Self-consistent modeling of charge redistributions in Josephson junctions

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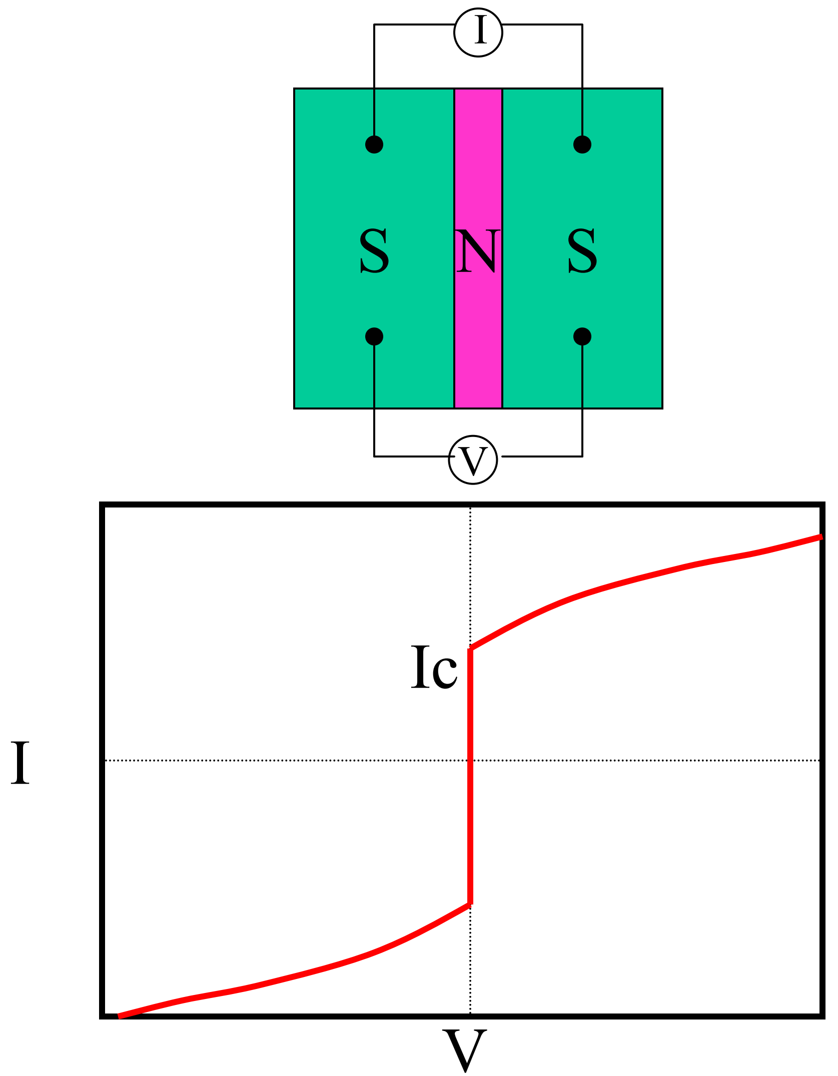
Most recent preprint: cond-mat/0001269

Funded by the Office of Naval Research

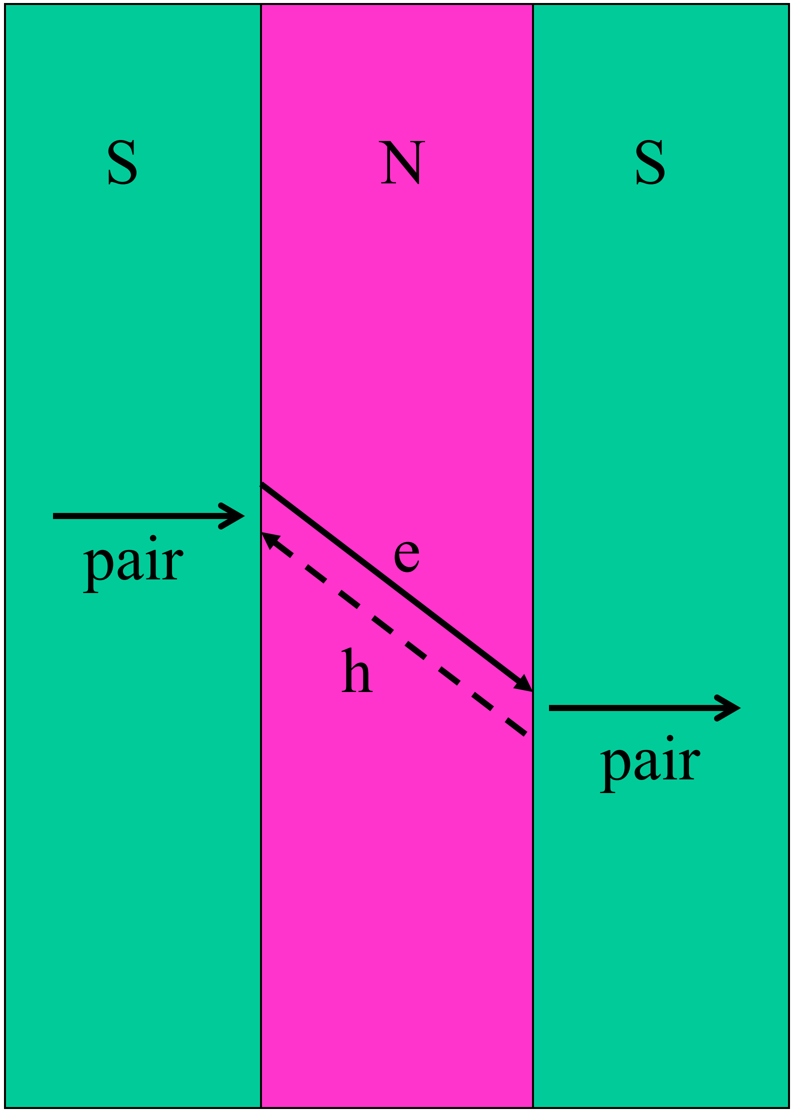
Josephson Proximity-Effect Junctions



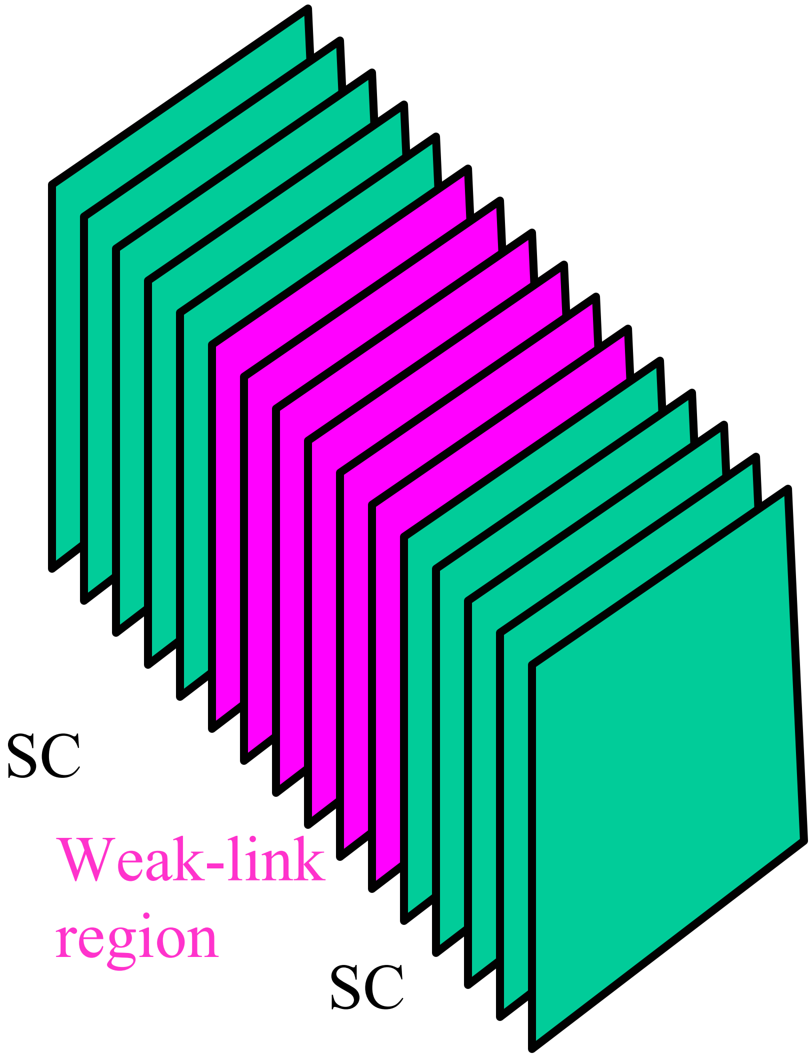
- A Superconductor-Normal metal-Superconductor sandwich where the weak link between superconductors occurs through the proximity effect.
- Andreev reflection at the N-S boundaries leads to sub-gap bound states that carry the pair current.
- Single-valuedness of the IV characteristic allows for non-latching technologies like RSFQ logic.
- If charge accumulates at the NS interfaces these junctions can behave like SINIS junctions.

Andreev Bound States

- At an N-S interface an incoming electron from the normal metal can be reflected into a superconducting pair and a hole (especially at low energies).
- Reflection off both N-S boundaries leads to a bound state in the weak-link region.
- Since Andreev reflection is strongest for voltages less than the superconducting gap, most bound states are sub-gap states localized within the barrier.
- It is the left and right-moving "pieces" of these bound states that carry the Josephson current when there is a phase difference across the junction.



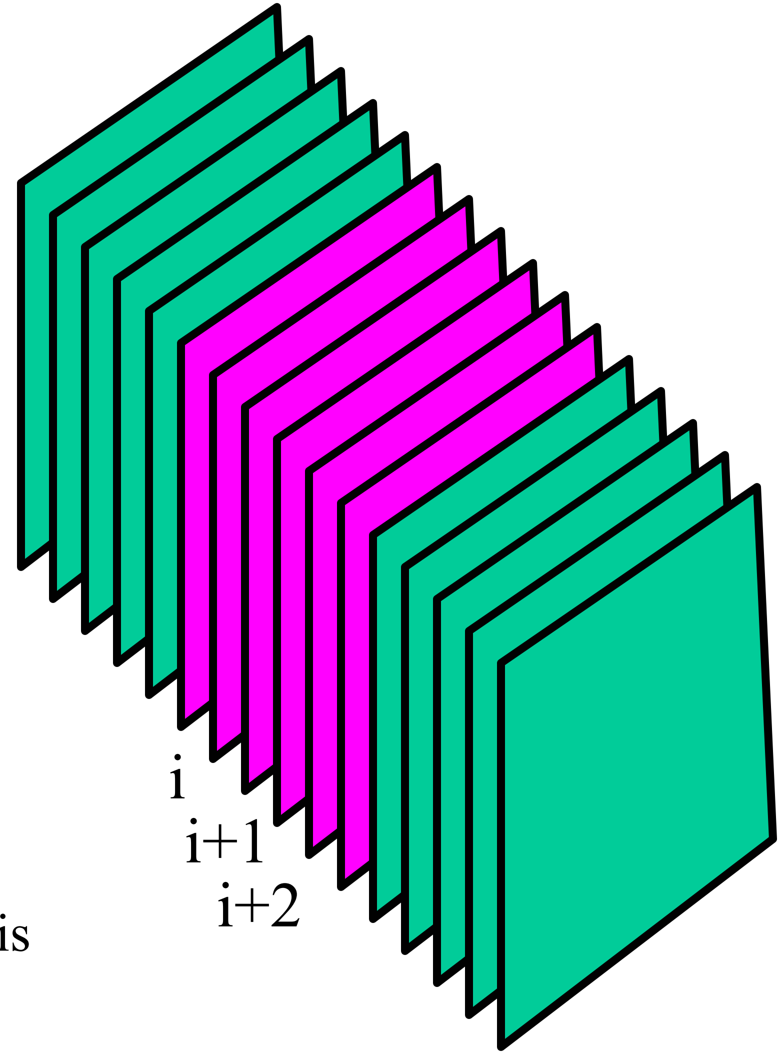
Optimization of the speed of a JJ



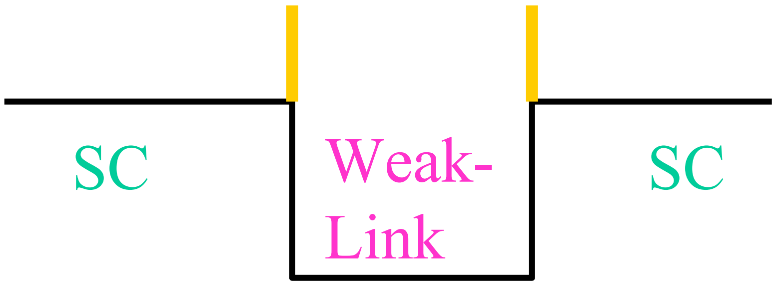
- Insulating barriers found in tunnel junctions have a high resistance and a low Josephson current.
- Metal barriers found in proximity-effect junctions have a low resistance and a high Josephson current.
- Is the speed optimized (i.e. the product IcRn maximized) when the barrier lies near the metal-insulator transition? What type of material produces the best Josephson junction weak-link region?
- We have adopted an efficient massively parallel materials-specific formalism to model and optimize the characteristics of a JJ.

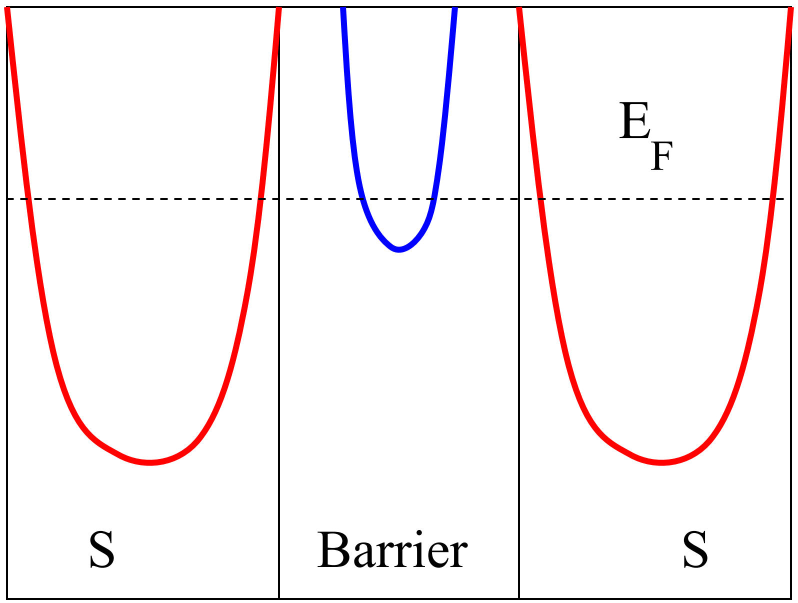
Many-Body Formalism

- Inhomogeneous system, with planes stacked along the z-direction.
- $H = -\Sigma\, t_{ij} c^*_{i\sigma} c_{j\sigma} + \Sigma\, U_i n_{i\uparrow} n_{i\downarrow}$
- Hopping, site energy, and the Coulomb interaction, can vary from one plane to another. Charge redistribution is allowed due to work-function mismatch.
- Local dynamical correlations are explicitly included for each plane via DMFT. The self-consistency relation is now modified to include effects that couple the effective medium between the planes.
- We illustrate the solution of the superconductor in the H-F approximation, which is identical to a *self-consistent solution* of the Bogulubov-deGennes equations (our method is 1000 times faster than conventional ones).



Conventional Models

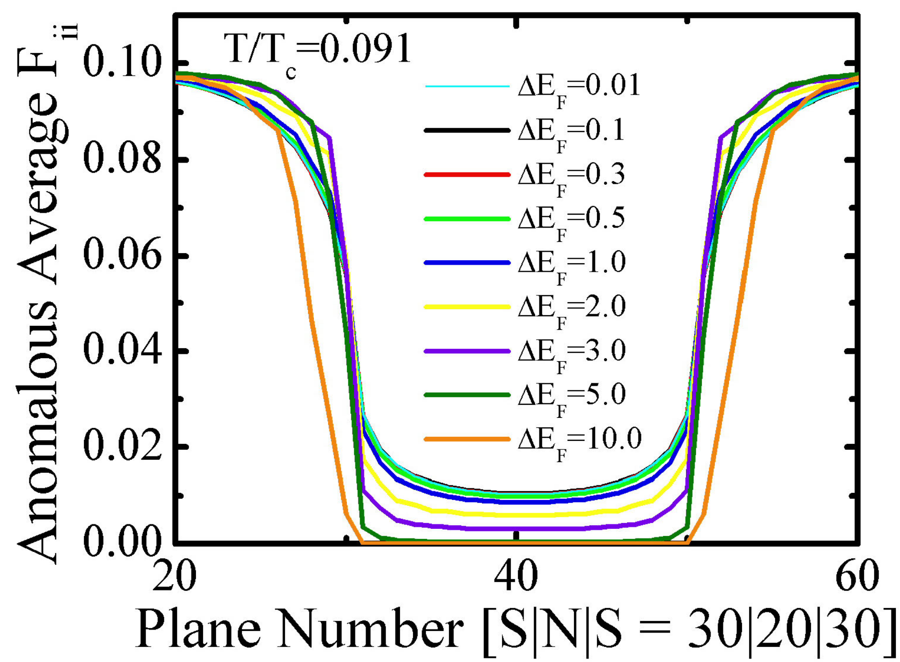


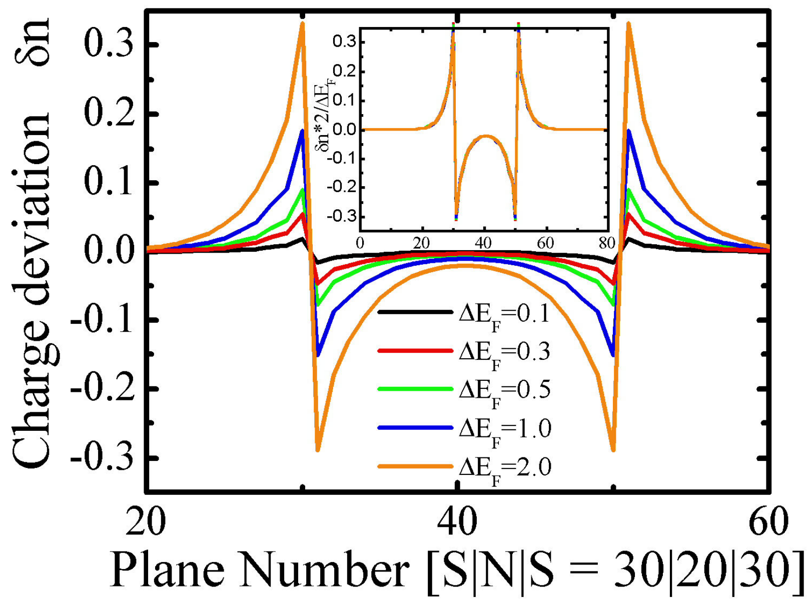


- BTK model, interface scattering, no self-consistency, no electron-electron interactions in the barrier, no bandstructure effects. Simple exercise of matching boundary conditions for plane waves.
- Generalizations to include bandstructure effects (Fermi wavevector mismatch, varying effective mass) are easy to include.
- Self-consistency and especially correlations have been much more difficult.
- **All of these effects are automatically included in our approach!**

Proximity Effect and Schottky Barriers

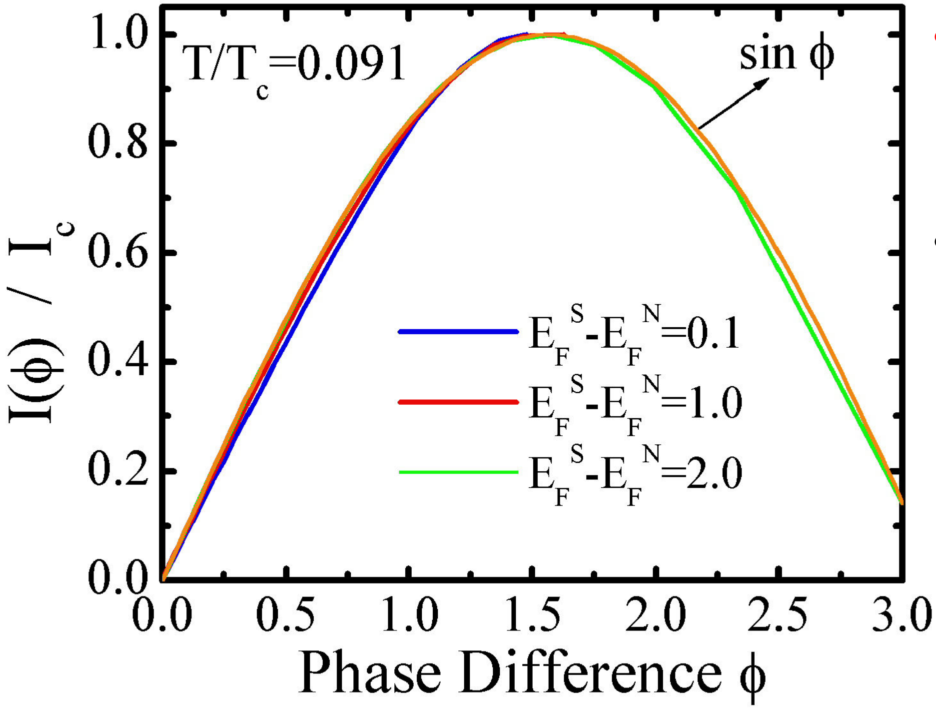
- Bulk superconductor has U= - 2 and half filling, which yields Tc=0.11, Δ = 0.198, and a coherence length of 10 lattice spacings. Barrier width is 20 lattice spacings.
- Note how the anomalous average does not depend too strongly on the Schottky barrier until it becomes large.



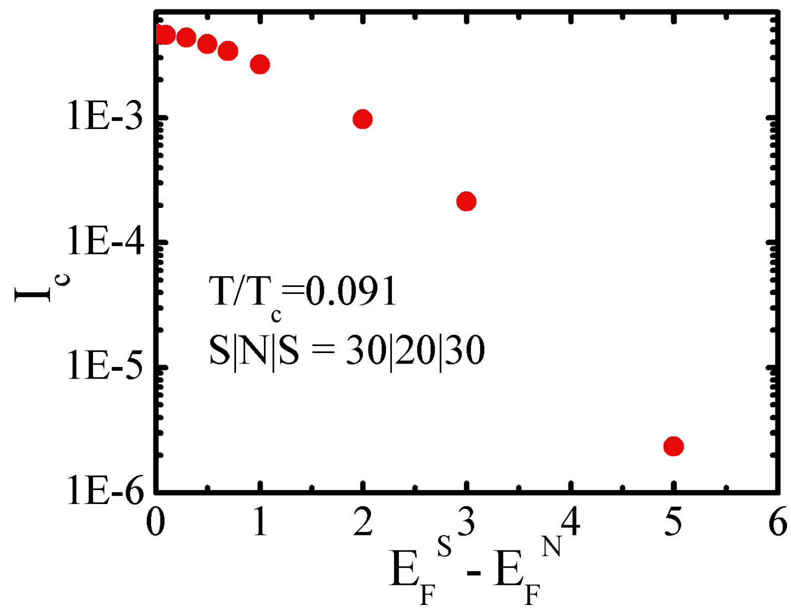


- The Schottky barrier scales with the work-function mismatch, but the anomalous average does not. As the Schottky barrier increases, the anomalous average sharpens.

Current-phase relation and Ic

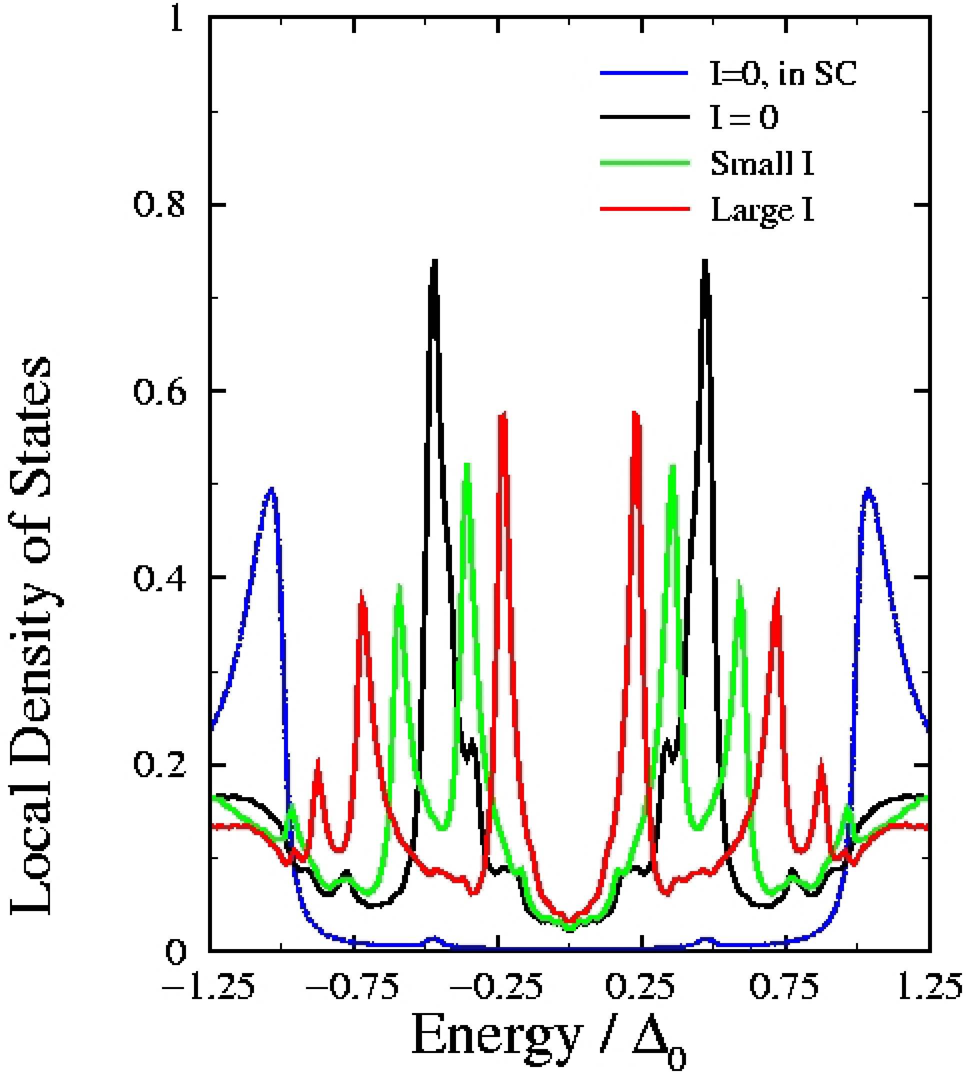


- Current-phase relation for SINIS junctions as a function of the work-function mismatch.
- Note how the curves have essentially a sinusoidal dependence for the SINIS systems with only a small dependence on the barrier height.
- Plot of the logarithm of the critical current Ic initially shows that it is not too strongly affected by the Schottky barrier, but then rapidly decreases as the barrier becomes large.



Many-Body Density of States

- The density of states is plotted at the center of the barrier with no current, small current, and large current. As the current increases, the splitting of the Andreev bound states into the left- and right-moving states becomes clear.
- For comparison, the density of states is shown just inside the superconductor, where the effects of the Andreev bound states can be seen arising from the self-consistency.



Issues for Grain Boundaries in HTS

- Charge redistribution at the interface
- Screening or charge “healing” length
- Short superconducting coherence length
- D-wave superconductivity
- Andreev bound state effects
- Proximity to an antiferromagnetic ordered phase
- Proximity to a Mott insulator
- Disorder
- Strain
- Other?

Conclusions

- Presented a new formalism that provides an efficient means to self-consistently determine the properties of Josephson junctions from a microscopic model. This allows for the smooth potential associated with charge redistribution to be self-consistently included in the description of an LTS SINIS junction.
- Self-consistency is critical for modeling junctions that have a redistribution of charge at the interface. The techniques employed here can be generalized to consider electrically active d-wave grain boundary junctions by modifying the symmetry of the SC order parameter and by examining very thin insulating barriers.
- Scaling phenomenon appears to hold for a number of parameters in the system, but the Ic and Rn values depend crucially on the self-consistency. These techniques can also be used to include many effects of correlations when one is near the metal-insulator transition which is also likely to be important in HTS grain boundaries.