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 $O(N_{\text{basis}}^3)$
   For TB or PW
2. Conjugate Gradient using FFT for evaluating $H \Psi$ $O(N_{\text{electron}} N_{\text{basis}} \ln N_{\text{basis}}$).
   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 $[H|\Psi\rangle]_a = T_a |\Psi\rangle_a + \sum_v V(G-G') |\Psi\rangle_v$.
• The first term is a scalar multiplication, the second becomes a scalar multiplication in the real space by the convolution theorem

$\sum_v V(G-G') |\Psi\rangle_v = FFT^{-1}[V |\Psi\rangle]$

Since $N_{\Psi} \ll N$, 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.

$H_{\text{TB}}(k) = \sum \exp[i(k \cdot \hat{R} - R)] T(\phi_\theta) K(\phi,\theta)$

where $T(\phi_\theta)$ is the rotation operator

$T(\phi_\theta) = \exp(-i\theta L_z) \exp(-i\phi L_y)$

$K$ 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


Sample Densities: PW – GaAs – Si

GaAs

Si


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.