

**The Angle Resolved Photoemission Pseudogap and Anomalous Background
of Underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ as Evidence for a Fermi Level Band Crossing**

Jason K. Perry and Jamil Tahir-Kheli

First Principles Research, Inc.

8391 Beverly Blvd., Suite #1711, Los Angeles, CA 90048

www.firstprinciples.com

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Abstract. We show that the unusual observations of a pseudogap in the normal state of underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BiSCO) using angle resolved photoemission spectroscopy (ARPES) is consistent with a new band structure for the cuprate superconductors in which the $x^2 - y^2$ and z^2 bands are seen to cross at the Fermi level. Limitations in the experimental method prevent the narrow 3D z^2 band from being fully resolved, leading instead to a broad background with “stepfunction” character. As a consequence, the Fermi surface is mis-assigned and a pseudogap of approximately d-wave symmetry develops.

A requirement of the BCS theory of superconductivity and its extensions is the formation of a non-zero gap at the Fermi energy if and only if the material is in the superconducting state ($T < T_c$). Thus the observation of an approximate $d_{x^2-y^2}$ gap in the normal state ($T > T_c$) of underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BiSCO) using angle-resolved photoemission spectroscopy (ARPES) is highly unexpected.¹ Present explanations for this phenomenon speculate that above T_c Cooper pairs are formed without long-range order of the wavefunction, producing a pseudogap without superconductivity. Below T_c , the wavefunction has long-range phase order and superconductivity appears. However a detailed theoretical formulation of Cooper pairing without coherence is lacking.

In this paper, we argue the ARPES pseudogap is *not* the result of Cooper pair formation above T_c , but arises simply from the crossing of two bands at the Fermi level. While conventional LDA band structure calculations do not predict the existence of two such bands, we demonstrated in a series of articles that correlation, which is well acknowledged to be missing in these calculations, changes the band structure more radically than previously assumed.² The new band structure is characterized by a narrow 3D $\text{Cu } d_{z^2}/\text{O}' p_z$ band (z^2) which crosses the broader, nearly 2D $\text{Cu } d_{x^2-y^2}/\text{O } p_\sigma$ band ($x^2 - y^2$) at the Fermi level. Our calculated band structure for optimally doped $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ (LaSCO) is shown in Figure 1. Significantly, a degeneracy of the two bands is allowed by symmetry along the $(0, 0) - (\pi, \pi)$ direction of the Brillouin zone. Elsewhere in the Brillouin zone the bands repel. This observation proves to be the essential ingredient in the Interband Pairing Theory (IBP) of high temperature superconductivity.³ This theory postulates the formation of a new type of Cooper pair (interband pair) comprised of a $k \uparrow$ electron from one band and a $-k \downarrow$ electron from another band in the vicinity of the $x^2 - y^2$ and z^2 symmetry allowed crossing. As described in the above references, IBP can explain a broad range of experimental data from simple band structure arguments. Such experimental data includes the observed d-wave Josephson tunneling (and by extension the ARPES d-wave superconducting gap), the temperature dependence of the Hall effect, the NMR, the mid-IR absorption, and the incommensurate neutron scattering.³

The origin of the pseudogap in our scenario is due to the difference in the 3D dis-

persion of the $x^2 - y^2$ and z^2 bands and the fact that ARPES is a method that maps a Fermi surface in 2D. Electrons ejected from k states with predominantly z^2 character produce a broad linewidth in ARPES and hence an unresolvable quasiparticle peak. A mis-assignment of the Fermi surface results and with it the pseudogap. This pseudogap is a direct measure of $x^2 - y^2/z^2$ band repulsion, which has approximately d-wave symmetry. From these considerations, described in detail below, we conclude the pseudogap is evidence for a Fermi level band crossing and is unrelated to the d-wave superconducting gap. We further show by calculation that the anomalous background spectrum present in all cuprate ARPES data is due to both primary and inelastically scattered secondary electrons associated with the narrow z^2 band.

ARPES on optimally doped and overdoped BiSCO yields a single holelike Fermi surface closed around (π, π) .⁴ At temperatures below T_c , the Fermi surface exhibits a d-wave gap with a node along the $(0, 0) - (\pi, \pi)$ direction.⁵ This gap disappears isotropically as the temperature is increased to T_c , as one would expect for a superconducting gap. For underdoped BiSCO, the situation is different as follows:

- 1.) The gap does not appear to be purely d-wave.⁶
- 2.) The temperature dependence of the gap is anisotropic.⁷
- 3.) The gap grows larger as the material is further underdoped and T_c is decreased.
- 4.) The gap persists through temperatures above T_c .¹

Based on our calculated band structure for LaSCO, we conclude the following:

- 1.) The $x^2 - y^2$ band is broadly dispersing in the CuO_2 planes (x and y directions) and narrowly dispersing normal to the planes (z direction). It is an approximately 2D band.
- 2.) The z^2 band is narrowly dispersing in the x and y directions and moderately dispersing in the z direction. It must be considered a 3D band.
- 3.) The two bands cross at or near the Fermi level. The crossing is allowed by symmetry along the $(0, 0) - (\pi, \pi)$ diagonal but avoided elsewhere in the Brillouin zone.

In order to reconcile this proposed band structure with the Fermi surface mapped by ARPES, one must consider the limitations in the ARPES method.⁸ The experimentally measured ARPES linewidth Γ_m , is a combination of the linewidth or lifetime of the photohole Γ_{hole} (hole state left behind by the excited electron) and the linewidth of the photoelectron Γ_{elec} (excited state of electron after photon absorption). It is given approximately by,

$$\Gamma_m = \Gamma_{hole} + (v_{i,z}/v_{f,z})\Gamma_{elec}, \quad (1)$$

where $v_{i,z}$ is the average Fermi velocity of the photohole in the z direction, and $v_{f,z}$ is the average Fermi velocity of the photoelectron in the z direction. While $\Gamma_{hole} \rightarrow 0$ at the Fermi level, Γ_{elec} is generally greater than or on the order of 1.0 eV.

For the very 2D $x^2 - y^2$ band, dispersion in the z direction is negligible compared to that in the x and y directions. Hence, $v_{i,z}$ is expected to be small relative to $v_{f,z}$. Thus $\Gamma_m \approx \Gamma_{hole}$, leading to a resolvable quasiparticle peak and a well defined Fermi surface crossing for k states with predominantly $x^2 - y^2$ character.

In contrast, the z^2 band is narrowly dispersing in the x and y directions but has larger dispersion in the z direction. For this band, there is no reason to expect that $v_{i,z}$ is not comparable to $v_{f,z}$. Thus, the contribution from the linewidth of the photoelectron cannot be neglected, leading to a broad peak cutoff by the Fermi function. For k states with predominantly z^2 character, there will be no resolvable quasiparticle peak but instead a signal that looks like a step function.

Given that only the $x^2 - y^2$ band leads to a well resolvable peak with ARPES, the band structure for LaSCO produces a Fermi surface shown in Figure 2, in excellent agreement with recent observations for this material.⁹ The z^2 band contributes only to a broad background signal. Such a signal has been a signature in ARPES on the cuprates, but has always been regarded with confusion.⁴⁻⁸ Careful experiments with light polarization and photon energy dependence may resolve if this background is due to z^2 character. Such experiments have been done to confirm that the major resolvable peak is in fact due to

$x^2 - y^2$ character.^{8,10} The analysis is unfortunately complicated by secondary inelastic scattering processes which may indeed dominate the background signal. Such processes have previously been considered and dismissed as the source of the background because the conventional band structure could not produce a large enough signal and the observed step function character.^{8,11} However, in Figure 3, we show the signal due to inelastic scattering from our calculated band structure for LaSCO leads to a background which is significantly larger than that obtained from the conventional $x^2 - y^2$ band structure. The inelastic scattering is proportional to the integrated density of states. Thus, the signal is dominated by the very narrow z^2 band with a large density of states within 0.1 eV of the Fermi level leading to the correct step function character near the Fermi level. The final ARPES lineshape is composed of primaries from both the $x^2 - y^2$ and z^2 bands as well as secondaries.

The observation of a pseudogap in the cuprates occurs when the true Fermi surface is dominated by z^2 character. The locus of (k_x, k_y) points that comprise the Fermi surface is determined by measuring spectra as one scans through the Brillouin zone from occupied k states to unoccupied k states. A quasiparticle peak appears as one approaches the Fermi surface and disappears as one scans through the Fermi surface. With our band structure, the dispersing quasiparticle peak will collapse in k space when we cross from states with predominantly $x^2 - y^2$ character (*i.e.* narrow linewidth) to states with predominantly z^2 character (*i.e.* broad linewidth). The extent (and possibly position) of the collapse of the quasiparticle peak is also subject to matrix element effects, which are different for $x^2 - y^2$ and z^2 . Should this crossover occur for k states below the Fermi level, the Fermi surface will be mis-assigned. For lower temperatures, the leading edge will be below the Fermi level, leading to the appearance of a pseudogap. At sufficiently high temperatures the $x^2 - y^2$ hole linewidth will be large enough that the leading edge of the spectra will be at the Fermi level, closing the pseudogap anisotropically with temperature.⁷

In order to explain the pseudogap in BiSCO, we need to qualitatively understand its band structure. While we have so far only calculated the band structure for LaSCO,

simple topological arguments can be used to understand BiSCO. The principal difference between the two materials is that BiSCO has two CuO_2 planes per unit cell instead of one. This means there will be bonding and antibonding combinations of both the $x^2 - y^2$ and z^2 bands leading to a total of four key bands instead of two. Of these, the two $x^2 - y^2$ bands are nearly degenerate (there is little z axis coupling between them), but the two z^2 bands should be reasonably split in energy such that only three bands (the two $x^2 - y^2$ bands and the antibonding z^2 band) are important at the Fermi level. The fourth bonding z^2 band should be lower in energy.

In Figure 4, we present a schematic of the dispersion of the three key bands along the symmetry lines $(0, 0) - (\pi, \pi)$ and $(\pi, 0) - (\pi, \pi)$. The shaded region in the figure for z^2 antibonding shows the spread in the dispersion of this band as a function of k_z . The two $x^2 - y^2$ bands will vary little as a function of k_z due to their approximately 2D character. Along $(0, 0) - (\pi, \pi)$, the different reflection symmetries of $x^2 - y^2$ versus z^2 allow the bands to cross. This crossing, which is crucial to IBP, can persist at the Fermi level over a range of dopings due to the z -axis dispersion of the z^2 band. From $(\pi, 0) - (\pi, \pi)$, only the $x^2 - y^2$ bonding and z^2 antibonding bands can cross and only if $k_z = \pi/c$ or $k_z = 0$. Elsewhere there is no symmetry to forbid mixing and the three bands must repel. This repulsion has approximately d-wave symmetry.

Figure 5 shows the approximate characters of the three bands in a 2D Brillouin zone. One can see that the top band has $x^2 - y^2$ antibonding character near (π, π) that changes over to z^2 antibonding character at $(0, 0)$ and $(\pi, 0)$. The middle band has $x^2 - y^2$ bonding character at (π, π) that changes over to z^2 antibonding for a small region and then changes again to $x^2 - y^2$ antibonding character at $(0, 0)$ and $(\pi, 0)$. The lowest band is z^2 antibonding at (π, π) that becomes $x^2 - y^2$ bonding at $(0, 0)$ and $(\pi, 0)$. For all relevant dopings of BiSCO, the Fermi surfaces of all three bands will be dominated by z^2 character.

Following our argument above, ARPES will mis-assign the Fermi surface as the locus of (k_x, k_y) points where character changes from antibonding z^2 to antibonding $x^2 - y^2$ in Band 2, as indicated by the dashed line. Along the $(0, 0) - (\pi, \pi)$ diagonal, there are always $x^2 - y^2$ states at the Fermi level since the $x^2 - y^2$ and z^2 bands can be degenerate here.

This leads to a zero gap (*i.e.* node) along the diagonal. Scanning from $(\pi, 0) - (\pi, \pi)$, the $x^2 - y^2$ states lie *below* the Fermi level due to band repulsion, producing a gap. Thus, the approximately d-wave pseudogap in BiSCO and related materials is due to a simple mis-assignment of the Fermi surface.

In regard to the relationship between the pseudogap and the superconducting gap, as argued elsewhere,³ the symmetry of interband pair to BCS pair scattering produces a d-wave superconducting gap which forces conventional BCS scattering to adopt this phase. The possibility of interband pair to interband pair scattering should produce an additional gap at the nodes, but this would be extremely difficult to observe with ARPES due to its strong k_z dependence. The confusion as to the pseudogap arises because when the material is underdoped, the pseudogap is larger in magnitude than the superconducting gap, completely obscuring its presence. As doping is increased, the pseudogap is expected to decrease in magnitude as the Fermi level nears the region where Band 2 switches to $x^2 - y^2$ antibonding character. Simultaneously, the superconducting gap is expected to increase in magnitude. At some point the superconducting gap is expected to be greater in magnitude than the pseudogap, thus obscuring its presence. Eventually the pseudogap will disappear entirely as the Fermi surface becomes increasingly $x^2 - y^2$ -like. This behavior is consistent with that observed for underdoped, optimally doped, and overdoped BiSCO.

It is important to note that since bands change character smoothly, we have not defined exactly what k point is the crossover from $x^2 - y^2$ to z^2 . The crossover momentum is dependent on the sizes of the $x^2 - y^2$ and z^2 ejection matrix elements and these clearly are dependent upon the incident photon energy. Thus, the controversy over recent observations of a different Fermi surface for BiSCO when the photon energy is ≈ 33 eV¹² are not in direct contradiction with the older $\approx 20 - 25$ eV results, but instead demonstrate that measuring Fermi surfaces using ARPES is not completely straightforward when the relevant bands include orbitals with real 3D dispersion.

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References

- ¹A.G. Loesser, *et al.*, Science **273**, 325 (1996); H. Ding, *et al.*, Nature **382**, 51 (1996).
- ²J.K. Perry and J. Tahir-Kheli, Phys. Rev. B **58**, 12323 (1998); J.K. Perry, J. Phys. Chem., in press (cond-mat/9903088); J.K. Perry and J. Tahir-Kheli, Phys. Rev. Lett., submitted (cond-mat/9907332). See also *www.firstprinciples.com*.
- ³J. Tahir-Kheli, Phys. Rev. B, **58**, 12307 (1998); J. Tahir-Kheli, J. Phys. Chem., in press (cond-mat/9903105); J. Tahir-Kheli, Phys. Rev. Lett., to be submitted; J. Tahir-Kheli and J.K. Perry, to be published. See also *www.firstprinciples.com*.
- ⁴H. Ding, *et al.*, Phys. Rev. Lett. **76**, 1533 (1996).
- ⁵Z.-X. Shen, *et al.*, Phys. Rev. Lett. **70**, 1553 (1993); H. Ding, *et al.*, Phys. Rev. B **54**, 9678 (1996).
- ⁶J. Mesot, *et al.*, to be published (xxx.lanl.gov/cond-mat/9812377).
- ⁷M.R. Norman, *et al.*, Nature **392**, 157 (1998).
- ⁸N.V. Smith, P. Thiry, and Y. Petroff, Phys. Rev. B **47**, 15476 (1993); Z.-X. Shen and D.S. Dessau, Phys. Rep. **253**, 2 (1995).
- ⁹A. Ino, *et al.*, J. Phys. Soc. Japan **68**, 1496 (1999).
- ¹⁰H. Ding, *et al.*, Phys. Rev. Lett. **76**, 1533 (1996).
- ¹¹L.Z. Liu, J. Phys. Chem. Solids **52**, 1471 (1991).
- ¹²Y.-D. Chuang, *et al.*, Phys. Rev. Lett. **83**, 3717 (1999); D.L. Feng, *et al.*, to be published (cond-mat/9908056); H.M. Fretwell, *et al.*, to be published (cond-mat/9910221); J. Mesot, *et al.*, to be published (cond-mat/9910430).

Figure Captions.

Figure 1. Calculated 3D band structure for optimally doped LaSCO (see reference 2). Band dispersion along (k_x, k_y) symmetry lines is given for $k_z = 0, \pi/c,$ and $2\pi/c$. Note the $x^2 - y^2$ and z^2 bands cross along the $(0, 0) - (\pi, \pi)$ symmetry line but repel near $(\pi, 0)$.

Figure 2. Calculated 2D Fermi surface (solid line) for optimally doped LaSCO that would be observed by ARPES. The true Fermi surface also contains 3D character, cross sections of which are represented by the dotted lines. This 3D component contributes to a broad background signal with no resolvable Fermi surface in the ARPES spectrum.

Figure 3. Integration over the occupied density of states for our calculated band structure for LaSCO vs. a conventional $(x^2 - y^2)$ only band structure. The ARPES background signal due to inelastic scattering is directly proportional to this curve. The background signal predicted from our band structure is in excellent agreement with that which is observed.

Figure 4. Schematic of the dispersion in BiSCO for the $x^2 - y^2$ bonding, $x^2 - y^2$ antibonding, and z^2 antibonding bands along the $(0, 0) - (\pi, \pi)$ and $(\pi, 0) - (\pi, \pi)$ symmetry lines. The two $x^2 - y^2$ bands cross the z^2 band along the $(0, 0) - (\pi, \pi)$ direction, but band repulsion opens up an energy gap in the $x^2 - y^2$ states along the $(\pi, 0) - (\pi, \pi)$ direction. The energy scale of the figure is $\approx 0.2-0.3$ eV.

Figure 5. Schematic of the character of the three key bands in BiSCO. The true Fermi surface (which is approximately indicated by the solid and dotted lines) has significant 3D character and cannot be easily pinned down. As a result, ARPES mis-assigns the Fermi surface as indicated by the dashed line. An approximate d-wave pseudogap is produced from this mis-assignment.

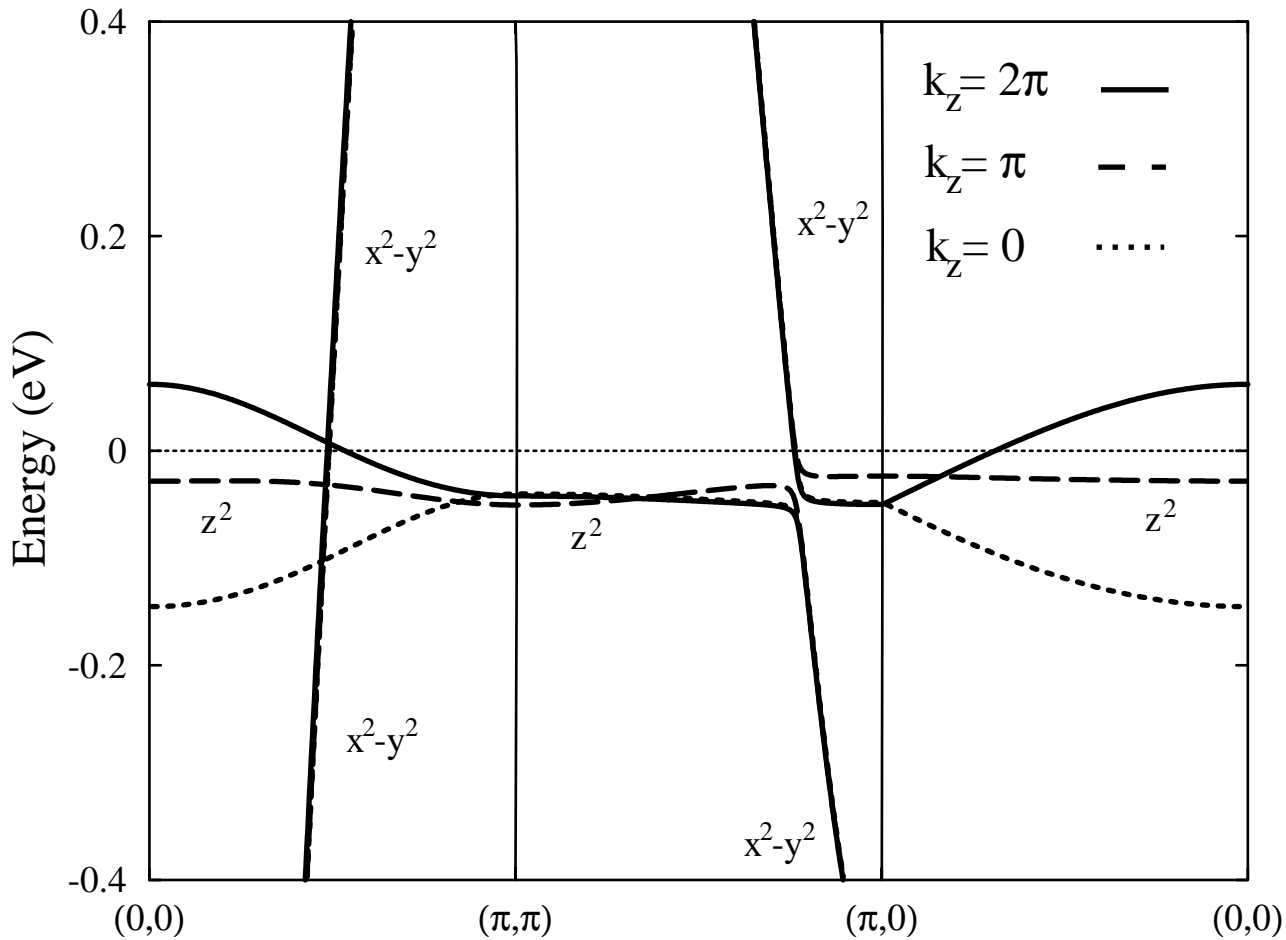


Figure 1

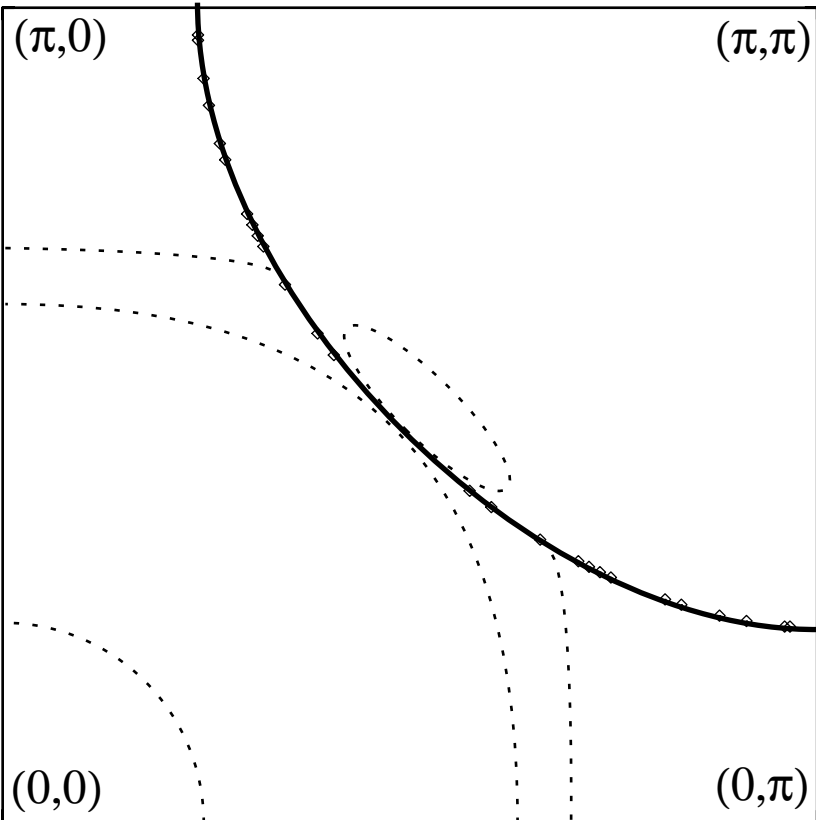


Figure 2.

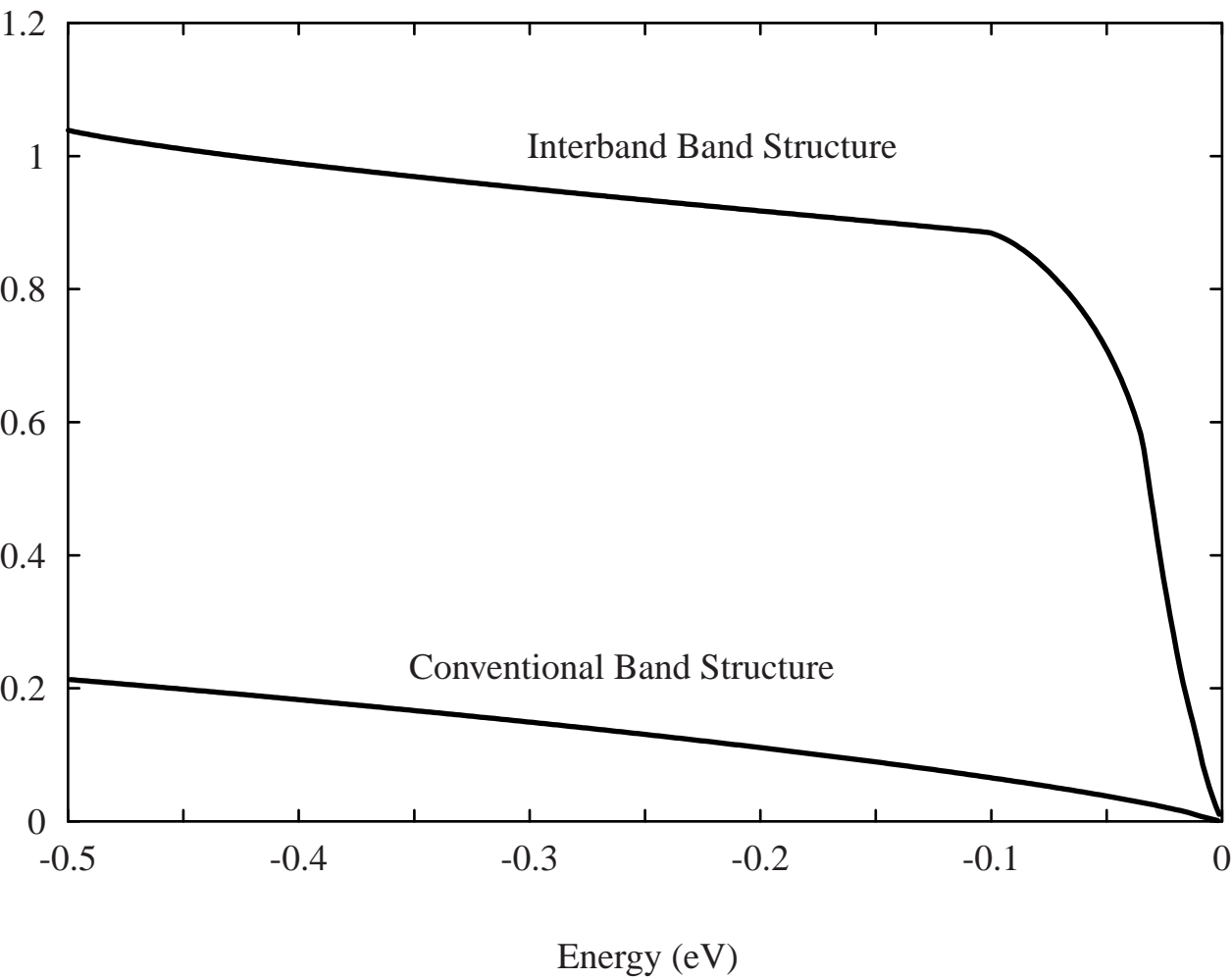


Figure 3.

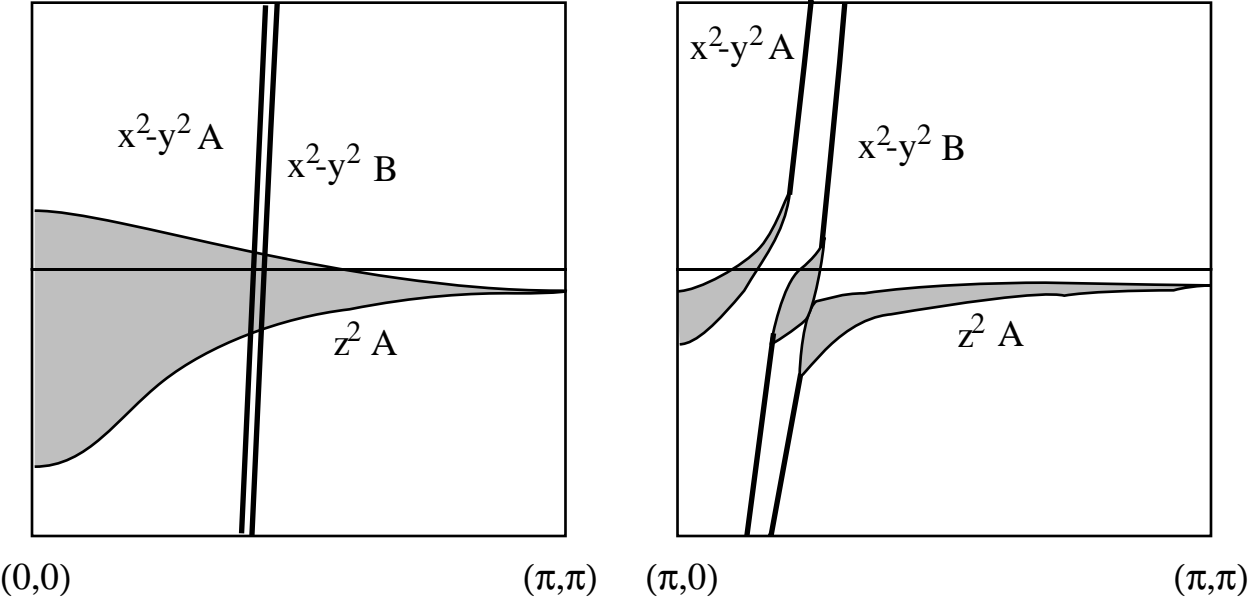


Figure 4.

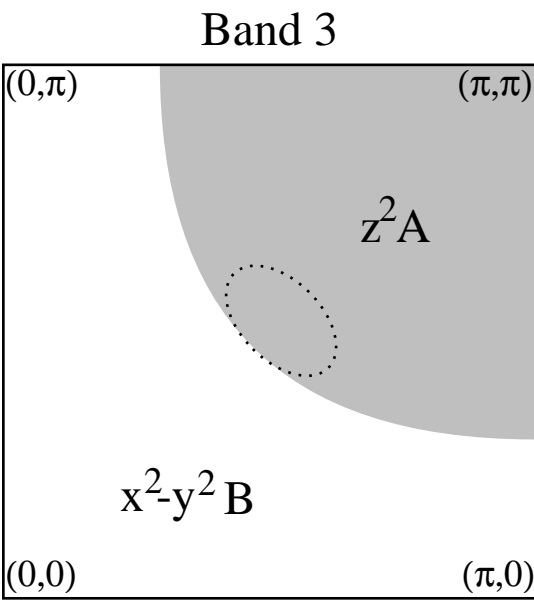
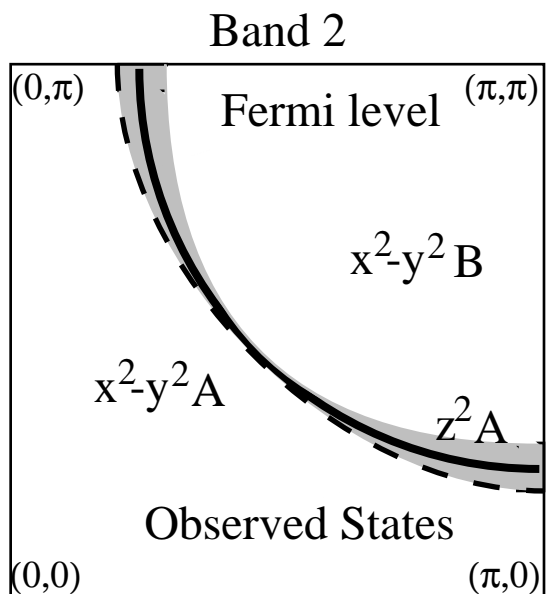
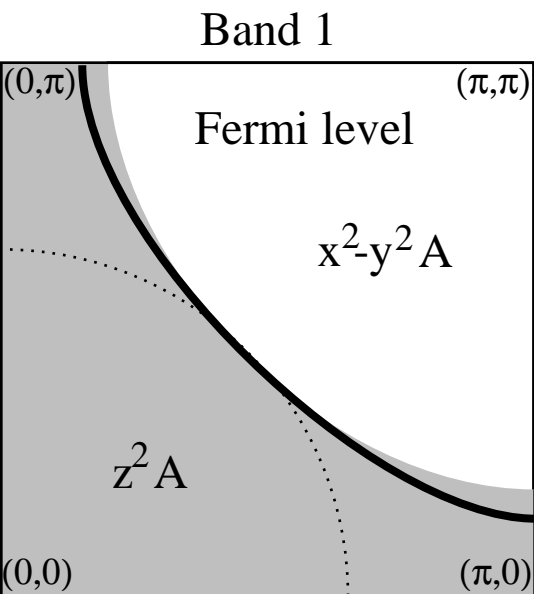


Figure 5.