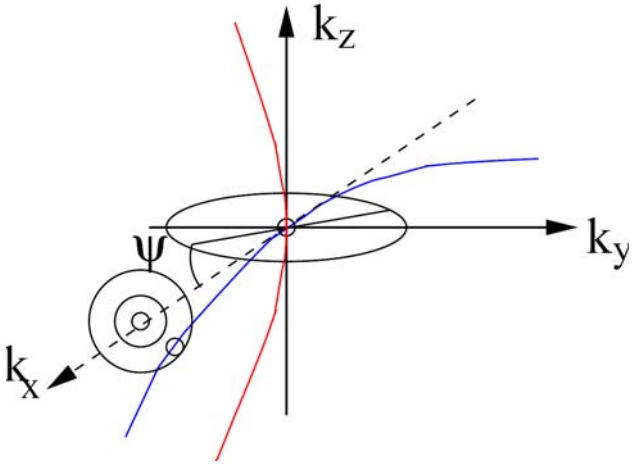
Then the effective Hamiltonian matrix is

$$\tilde{H}_{eff}=\left[-V_4-\frac{V_4\left(\Delta_x^2+\Delta_z^2\right)}{V_4^2-V_3^2}\right]\hat{1}+\begin{pmatrix}\Delta_y+\dfrac{V_4\left(\Delta_z^2-\Delta_x^2\right)}{V_4^2-V_3^2} & \dfrac{2V_3\Delta_x\Delta_z}{V_4^2-V_3^2}\\ \dfrac{2V_3\Delta_x\Delta_z}{V_4^2-V_3^2} & -\Delta_y-\dfrac{V_4\left(\Delta_z^2-\Delta_x^2\right)}{V_4^2-V_3^2}\end{pmatrix}. \qquad (8)$$

This is the approximate version of Eq.(7) relevant to the lower two states, with k not too far from the K point, and E not too far from $-V_4$. The resulting formula for the eigenvalue is

$$E=-V_4-\frac{V_4\left(\Delta_x^2+\Delta_z^2\right)}{V_4^2-V_3^2}\pm\left\{\left[\Delta_y+\frac{V_4\left(\Delta_z^2-\Delta_x^2\right)}{V_4^2-V_3^2}\right]^2+\left[\frac{2V_3\Delta_x\Delta_z}{V_4^2-V_3^2}\right]^2\right\}^{1/2}. \qquad (9)$$

This formula shows that, in order for the two states not to split, two conditions must be satisfied, namely $\Delta_x\Delta_z=0$ and $\left(V_4^2-V_3^2\right)\Delta_y=V_4\left(\Delta_x^2-\Delta_z^2\right)$. There are two ways for this to happen: (1) $\Delta_x=0$ and $\Delta_y=-V_4\Delta_z^2/\left(V_4^2-V_3^2\right)$, or (2) $\Delta_z=0$ and $\Delta_y=V_4\Delta_x^2/\left(V_4^2-V_3^2\right)$. These define two different paths, both passing through K, on which the degenerate states remain "accidentally" degenerate. Both of these paths lie on symmetry planes, $\Delta_x=0$, or $\Delta_z=0$, where symmetry forces a vanishing off-diagonal element, since the two states that stick together now belong to different irreducible representations (they have opposite parity under reflection in the symmetry plane. A schematic view of the two lines, (1) in red, lying in the plane $k_x=\pi/a$ and (2) in blue, lying in the plane $k_z=0$, is shown to the right. What happens to wavefunctions $|\psi_k\rangle$ when they evolve adiabatically on paths that surround these lines of degeneracy? The answer, as we expect from related problems such as the "Dirac points" in graphene, is that they change sign when the path goes once around a single line. But if the path goes around two lines, there is no sign change. These results can be seen explicitly by looking at the eigenstates of $\tilde{H}_{eff}$, Eq.(8). Consider a circular path surrounding one of the degeneracy lines. To be specific, the figure shows a line in the k_y-k_z plane at a fixed positive displacement $k_x=2\pi/a+\Delta_x$ from the K point which is the origin in this figure. The equation of this circle is $\Delta_x=\Delta_0$=const; $\Delta_y=\Delta_1\cos\phi$, and $\Delta_z=\Delta_1\sin\phi$. The non-constant part of the Hamiltonian matrix (8) is



$$\widetilde{H}_{eff,1}\begin{pmatrix} \Delta_1\cos\phi + C_4\left(\Delta_1^2\sin^2\phi - \Delta_0^2\right) & 2C_3\Delta_0\Delta_1\sin\phi \\ 2C_3\Delta_0\Delta_1\sin\phi & -\Delta_1\cos\phi - C_4\left(\Delta_1^2\sin^2\phi - \Delta_0^2\right) \end{pmatrix}.$$

$$= \delta E\begin{pmatrix} \cos\gamma & \sin\gamma \\ \sin\gamma & -\cos\gamma \end{pmatrix} \text{ where } \tan\gamma = \frac{2C_3\Delta_0\Delta_1\sin\phi}{\Delta_1\cos\phi + C_4\left(\Delta_1^2\sin^2\phi - \Delta_0^2\right)}. \qquad (10)$$

Here the constants are defined as $C_3 = V_3/\left(V_4^2 - V_3^2\right)$ and $C_4 = V_4/\left(V_4^2 - V_3^2\right)$. How do the eigenvectors of this matrix evolve as the angle ϕ increases from *0* to 2π? If γ also increases from *0* to 2π, then the eigenvectors change sign. Issues of this kind are discussed in note 1. Note that as ϕ increases from *0* to 2π, the off-diagonal elements evolve as the *y*-component of a full circle, but it is not guaranteed that the diagonal elements evolve as the x-components of such a circle. It depends on whether Δ_1 is greater than $C_4\Delta_0^2$ or not. This is the same as the question whether the radius of the circle is large enough that it surrounds the blue degeneracy line or not. If yes to both, then there is a sign change of the eigenfunction. The math is discussed in more detail in note 1. Thus we see that the aluminum Bloch functions governed by Eq.(10) have a phase shift of π (Berry phase) if they evolve adiabatically around the line of degeneracy.

The next question is a path like the one shown in the center of the figure above, where the path surrounds two different lines of degeneracy. The equation of such a path is $\Delta_x = \Delta\cos\theta$; $\Delta_y = \Delta\sin\theta\cos\phi$, and $\Delta_z = \Delta\sin\theta\sin\phi$, where ϕ is the tilt angle of the path relative to the *y* axis, and θ is the path angle. The non-constant part of the effective Hamiltonian matrix is

$$\widetilde{H}_{eff,2} = \begin{pmatrix} \Delta\cos\theta - C_4\Delta\sin^2\theta\cos 2\phi & C_3\Delta^2\sin^2\theta\sin 2\phi \\ C_3\Delta^2\sin^2\theta\sin 2\phi & -\Delta\cos\theta + C_4\Delta\sin^2\theta\cos 2\phi \end{pmatrix}. \qquad (11)$$

Because the matrix elements involve cos*2*ϕ and sin*2*ϕ, they circulate an even number of times, so the sign of the eigenvector changes an even number of times, and the eigenvector returns to itself with no Berry phase after the circular path around two degeneracy lines is complete. This result is not surprising, but it is reassuring to see it explicitly in a specific example.

Now let us return to the question of the accidental degeneracy of the A_1 and B_1 states along the symmetry line connecting W to X. The 4 x 4 Ashcroft-Harrison matrix Eq.(7) along this line is

$$\widetilde{H}\left(2\pi/a, \pi/a + \delta_y, 0\right) = \left(\varepsilon_0 + \delta^2\right)\hat{1} + \begin{pmatrix} 2V_3 + V_4 & \Delta_y & 0 & 0 \\ \Delta_y & -2V_3 + V_4 & 0 & 0 \\ 0 & 0 & -V_4 + \Delta_y & 0 \\ 0 & 0 & 0 & -V_4 - \Delta_y \end{pmatrix}. \qquad (12)$$

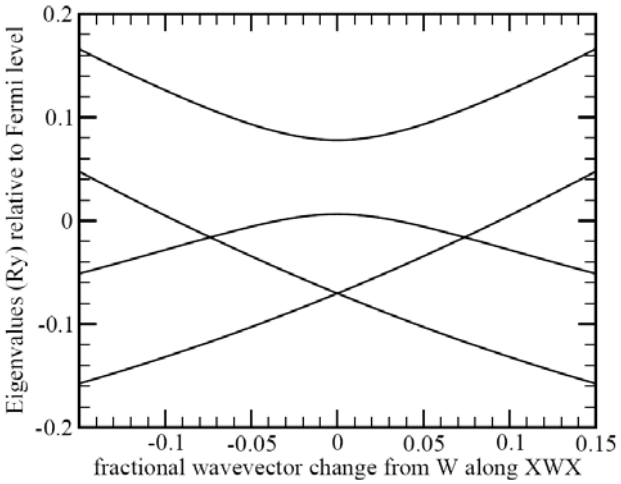
The upper 2 x 2 subblock is the A_1 subspace, and the third and fourth states are the B_2 and B_1 states respectively. The band crossing shown in Ashcroft's picture is at negative Δ_y, where the rising B_1 state crosses the lower (falling) A_1 state. The eigenvalues are: $E_{A_1} = \varepsilon_0 + \delta^2 + V_4 - \sqrt{4V_3^2 + \Delta_y^2}$ and $E_{B_1} = \varepsilon_0 + \delta^2 - V_4 - \Delta_y$. The corresponding eigenvectors are columns of the unitary matrix

$$Y^{+}=\begin{pmatrix}\cos(\chi/2) & \sin(\chi/2) & 0 & 0\\ \sin(\chi/2) & -\cos(\chi/2) & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix} \text{ where } \sin\chi=\frac{V_3^2-V_4^2}{V_3^2+V_4^2}. \tag{13}$$

If we use a dimensionless wavevector η defined as $\vec{k}=(2\pi/a)(1,.5+\eta,0)$, instead of $\Delta_y=(2\pi/a)\delta_y$ which has dimensions of energy, then the point of accidental degeneracy is at

$$\varepsilon=\frac{V_4^2-V_3^2}{\left(\frac{2\pi}{a}\right)^2 V_4}\approx 0.0750\,, \tag{14}$$

about 15% of the way from K toward W. A plot of these bands along this symmetry line is shown to the right. It is symmetric around the W point, which is perhaps not obvious from the picture of the Brillouin zone. Going from W toward the left, $\vec{k}$ evolves toward the X point at the center of the square face of the zone. Going from W along the same path to the right, $\vec{k}$ is outside the first Brillouin zone, but moving directly toward an X point at (2π/a)(1,1,0) = (2π/a)(0,0,1) lying on the face of a copy of the Brillouin zone. In the bands plotted to the right, where the central wavevector is W, negative η has the B_1 branch rising and intersecting the lower A_1 branch; positive η goes from W toward the right hand copy of the X point, with the B_2 branch rising and intersecting. This change of symmetry label from B_1 to B_2 occurs because the orientation of *x* and *z* is switched in this second copy of the square face, and the character table for C_{2v} shows that B_1 and B_2 are interchanged when *x* and *z* are interchanged.



It is a generic result that for real-symmetric matrices, accidental degeneracies require special choices of two independent parameters. In 3-dimensional crystals, there are three directions in $\vec{k}$ -space that can be varied. Thus we should look for a line in $\vec{k}$ -space where this accidental degeneracy persists (or possibly more than one line, as we found when we looked at the W-point E doublet.) To find this line, we first need to rotate the matrix $\tilde{H}$ to the new basis $\tilde{\tilde{H}}=Y\tilde{H}Y^{+}$ which is diagonal at the symmetric accidental degeneracy that we just found on the line between W and X. The result is $\tilde{\tilde{H}}=\tilde{\tilde{H}}_0+\tilde{\tilde{H}}_1$ where $\tilde{\tilde{H}}_0$ is the diagonal matrix at the degeneracy point and $\tilde{\tilde{H}}_1$ contains the deviation caused by moving the wavevector by $\vec{\Delta}_0+\vec{\Delta}_1$, where $\vec{k}=(2\pi/a)(1,.5+\eta,0)=\vec{W}_1+\vec{\delta}_0$ and $\vec{\Delta}_0$ is 2π/a times the wavevector $\vec{\delta}_0$ just found. The results are

$$\tilde{\tilde{H}}_0=\left(\varepsilon_0+\delta_0^2\right)\hat{1}+\begin{pmatrix}2V_4+V_3^2/V_4 & 0 & 0 & 0\\ 0 & -V_3^2/V_4 & 0 & 0\\ 0 & 0 & V_3^2/V_4-2V_4 & 0\\ 0 & 0 & 0 & -V_3^2/V_4\end{pmatrix} \text{ and}$$

$$\tilde{\tilde{H}}_1 = \begin{pmatrix} \sin\chi\Delta_{1y} & -\cos\chi\Delta_{1y} & T_1\Delta_{1x} & T_2\Delta_{1z} \\ -\cos\chi\Delta_{1y} & -\sin\chi\Delta_{1y} & -T_2\Delta_{1x} & T_1\Delta_{1z} \\ T_1\Delta_{1x} & -T_2\Delta_{1x} & \Delta_{1y} & 0 \\ T_2\Delta_{1z} & T_1\Delta_{1z} & 0 & -\Delta_{1y} \end{pmatrix} \text{ where } \begin{matrix} T_1 = \sqrt{2}\left(\cos\frac{\chi}{2} + \sin\frac{\chi}{2}\right) \\ T_2 = \sqrt{2}\left(\cos\frac{\chi}{2} - \sin\frac{\chi}{2}\right) \end{matrix} \quad (15)$$

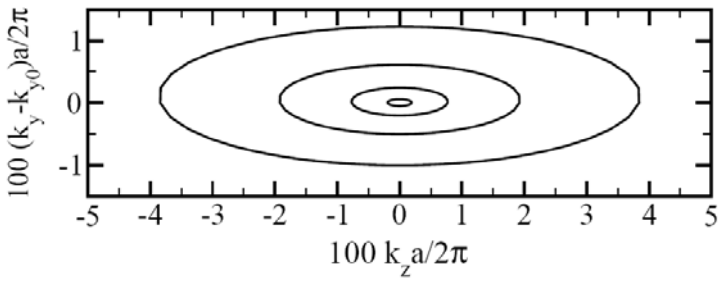
This is still an exact transformation of the original Ashcroft-Harrison 4-band model. At this point, our interest is to see what happens for small excursions $\left|\vec{\Delta}_1\right|$ away from the point of degeneracy at $\vec{\Delta}_1 = 0$, for energies near that of the accidental doublet of $\tilde{\tilde{H}}_0$ at $E = \varepsilon_0 + \delta_0^2 - V_3^2/V_4$. This doublet derives from the 2nd and 4th entries of $\tilde{\tilde{H}}_0$. To first order it is sufficient to truncate to a 2 x 2 matrix formed by crossing out rows and columns 1 and 3 of Eq.(15). The result is

$$\tilde{\tilde{H}}_{truc} = \left[\varepsilon_0 + \delta_0^2 - V_3^2/V_4 - \frac{1+\sin\chi}{2}\Delta_{1y}\right]\hat{1} + \begin{pmatrix} \frac{1-\sin\chi}{2}\Delta_{1y} & T_1\Delta_{1z} \\ T_1\Delta_{1z} & -\frac{1-\sin\chi}{2}\Delta_{1y} \end{pmatrix}. \quad (16)$$

This contains all the information about the first-order splitting of the degeneracy. The eigenvalues are

$$E = \left[\varepsilon_0 + \delta_0^2 - V_3^2/V_4 - \frac{V_3^2}{V_3^2+V_4^2}\Delta_{1y}\right] \pm \frac{\sqrt{\left(V_4^2\Delta_{1y}\right)^2 + 8\left(V_3^2\Delta_{1z}\right)^2}}{V_3^2+V_4^2}. \quad (17)$$

This tells us that the degeneracy is lifted to first order in the k_y and k_z directions, giving an anisotropic Dirac dispersion. The shape of the constant energy surfaces is shown below in the plane $\Delta_{1x} = 0$, at constant increments of energy. Note that the splitting does not depend on the absolute magnitude of the Fourier coefficients of the potential, only on the relative size V_3/V_4. In the k_x direction, there is no splitting. There is a line of Dirac points perpendicular to the square Brillouin zone faces. In higher order, Eqs. (15) show that the accidental degeneracy line will not depart from the symmetry plane $\Delta_{1z} = 0$. On this plane, the 4th eigenstates is odd under reflection in the plane and the other 3 are even. This makes the off-diagonal element in any 2 x 2 truncation rigorously zero. The remaining parameters Δ_{1x} and Δ_{1y} must be tuned to make the diagonal elements equal, giving a line in Δ_{1x}, Δ_{1y} space. The energy of this line of Dirac points increases toward the Fermi energy as it moves away from the WX symmetry line (this happens when Δ_{1y} is negative) and pops through the Fermi surface, as noticed by Ashcroft.



Finally, let us look at eigenfunctions. Using the particular Ashcroft choices of V_3 and V_4, we can write the 2 x 2 Hamiltonian in "real units" as

$$\tilde{\tilde{H}}_{truc} = \left[\varepsilon_0 + \delta_0^2 - V_3^2/V_4 - .0921\frac{2\pi}{a}\left(k_y - k_{y0}\right)\right]\hat{1} + \frac{2\pi}{a}\begin{pmatrix} .908\left(k_y - k_{y0}\right) & .607k_z \\ .607k_z & -.908\left(k_y - k_{y0}\right) \end{pmatrix}. \quad (19)$$

This is the form used for the energy contour plot. If we define new variables, the matrix simplifies to

$$\tilde{\tilde{H}}_{truc} = E(\vec{k}_0)\hat{1} + \frac{2\pi}{a}\delta\begin{pmatrix}\cos\xi & \sin\xi \\ \sin\xi & -\cos\xi\end{pmatrix} \quad \text{where} \quad \begin{aligned}\delta\cos\xi &= .908(k_y - k_{y0}) \\ \delta\sin\xi &= .607k_z\end{aligned} \tag{20}$$

Lines of constant δ are ellipses in the k_y-k_z plane. As the angle ξ circulates from *0* to 2π, an elliptical path around the Dirac point is followed, and the eigenfunction acquires a Berry phase $\exp(\pm i\pi)$.