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3 Auger Recombination Code Development

3.1 Theory of Wannier FUnctions

The idea behind Wannier functions is to take the extended, Bloch like states that we use in our first principles code and reduce them to localized states in real space. You can loosely think about this in terms of Fourier transforms between wave functions in k and real space. In k space, wave functions are spread out over entire supercells which will correspond to localized wave functions in real space. The question is how to actually find these analytically.

We run into two problems with the arbitrary nature of Wannier functions. The first is the familiar phase factor that can be added to any wave funciton. The second is the Gauge choice of specifically defining the Bloch functions. This is slightly different than the phase choice, and leads Wannier functions to be doubly arbitrary. So what method can we use to actually choose them and to make sure that they are localized.

One method for choosing the gauge is to make sure that the gauge is *smooth*. That is, the wave function doesn't jump around all that much. You might think

that the Bloch wave functions are going to be smooth, but because of crossings and degeneracies they probably are not going to be. In these cases, we can define Unitary matricies that get rid of those discontinuities and apply them to our Bloch Functions. These may no longer be eigenvalues of the Hamiltonian, but that's okay, we can always transform back eventually. These new Bloch functions have a smooth gauge, which will lead to localized Wannier Functions.

But that's only part of the story. We still need some sort of minimization condition to make sure that they are localized. So what we do is define a localization minimization condition involving the position operator. From here, we rewrite that in terms of the Bloch functions and figure out how to actually minimize this condition.

When the bands are entangled there are some special considerations that we need to go through.

Local Minima

Reason why this method for Wannier is the best one?

Discussion of Bloch's Theorem

Discussion of Fourier Transforms . . . luckily, the Fourier transform is unitary and therefore will preserve the norms of the Hilbert Space.

3.2 Approximations for Tractable Calculations

3.3 Refactoring and Optimization

3.4 Parallelism and Optimization

3.5 Future Work

4 Scintillator Materials

4.1 History of Scintillators and the Nonlinearity Problem

4.2 Why Sodium Iodide

Sodium Iodide is a simple, cubic crystal that is easy to grow in large quantities. (CITATION + discussion more in depth). It was one of the first materials to be shown to have scintillating properties when (CITATION + STORY). Because it has been so heavily studied and because it is easy to produce, sodium iodide was used in many of the first radiation portal monitor devices commissioned by the government.

Unfortunately, sodium iodide is also one of the most *non-proportional* scintillating materials we know about **??**. This has lead to the problem of high false alarm rates among the RPM used in the United States. While many properties are known about sodium iodide, Auger recombination has proven difficult to understand because of the aforementioned theoretical and experimental hurdles. To our (my?) knowledge, there is no theoretical studies of sodium iodide.

Experimental measurements of Auger recombination in sodium iodide have widely varying results. ::Review literature on Sodium Iodide here. The following are the papers you cite in paper::

- G. Bizarri, N. Cherepy, W. S. Choong, G. Hull, W. Moses, S. Payne, J. Singh, J. Valentine, A. N. Vasilev, and R. Williams, IEEE Trans. Nucl. Sci. 56, 2313 (2009).
- W. W. Moses, S. A. Payne, W.-S. Choong, G. Hull, and B. W. Reutter, IEEE Trans. Nucl. Sci. 55, 1049 (2008).
- S. Payne, W. W. Moses, S. Sheets, L. Ahle, N. Cherepy, B. Sturm, S. Dazeley, G. Bizarri, and W.-S. Choong, IEEE Trans. Nucl. Sci. 58, 3392 (2011).

(KMC studies on this?)
(Discussion of expectations with phonon-assisted vs. direct?)
Because of the need for accurate Auger recombination numbers for KMC modeling by (GROUP) and because of the large variance among experimental measurements, sodium iodide is an ideal candidate for study using our first-principles methods.