Superconductivity in a doped topological insulator

1. Superconductivity in $Cu_xBi_2Se_3$ and its implication for pairing in the undoped topological insulator
   Y.S. Hor, A.J. Williams, J.G. Checkelsky, P. Roushan, J. Seo, Q. Hu, H.W. Zandbergen, A. Yazdani, N.P. Ong and R.J. Cava,
   arXiv:0909.2890, Phys. Rev. Lett. **104**, 057001 (2010).

2. Observation of unconventional band topology in a superconducting doped topological insulator, $Cu_xBi_2Se_3$: Topological or non-Abelian superconductors?
   L. Wray, S. Xu, J. Xiang, Y. Xia, D. Qian, H. Lin, A. Bansil, Y. Hor, R. Cava and M.Z. Hasan,
   arXiv: 0912.3341.

3. Odd-parity topological superconductors: Theory and application to $Cu_xBi_2Se_3$
   Liang Fu and Erez Berg,
   arXiv: 0912.3294.

Recoomended and a Commentary by Patrick A. Lee, MIT.

The theoretical predictions [1–3] of topological insulators (TI) and the rapid experimental development [4–7] in the past few years have led to an explosion of activities and interest in this subject. One of the most exciting proposals is the suggestion by Fu and Kane [8] of coating a three dimensional TI with a conventional superconductor. They show that unconventional superconductivity may be induced in the surface state of the TI and its vortex carries a gapless Majorana state. Such a state obeys non-abelian statistics and is of great interest in its own right. A potential link to topological quantum computing adds to the intrigue. Of the several materials studied, the layered compound Bi_2Se_3 [6] and its cousin Bi_2Te_3 [7] are of special interest because the surface state is a single Dirac core. Furthermore, much is known about these materials due to their favorable thermoelectric properties. Thus it is a welcome surprise when Nature obliges and Bi_2Se_3 turns out to be a 3.8 K superconductor when 10 to 15% Cu is added per formula unit.

The initial discovery by Hor *et al.* raised a lot of questions. Hall effect measurements indicated that the carrier density is very low, $\sim 2 \times 10^{20}$ cm^{-3}. This is a fraction of what is expected if each intercalated Cu were to donate a single electron. Thus the nature of the doping and the homogeneity of the sample may be called into question. These questions are largely answered by the ARPES data by Wray *et al.* They showed that the bulk conduction band is indeed partially filled by the copper doping, but the Fermi volume is extremely small, corresponding to 0.5% carrier per unit cell, even smaller than that derived from the Hall data. The authors suggest that about 1/3 of the Cu enters the sample through substitutional defects with Bi and donates two holes per Cu. Thus Cu acts both as donors and acceptors of electrons and a delicate balance leads to the small carrier density.

Remarkably the ARPES data indicate that even though the Fermi energy lies 300 meV above the bottom of the bulk conduction band, the surface state remains split off below the conduction band and visible as a sharp excitation (see Fig. 4 in Wray *et al.*). This is important if one envisions using Cu doping to create the superconducting coating needed to produce the Majorana states as mentioned earlier.

Meanwhile a theory paper by Fu and Berg pointed out the potential for another interesting development. They argue that the bulk superconductivity observed in $Cu_xBi_2Se_3$ may be of an exotic variety, called the odd-parity topological superconductor. Soon after the notion of TI was introduced, the classification was extended to Bogoluibov-deGenne Hamiltonians which describe time reversal invariant superconductors [9–11]. Just as in TIs, the observational consequences are the existence of a topologically protected time-reversed (Kramers) pair of edge or surface states which are now Majorana modes. One significant difference is that in a TI two surface modes can combine and split their energies, so that even and odd Kramers pairs of surfaces states fall into equivalent classes and the classification is Z_2. In 3D topological superconductors, the built-in particle hole symmetry of the BdG Hamiltonian gives additional protection so that integer classification Z with! integer number of Kramers pairs of surface states is possible. It turns out that a few examples of topological superconductors are already known. The first is the triplet $p_x \pm ip_y$ pairing where up and down spins are paired into the odd parity states $p_x \pm ip_y$, respectively. Here two counter propagating edge states are expected. Sr_2RuO_4 would have fallen into this class except that the observation of spontaneous breaking of time reversal symmetry disqualifies it. Another example is the fully gapped B phase in superfluid He^3. Here the existence of gapless Andreev bound states on the surface was predicted theoretically [12] even though its topological origin was not fully appreciated. It is fair to say that topological superconductors in solids have not yet been identified. Since odd parity pairing is involved the common belief is that one may need to look for exotic superconductors where pairing is not driven by phonons. A novelty of the paper by Fu and Berg is to point out that under suitable circumstances, odd parity pairing may emerge from on-site pairing interactions typical of conventional electron-phonon couplings.

The starting point of the Fu-Berg work is the recognition that the bulk conduction band in Bi_2Se_3 originates from strong spin orbit coupling and forms a three dimentional Dirac structure [13]. The four component wavefunction arises from electron spin and two orbitals. From first principle calculations these orbitals have been identified as primarily the p_z orbitals associated with the top and bottom Se atoms in the five layer unit cell [6,14]. Thus the conduction band is doubly degenerate, but as in any strongly spin-orbit coupled system, the degeneracy is not labeled by spin but by linear superposition of spin and orbit, forming the four component Dirac spinon representation.

Fu and Berg started with a phenomenological Hamiltonian with onsite attraction U. They introduced an inter-orbital attraction V so that when $V > U$, the inter-orbital attraction exceeds the intra-orbital one. We could imagine that $U = V$ is due to electron-phonon coupling and U and V become unequal if we include the residual repulsion (μ^* in BCS theory). For example, $V > U$ may come from weaker repulsion for inter-orbital interaction and is not unreasonable. They then examined different pairing possibilities in the basis of spin and orbitals. In addition to the usual spin singlet even parity pairing which involves both orbitals, the existence of the orbital degrees of freedom allows the possibility of spin triplet *on-site* pairing $\Delta_{1,2}^{(\boldsymbol{r})} = \langle c_{\uparrow 1}(\boldsymbol{r}) c_{\downarrow 2}(\boldsymbol{r}) + c_{\downarrow 1}(\boldsymbol{r}) c_{\uparrow 2}(\boldsymbol{r}) \rangle$, where $1, 2$ labels the p_z orbitals mentioned earlier. It turns out that for $V > U$, the triplet pairing is more favorable than the conventional singlet pairing.

It is interesting to view the pairing in the basis of the doubly degenerate eigenstates which diagonalize the bulk conduction band. The pairing will be between time reversed pairs of eigenstates. Since inversion symmetry is present, we expect the inter-orbital triplet pairing will show up in this basis as 2×2 matrix gap functions which are odd in $\boldsymbol{k}$ and most likely closely related to the B phase of He^3. From this point of view, it is remarkable that odd momentum pairing can be competitive with conventional singlet even momentum pairing. The main ingredient is the admixture of the wavefunction in terms of orbit and spin. Even if this particular example does not work out in reality, there is hope that odd parity pairing may be stabilized in some other strong spin-orbit coupled situation.

While we do not know which pairing state occurs in $Cu_xBi_2Se_3$, it appears that we are in a win-win situation. If the pairing is conventional singlet, one may hope to realize the Fu-Kane proposal to create Majarana particles. If the pairing is odd-parity, as suggested by Fu and Berg, this will be the first example of a topological superconductor in a solid. While much work lies ahead, the future does hold a lot of promise for the doped TIs.

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