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Superconductivity in a 3D tight-binding model for Ba-122[1]

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Theoretical investigations of the superconducting state in the iron pnictides have shown that weak-coupling approaches based on a tight-binding parametrization of the LDA band structure can be successfully applied to describe both magnetism and superconductivity in these materials. FLEX, RPA, and fRG studies find in most cases a superconducting state with s-wave symmetry that exhibits a π-phase shift between the gap on the electron and the hole Fermi surfaces, often called a sign-changing s-wave state. Besides this general agreement about the symmetry of the superconducting state these studies have also revealed that the momentum dependence of the gap, including the possibility of gap nodes, is highly sensitive to details of the electronic structure, in particular to the orbital composition of the Fermi surface. Since superconductivity in these materials is restricted to the FeAs layers that, at least for the 1111 compounds, are well separated and only weakly coupled most tight-binding models used to study the superconducting state have been limited to two dimensions. On the other hand the 122 compounds as well as the binary compounds show a very pronounced 3D electronic structure with changing orbital weights on the Fermi surfaces along the k_z direction. An RPA based calculation of the spin susceptibility for the Ba-122 material demonstrates that the necessary averaging over the full three dimensional Brillouin zone leads to a broader and more commensurate spin response compared to a corresponding two dimensional calculation in agreement with experimental observations. In addition changes of the orbital character of the Fermi surface lead to a complicated three dimensional gap structure exhibiting V-shaped or near horizontal nodes on the hole sheets near the zone boundary that can in part explain the puzzling transport measurements.

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