Calculation of Quasiparticle Properties and Optical Responses Using BerkeleyGW

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1 Personal Introduction

Hello, my name is Alex Anderson. I am a first year physics graduate student. I grew up in the Chicago area and I went to Washington University in St. Louis where I double majored in math and physics. As an undergrad, my primary research involved studying the behavior of classical mechanics when complex numbers are introduced. (See here for a bare-bones website about some of my previous work [1]). I have always enjoyed programming in the past and I am looking forward to learning more. I hope to be able to use the computing skills that I learn in this class to make predictions about quantum mechanical systems.

2 Density Functional Theory and the GW Approximation

Density Functional Theory (DFT) is a quantum mechanical modeling method used to investigate the electronic structure of many body systems. [2]

The theory reduces the intractable many body problem of interacting electrons into a problem involving non-interacting electrons moving in an unknown effective potential that takes into account the interactions. While the exact form of this potential is not known, there are a number of approximations used such as the local-density approximation (LDA) and the generalized gradient approximation (GGA).

While DFT is well suited to finding the ground state electron configuration, further methods must be applied to extract more information. For instance, the GW approximation [3] (GWA) helps one calculate quasiparticle properties of a wide range of material systems. The Berthe-Salpeter equation (BSE) is used to calculate the optical responses of materials.

3 The Berkeley GW Package

The BerkeleyGW package [4] is a set of computer codes that calculates electronic properties of a variety of materials. The package takes as input the mean-field results from DFT calculations and has routines that calculate three major quantities. It deals with polarizability, self-energy corrections to the DFT eigenenergies, and correlated electron-hole excitations.

4 Comparison Between Simulation and Experiment

There are a wide range of problems that can be addressed using density functional theory. Some typical results for the valence bands of Ge are shown in the following figure taken from [5] (a more full list of references on the methods can be found under resources here [4]).

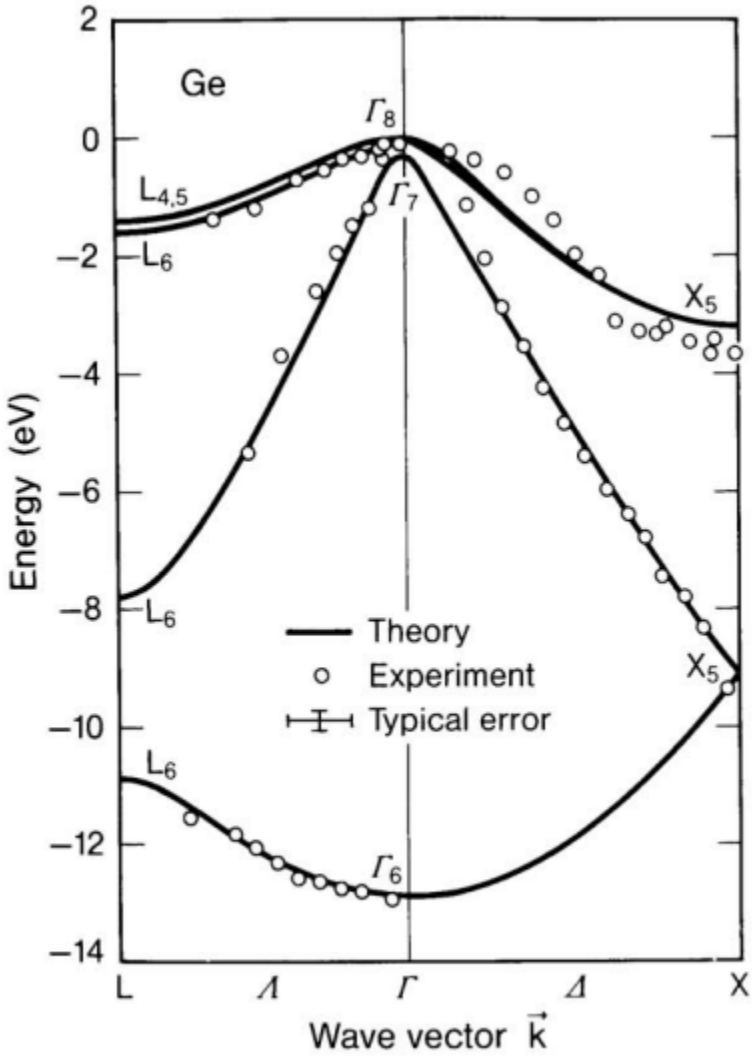

FIGURE 5 The calculated valence bands in Ge are compared to the results of angle resolved photoemission measurements from Ref. 30.

Further, there are many problems where DFT does not give the best results and so there is extensive work in doing additional calculations to improve the quality of DFT results and to extend the method to new problems. There are a huge number of

5 Implementation of Parallelism

The BerekeleyGW package uses a number of standard libraries to execute computationally intensive steps. In particular, BLAS, MPI, LAPACK, ScaLAPACK and FFTW are required. To give an instance of the parallelism used in this software package, let us consider the subroutine that calculates polarizability. There are three main linear algebra tasks. First, elements of a matrix need to be calculated. Second, two matrices need to be multiplied. Third, a matrix needs to be inverted. The first step is embarassingly parallel as the matrix elements are uncoupled. This work is easily distributed among processors. The other steps use ScaLAPACK in order to execute the matrix operations. The work scales easily up to around 100,000 processors because the systems of interest. As this program was developed at Berkeley, it is often run on Hopper [**?**] The following figure shows the amount of time necessary to execute a calculation as the number of cps is increased. Notice that while the graph starts as linear, there are diminishing marginal returns as the number of CPUs is increased. The figure is taken from [6].

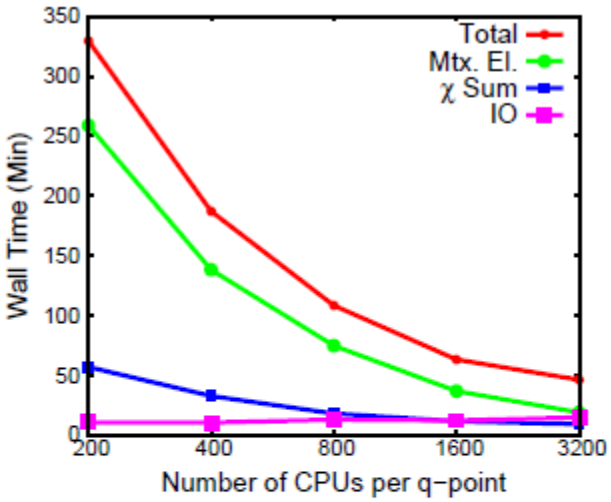

Figure 11: The wall-time required *vs.* the number of CPUs per **q**-point used for a `epsilon` calculation on the (20,20) single-walled carbon nanotube. There is near linear scaling up to 1,600 CPUs. Since there is an additional layer of trivial parallelization over the 32 **q**-points required, the `epsilon` calculation scales to over 50,000 CPUs. See text for parameters used.

More details about the implementation can be found in (Ref. [6]).

References

[1] Alex Anderson. Alex anderson's personal website. http://panic.berkeley.edu/~aga/, Nov 2012.

[2] Wikipedia. Density functional theory. http://en.wikipedia.org/wiki/Density_functional_theory, Feb 2013.

[3] Wikipedia. Gw approximation. http://en.wikipedia.org/wiki/GW_approximation, Feb 2013.

[4] Marvin L. Cohen Mark S. Hybertsen David A. Strubbe, Steven G. Louie. Berkeleygw. http://berkeleygw.org/, Feb 2013.

[5] Mark S. Hybertsen and Steven G. Louie. Theory and calculation of quasiparticle energies and band gaps. *Cond. Mat. Phys.*, 13:223–247, 1987.

[6] David A. Strubbe Manish Jain Marvin L. Cohen Steven G. Louie Jack Deslippe, Georgy Samsonidze. Berkeleygw: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures. *Comput. Phys. Commun.*, 183:1269, 2012.