Bandstructure Assignment

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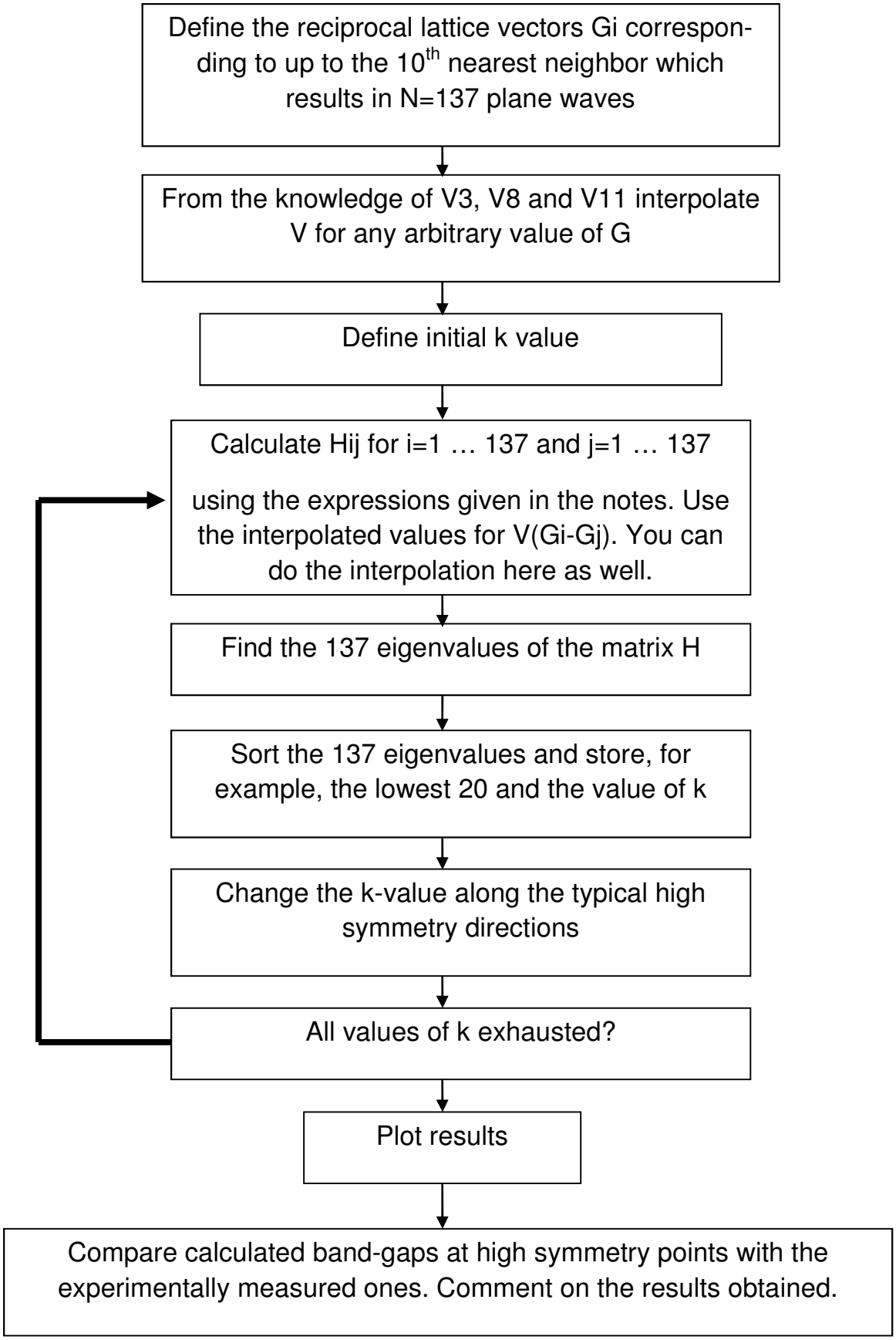
Knowing the electronic structure is essential for the understanding key properties of materials such as bandgaps, effective masses, etc. The bandstructure calculation methods can be categorized into two classes: (a) *ab initio* methods and (b) semi-empirical methods. The *ab initio* methods are first principle calculations and they give best results, but they are difficult to implement. On the other hand, the semi-empirical methods are more easy to implement but are less accurate and depend upon a number of fitting parameters. Amongst the variety of semi-empirical band-structure calculation methods, the most popular ones are: empirical pseudopotential method, semi-empirical tight-binding method and the k.p method. The k.p method is the best for determining the effective masses near the band minima and the empirical pseudopotential method is best suitable for determining the optical gaps.

In this exercise, you are required to develop an empirical pseudopotential code in MATLAB that calculates the bandstructure for Si, Ge and GaAs. Note that Si and Ge are covalent materials whereas GaAs is zincblende material. In your implementation procedure use 137 plane waves that are discussed in the powerpoint slides and the word document with the description of the empirical pseudopotential method. The implementation procedure is as shown on the next page.


Define the reciprocal lattice vectors Gi corresponding to up to the 10th nearest neighbor which results in N=137 plane waves
From the knowledge of V3, V8 and V11 interpolate V for any arbitrary value of G
Define initial k value
Calculate Hij for i=1 … 137 and j=1 … 137
using the expressions given in the notes. Use the interpolated values for V(Gi-Gj). You can do the interpolation here as well.
Find the 137 eigenvalues of the matrix H
Sort the 137 eigenvalues and store, for example, the lowest 20 and the value of k
Change the k-value along the typical high symmetry directions
All values of k exhausted?
Plot results
Compare calculated band-gaps at high symmetry points with the experimentally measured ones. Comment on the results obtained.