Theoretical modeling of MgB_2 Josephson junctions

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Office of Naval Research Superconducting Electronics program review (2006)

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Challenges to
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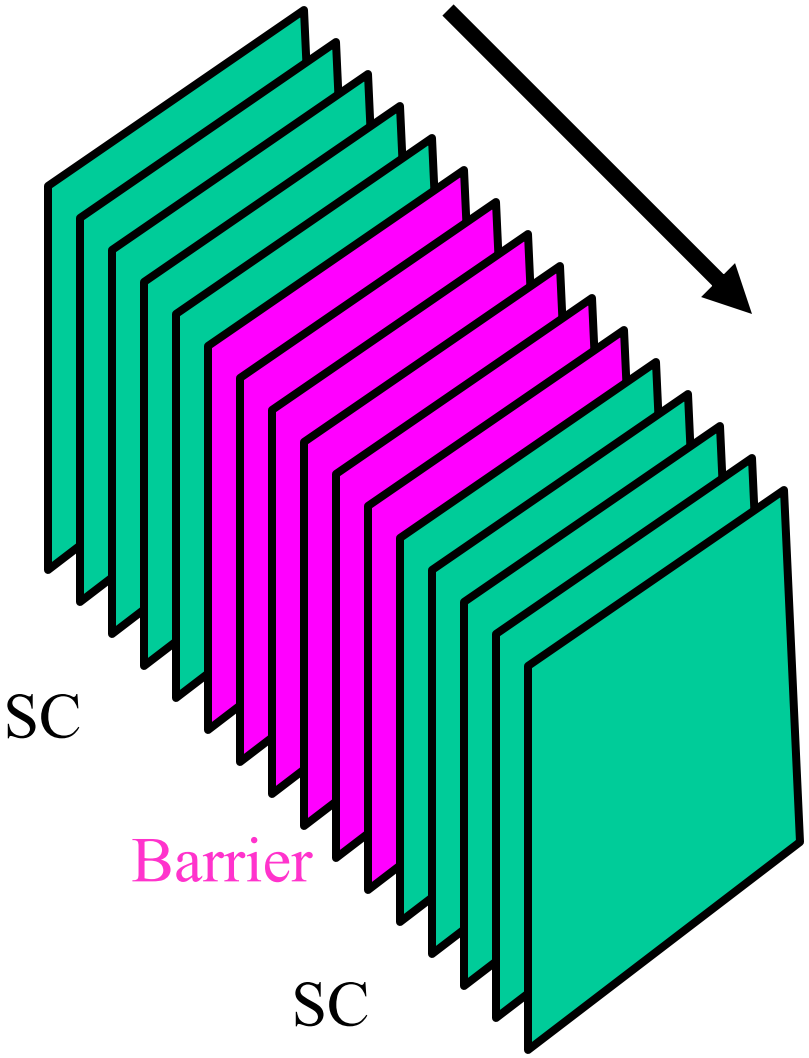
Overall goals of project

- Provide real-materials-specific modeling of Josephson junctions based on MgB_2. Determine the critical current density, the resistance-area product, and the figure of merit.
- Identify the types of barriers and leads that have the best performance. Should the SC be dirty or clean? What is a good barrier material---ion damaged SC, MgO, AlO_x, BN, or something else?

Current research problems

- Formulating a four-band tight-binding model in the bulk and applying it to MgB_2 systems in devices.
- Determining the changes to the interface on atomically pure candidate barrier materials---MgO is our first test case.
- Calculate Josephson junction properties for both ion-damaged and MgO junctions.
- All of this work requires significant modifications and generalizations of our currently existing codes, so we are also working on efficient algorithm development too.

Josephson junctions for digital electronics



- Sandwich of superconductor-barrier-superconductor with current moving perpendicular to the planes. We examine MgB_2, and model the active B sites, which contribute to all of the states at the Fermi energy.
- Two-gap structure in the SC makes the modeling more complicated.
- Band insulator barriers: AlO_x, MgO, BN, etc.
- Ion-damaged MgB_2 barrier.

Why MgB_2-based junctions?

- Medium-high Tc allows for operation well above 4K, which makes refrigeration obstacles less of an issue.
- S-wave gaps do not have the problems seen with HTSCs and their d-wave gaps. But there is a big gap and a small gap, and the small gap is the easily accessible one for c-axis junctions.
- Larger gaps potentially allow for higher operating speeds than Nb-based junctions.

Challenges to MgB_2-based JJs

- What barrier will have the best Josephson properties, will be easy to manufacture, and will not be degraded over time?
- What problems arise with the two-gap structure, and will this affect the ability to make operating devices?
- Since the processing of MgB_2 thin films is complicated, how does one grow the top electrode for a trilayer process with the same level of quality as the bottom layer? Is this necessary for good performance?

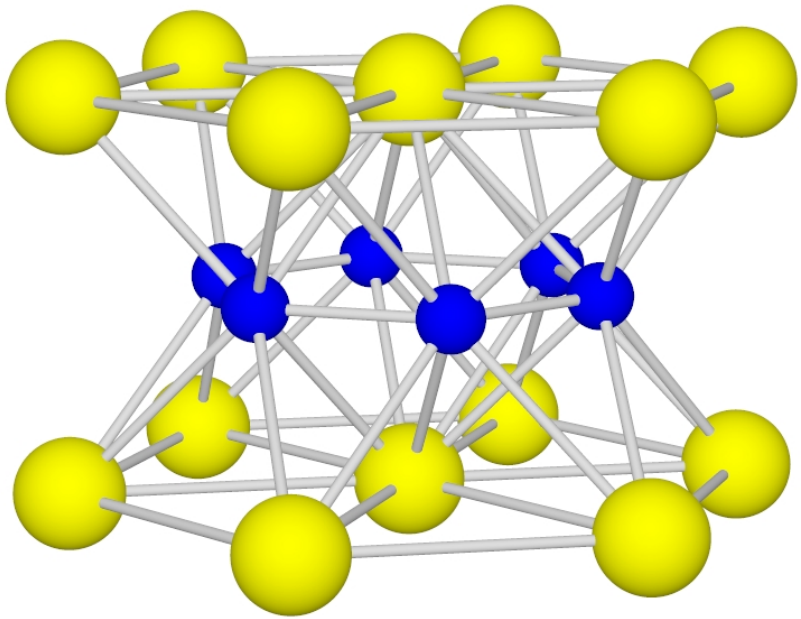
Current successes

- High quality thin films can be grown via the Penn-State process. Tcs can be even higher than in the bulk!
- Functioning JJs have been demonstrated in three different categories: (i) ramp-edge junctions which go into the a-axis and the large gap; (ii) ion-damaged junctions in a planar structure; and (iii) trilayer junctions with barriers like AlO_x or MgO.
- *But there isn't yet a well-defined and accepted method to make high-quality junctions.*

Our approach

- Map DFT band structures for the bulk materials onto tight-binding models that only connect nearest-neighbor planes along the c-axis. Do this for both the SC and the barrier.
- Perform interface DFT calculations to determine how the tight-binding parameters change and to determine the charge transfer at the interfaces.
- Incorporate these effects into an inhomogeneous DMFT transport code to determine the current density, resistance-area product, and figure of merit for a junction. (Scattering by charge defects is easily included.)

Lattice structure of MgB_2

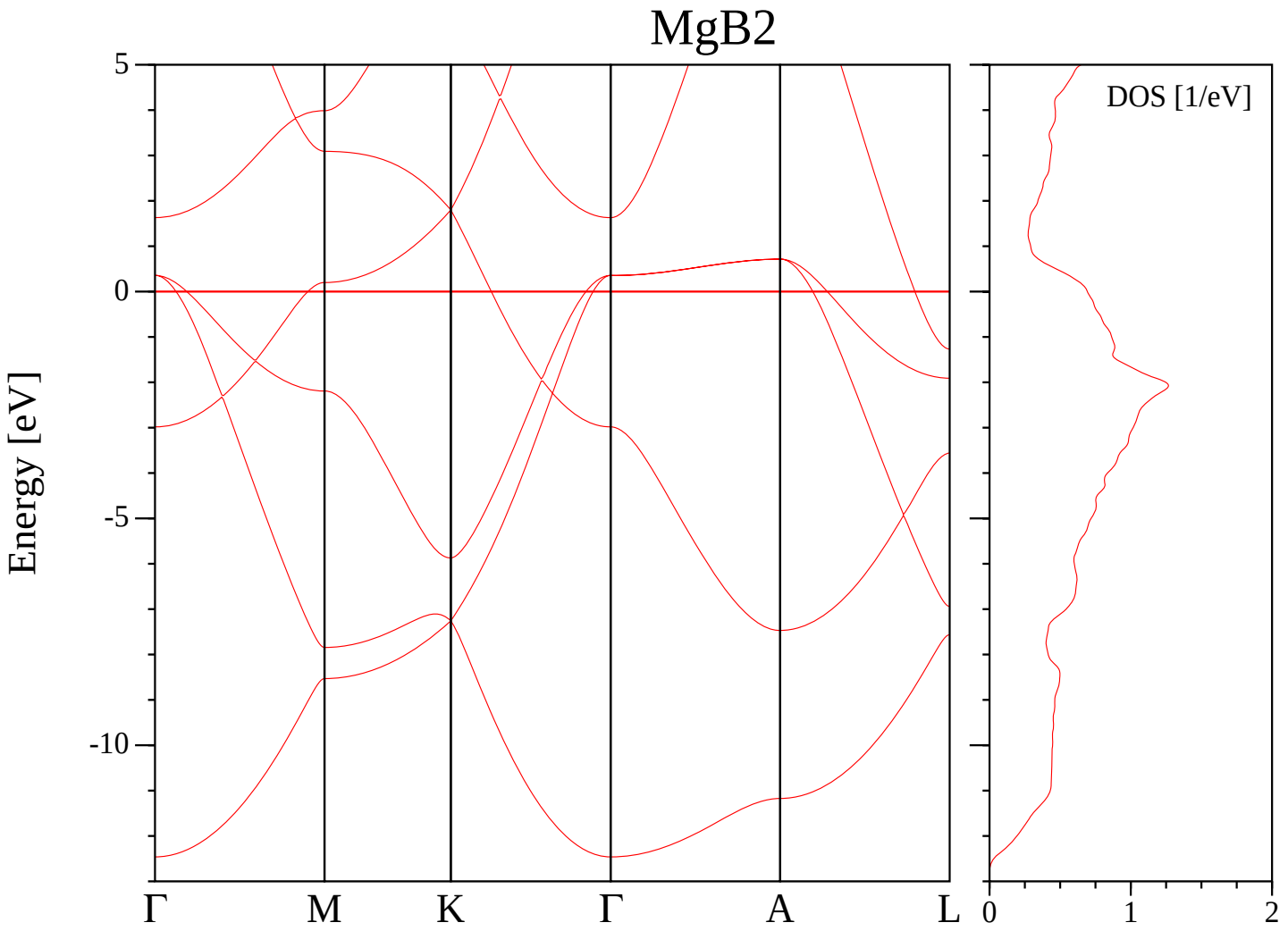


Alternating hexagonal planes of Magnesium (yellow) and Boron (blue).

Epitaxial growth is easiest along the c-axis direction. There are twice as many borons in its plane as magnesiums in its plane. The system, especially the boron plane, has many similarities with graphite in its structure.

The electrons either sit in bands localized within the hexagonal Boron planes, or move between the Boron planes.

DFT bandstructure bulk MgB_2

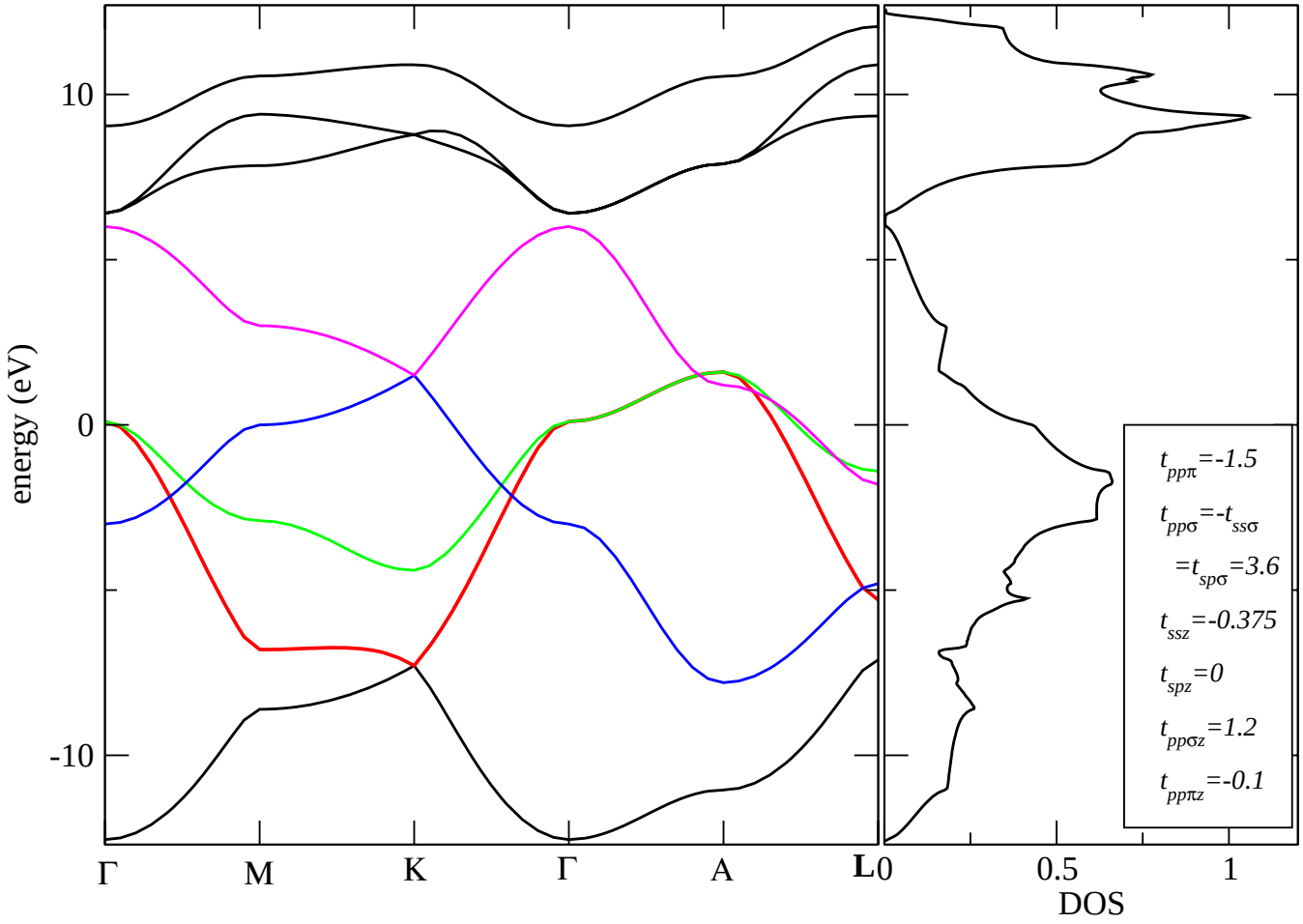


Four bands cross the Fermi energy (0 on the graph).

Tight binding fit to bandstructure and DOS

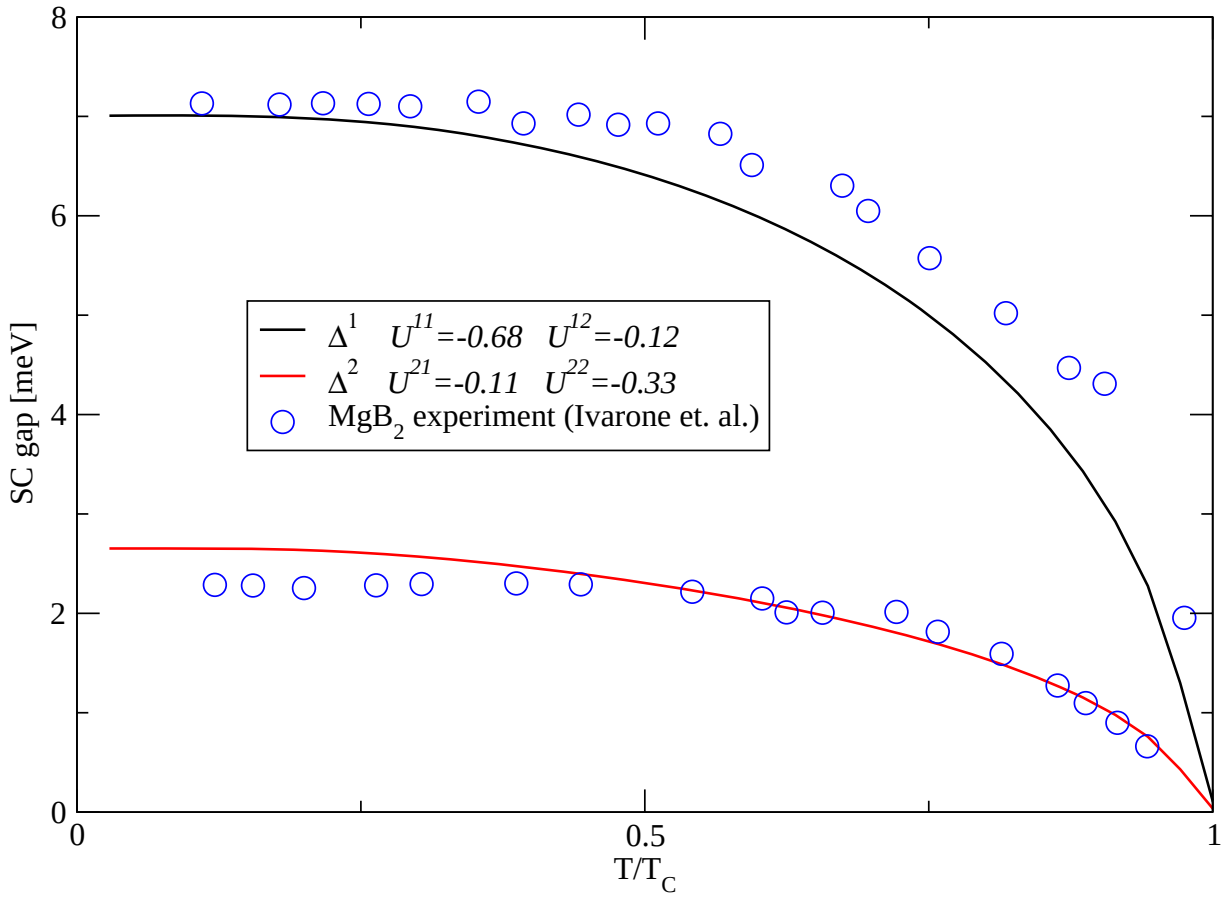
This preliminary fit was made by fitting the band widths and the gaps between bands at certain high-symmetry points. Here the DOS is about 20% high.

We will also try to fit the DOS and the slope of the bands at the Fermi energy, and see which approach yields better results.



Two-gap structure in the ordered phase

This is the typical fit that we find when we adjust the pairing interaction between each band and within the bands. Currently we need to adjust the overall magnitude to get the right Tc. We may modify our procedure to include the actual a2F found with DFT.



Effect of ion-damage

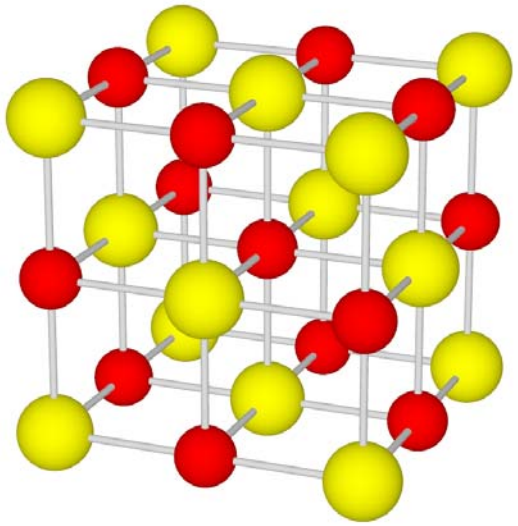
- We model ion damage with the FK model. The concentration of defects is given by w_1. The expectation is the two gaps should become similar in size as the damage increases.
- DFT says that once Tc drops to about 20K, we go into the dirty limit where the gaps are reduced in size but isotropic.
- We would like to see if such an evolution can be seen from our theory and compare with the ASU experiments on Tc versus ion damage.

Ion-damaged JJs.

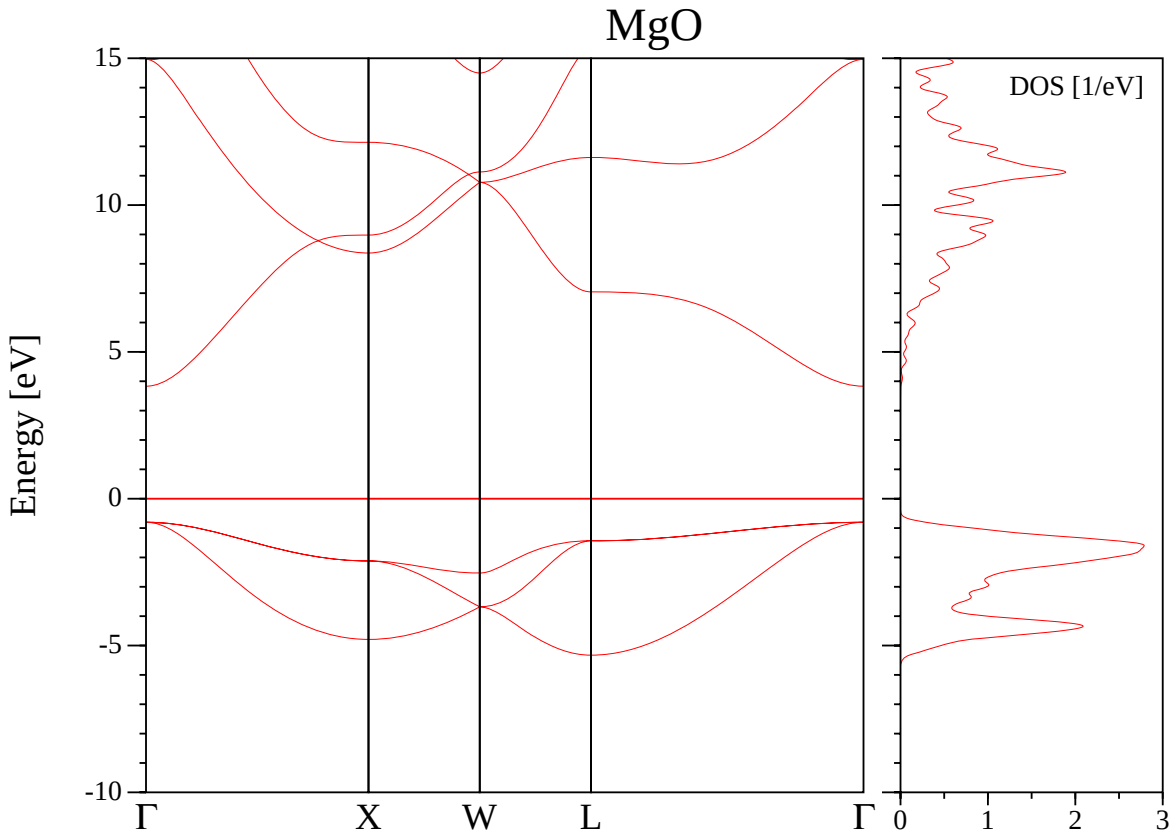
- Our first JJ calculation will be for ion-damaged JJs, because they are the simplest system to work with. We just take our bulk MgB_2 system, and add charge scattering defects in the barrier region with some given strength of scattering.
- We hope to be able to start getting results from these calculations within the next six months.
- This is to be viewed as a simple test-case for the code, because our junctions will be trilayer ion-damaged junctions, while most experimental ion-damaged junctions are planar.

Magnesium oxide barrier (band structure)

Mg=yellow and O=red



Rocksalt structure

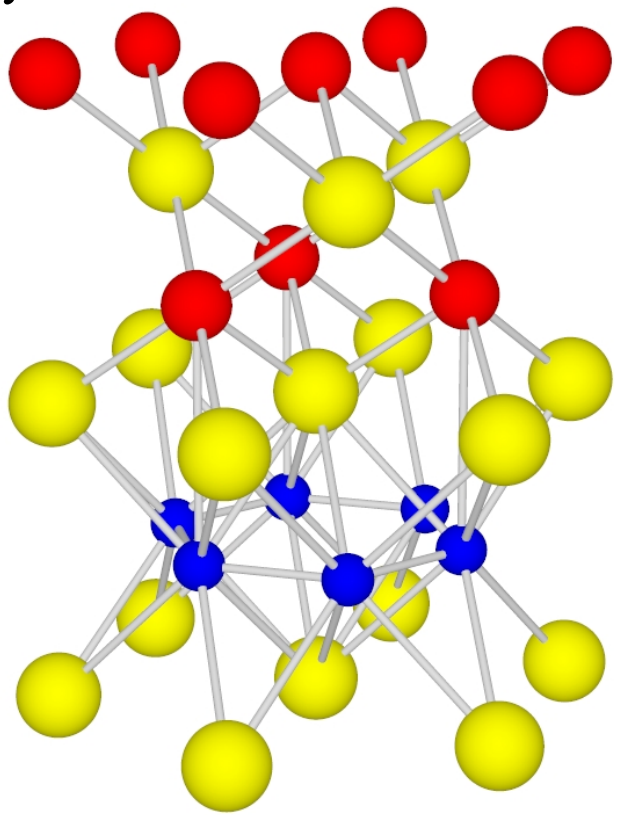


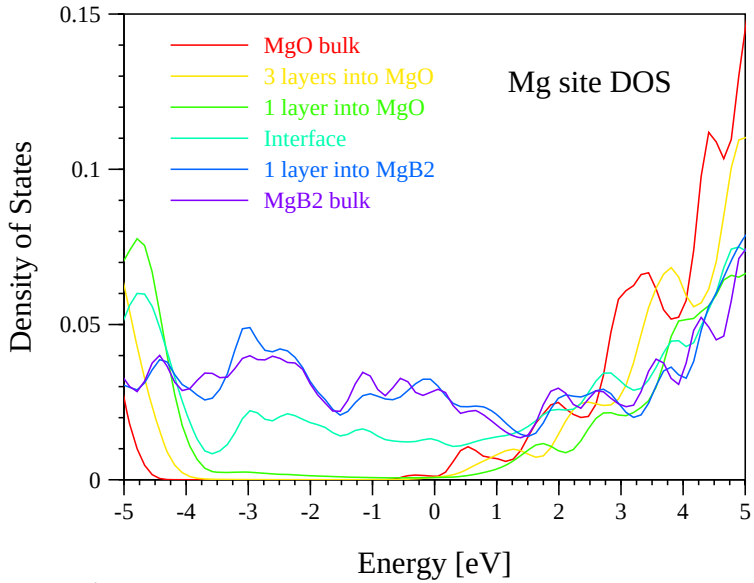
Well lattice matched along the [111] direction

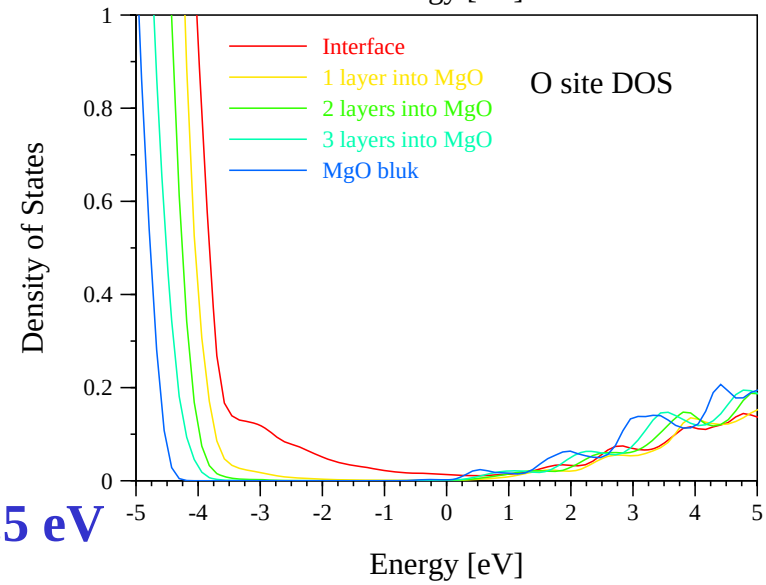
(about a 5 eV gap)

Interface between MgB_2 and MgO

Calculate a fully relaxed interface, with atoms able to be rearranged to lower their energy







Barrier height can be much less than 2.5 eV

MgO-barrier junctions

- The band structure for MgO does not separate into a planar energy plus a dispersion along the z-axis. Hence, we must modify our algorithm to sum over the two-dimensional Brillouin zone rather than just integrating over the 2d DOS. This is a technical and numerical complication that will require significant algorithm development.
- In MgB_2, we can focus on the B sites alone, because they contain all the states near the Fermi energy. In MgO, we can focus only on the O states for the valence band, but the conduction band has some mixing with Mg states. We will need to determine whether this mixing is important to include in the modeling.
- This work should have direct experimental relevance with attempts of experimental groups to make a technologically viable trilayer process (either natural barriers or purposely grown)

Other junctions

- We would like to know about other promising barriers for making junctions.
- Experimentalists have tried AlO_x, which can be difficult to model if it is not stoichiometric, AlN, and oxidizing MgB_2 by exposure to air (likely MgO barriers).
- There may be other possible barriers that can be tried. Boron nitride is one interesting possibility. The compound has a hexagonal planar structure, which may be feasible to grow on top of MgB_2.

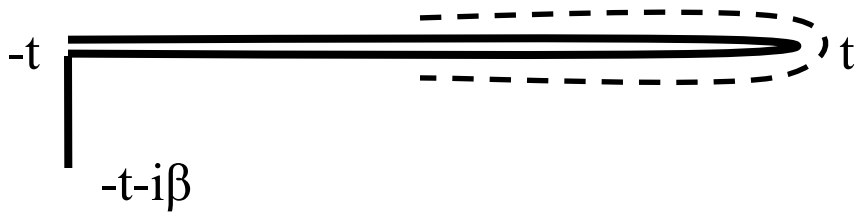
And now for something completely different

Nonlinear response

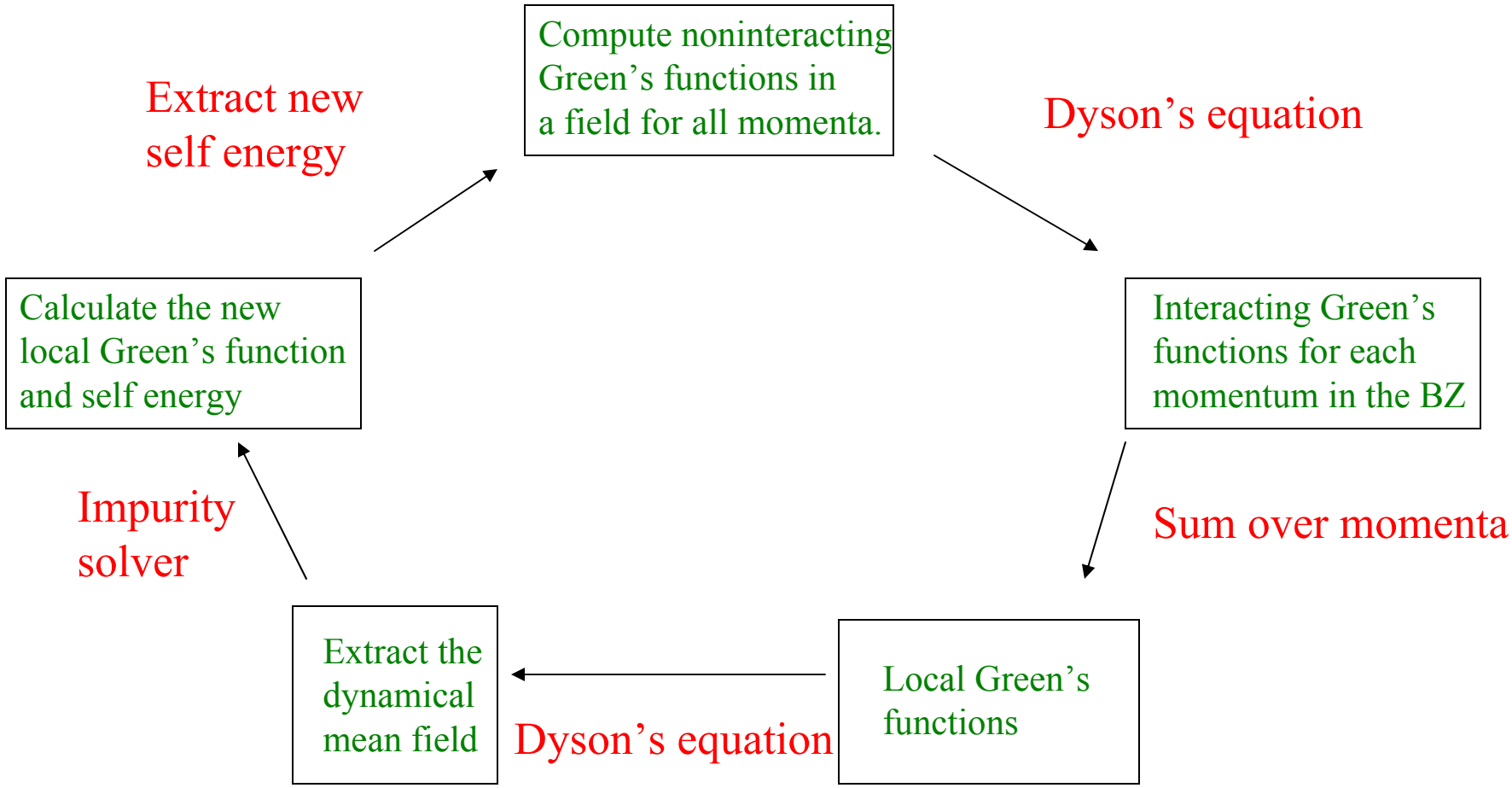
- Often the **nonlinearities** of a device determine it's ultimate performance.
- So-called "smart" materials usually involve **strongly correlated systems** because their materials parameters can be tuned by doping, pressure, or temperature variations.
- Many devices of interest to the Navy will be subject to **large electromagnetic fields** or **field pulses**, which can affect their performance.

Nonequilibrium formalism

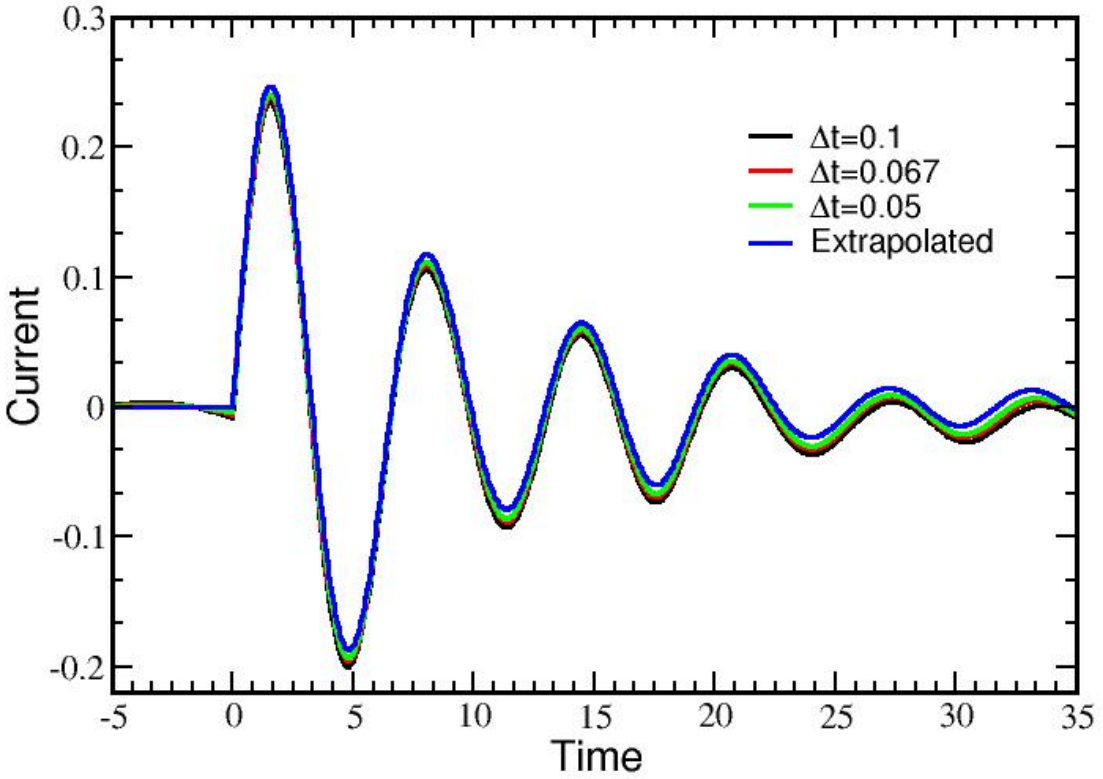
- In a nonequilibrium situation, the quantum-mechanical operators must be evolved **forward in time**, and then de-evolved **backward in time**, in order to determine operator averages with respect to the original equilibrium distribution.
- A Keldysh-like formalism is used to calculate the so-called **contour ordered Green's function**. In our case, the field is turned on at **t=0**, as indicated by the dashed line.



Exact nonequilibrium many-body algorithm with interactions

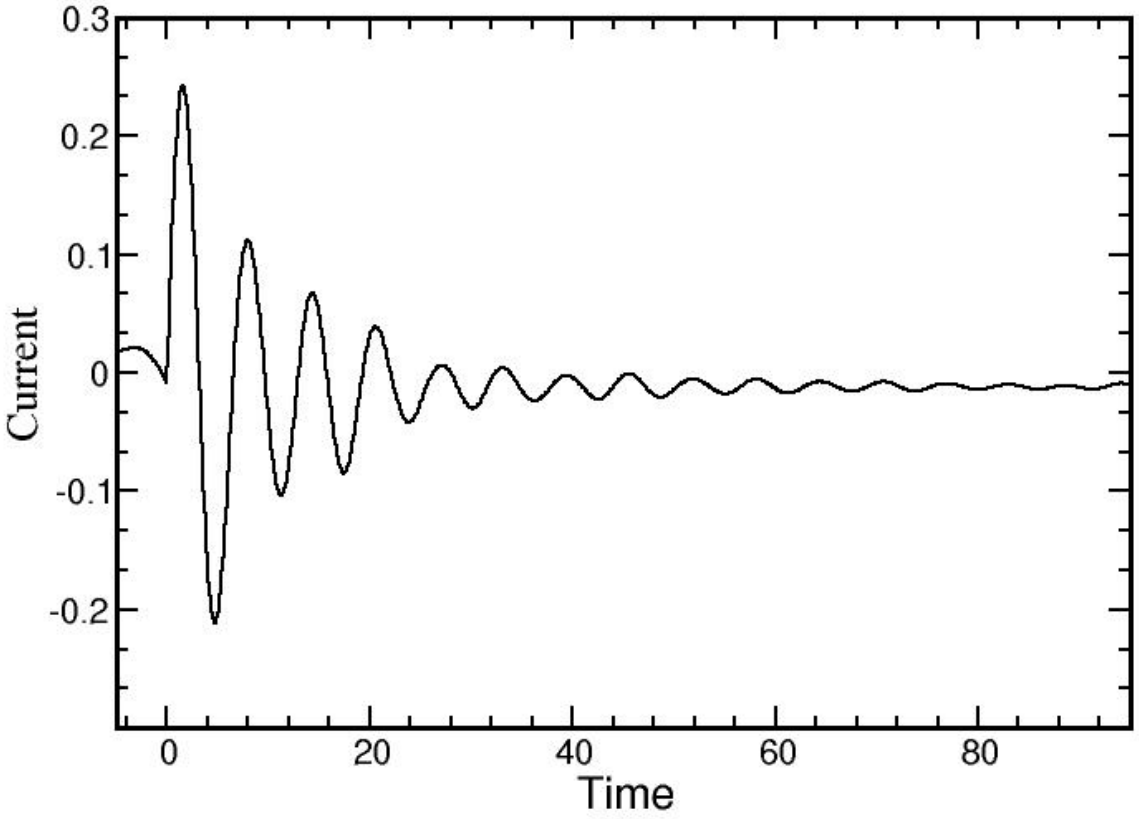


Nonlinear current response for a strongly scattering metal



The field is turned on at T=0 (E=1). Note how the current starts with a large oscillation and then damps out. We have not yet been able to settle the question of whether the oscillations survive at long times, or ultimately decay. These results scale well with our discretization size.

Long-time response



The long-time response may be oscillatory, but it is hard to tell from these results alone, because we cannot rule out two decay time scales, a short initial one, and then a long one for large times.

Future plans

- All algorithm development has been completed, and codes have been debugged.
- We are finishing up our production runs of codes (hopefully with time from a Capabilities Acquisition Project phase II allocation of computer time.
- Project will wind up when production runs are finished.