TBPW: A Modular Framework for Pedagogical Electronic Structure Codes

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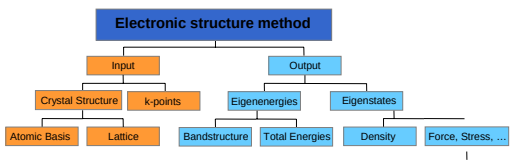
Motivation

All electronic structure codes have much in common, including a basic paradigm and set of components. The purpose of the code is to provide a framework to demonstrate the similarities, a pedagogical example of the development of such codes, and a pedagogical tool for teaching and understanding electronic structure.

Framework

- Provides common tools for crystal structures, k-point sampling, input/output, and graphics, along with examples of different bases and methods for diagonalization of the kamiltonian.
- Provides basic atomic simulation data structures.

Common Components



Electronic Structure Capabilities

TBPW is written from the ground-up in a modular style using Fortran 90. This code is composed of three distinct parts: common tools, tight binding (TB) and plane wave (PW) methods.

TB – Tight-Binding

Implemented using a rotation matrix formalism allows the use of orbitals with arbitrary angular momentum.

PW – Plane-Wave

Implemented using empirical pseudopotentials (non-self-consistent). Options of diagonalization via direct-inversion, or conjugate gradient method with optional fast Fourier transform (FFT).

Diagonalization Methods

Two alternative ways of diagonalization are provided:

1. Standard LAPACK routine $O(N_{basis}^3)$
   For TB or PW
2. Conjugate Gradient using FFT for evaluating $H\Psi$ $O(N_{electron} N_{basis} \ln N_{basis})$.
   For PW only

Conjugate Gradient scheme

- Constrained minimization of a quadratic functional , $\langle\Psi|H|\Psi\rangle$, with $|\Psi\rangle$ finally converging to the lowest eigenvector allowed by the constraints.
- The constraints reduce efficiency, but in practice sufficient accuracy is obtained.

Why FFT?

The Hamiltonian is constructed in the plane-wave basis, where a potential is not diagonal but the kinetic energy is. $H|\Psi\rangle = T|\Psi\rangle + V|\Psi\rangle$, or $[H\Psi]_G = T_G\Psi_G + \Sigma_{G'}V(G-G')\Psi_{G'}$

- The first term is a scalar multiplication, the second becomes a scalar multiplication in the real space by the convolution theorem

$$\Sigma_{G'}V(G-G')\Psi_{G'} = FFT^{-1}[V_r\Psi_r]$$

Since $N_B << N$, FFT is inexpensive compared to a full $O(N^3)$ diagonalization.

Relation to other codes

This is a simple example of the algorithm as used in ABINIT – similar to the one used in VASP

Tight Binding Method

Slater-Koster scheme implemented in a rotation matrix form that permits use of real (or complex) spherical harmonic basis with arbitrary angular momenta.

- Hamiltonian matrix elements are given by

$$H_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} \exp\left(i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)\right)\left[T^*(\phi_{ij},\theta_{ij})K(R_{ij})T(\phi_{ij},\theta_{ij})\right]_{\alpha\beta}$$

where $T(\phi_{ij},\theta_{ij})$ is the rotation operator

$$T(\phi_{ij},\theta_{ij}) = \exp(-i\theta_{ij}L_y)\exp(-i\phi_{ij}L_z)$$

K is the Slater-Koster matrix in the standard configuration.

- Easy input for widely used parameters such as the Harrison "universal parameters"

Relation to other codes

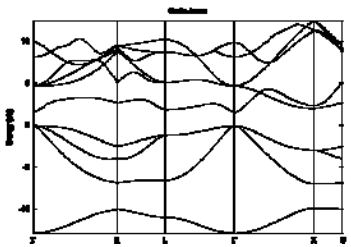
A simple example of local orbitals – as used in SIESTA

Input/Output

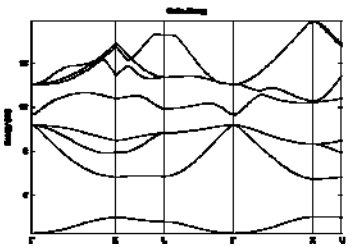
Input: Keyword format with structure and keywords similar to **SIESTA** – also close to **ABINIT**

Output: Standard data files or convenient plots using **Gnuplot** – density on a grid – can use **Xcrysden** and other plotting packages

Sample Bands: Gallium Arsenide – TB - PW

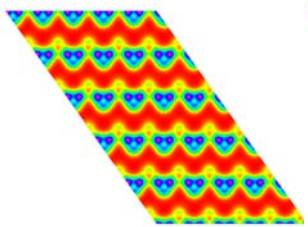


TB parameters from
J.-M. Jancu et al, *Phys. Rev. B* **57** 6493 (1998)

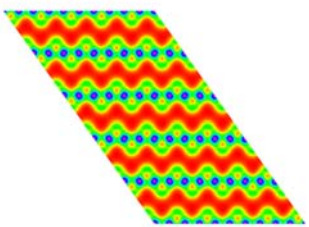


PW empirical pseudopotential from
Zhang, et al., *Phys. Rev. B* **48** 11204 (1993).

Sample Densities: PW – GaAs – Si



GaAs



Si

Plotted using Xcrysden. See A.Kokalj, Comp. Mater. Sci., 2003, Vol. 28, p. 155. Code available from http://www.xcrysden.org/

Conclusions

- A useful code for Teaching – Used in Summer schools
- A useful code for many calculations – semiconductor bands, nanotubes, . . .
- Electronic structure codes fit well into the component based code paradigm
- Fortran 90 is sufficient for component based programming, but requires careful planning.