Abstract Submitted
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Superconducting instability of a non-magnetic metallic band in an antiferromagnetic background[1] FERNANDO REBOREDO, Oak Ridge National Laboratory — In superconducting cuprates there is experimental consensus that, for low doping, holes occupy a band primarily formed by the p_x and p_y oxygen orbitals in the CuO2 planes. However, it is very difficult to determine whether this band is formed by σ or a π bonds with the d orbitals of copper. In electron doped cuprates, the location of the carriers less clear. Most ab-initio methods based in a mean field approach lack of the accuracy required to determine the location of the carriers introduced by doping due to errors in exchange, correlation and self-interaction. Nevertheless, these methods have been used to support models that consider only one Cu orbital and the σ oxygen bonds. In this talk we consider what could happen if the carriers go elsewhere and discuss attempts to determine the location of these carriers with diffusion Monte Carlo. It is shown that if the holes occupy the π bonds or the electrons remain centered at the cation outside the planes, a non-magnetic metallic band would form. In the presence of an antiferromagnetic background this band will be coupled to the planes by the exchange interaction in second order, developing a superconducting instability similar to the one described by BCS theory.

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Fernando Reboredo
Oak Ridge National Lab

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