Introduction to Research Topics

Ongoing and Planned

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Overview

- Solving Kohn-Sham problem
  - PWDFT.jl, parallelization, etc
  - Real-space based basis: finite-difference, Lagrange basis, adaptive grid, ...
  - FLAPW
  - Spectral finite element method
- Faster calculation: DFTB
- Density functional perturbation theory, phonons, response functions
- Time-dependent density functional theory
- Machine-learning related
- Kinetic Monte Carlo for surface reactions
- CFD + phase field nanomaterials formation (nucleation theory, combining Navier+Stokes and Allen-Cahn equations, reaction-diffusion equations for material science), shape control of nanomaterials

TOPIC: Solving Kohn-Sham problem

- We are trying to find what are really computed behind the software packages such as Quantum ESPRESSO, VASP, ABINIT, Gaussian, etc.
- We are trying to implement (write codes) that solve the Kohn-Sham problem.

The Kohn-Sham energy functional

Total energy:

$$E\left[\{\psi_i(\mathbf{r})\}\right] = -\frac{1}{2}\int \psi_i(\mathbf{r})\nabla^2\psi_i(\mathbf{r})\,\mathrm{d}\mathbf{r} + \int \rho(\mathbf{r})\,V_{\mathrm{ext}}(\mathbf{r})\,\mathrm{d}\mathbf{r} + \tag{1}$$

$$\frac{1}{2}\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}' + E_{\mathrm{xc}}\left[\rho(\mathbf{r})\right] \tag{2}$$

Electron density

$$\rho(\mathbf{r}) = \sum_i f_i\,\psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) \tag{3}$$

External potential:

$$V_{\mathrm{ext}}(\mathbf{r}) = \sum_I \frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|} \tag{4}$$

Kohn-Sham equation

$$\hat{H}_{\mathrm{KS}}\,\psi_i(\mathbf{r}) = \epsilon_i\,\psi_i(\mathbf{r}) \tag{5}$$

$$\hat{H}_{\mathrm{KS}} = -\frac{1}{2}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) + V_{\mathrm{Ha}}(\mathbf{r}) + V_{\mathrm{xc}}(\mathbf{r}) \tag{6}$$

$$V_{\mathrm{Ha}}(\mathbf{r}) = \int \frac{\rho(\mathbf{r})}{\mathbf{r}-\mathbf{r}'}\,\mathrm{d}\mathbf{r}' \tag{7}$$

$$\nabla^2\,V_{\mathrm{Ha}}(\mathbf{r}) = -4\pi\rho(\mathbf{r}) \tag{8}$$

$$V_{\mathrm{xc}}(\mathbf{r}) = \frac{\delta E[\rho(\mathbf{r})]}{\delta\rho(\mathbf{r})} \tag{9}$$

Various ways to "discretize" Kohn-Sham problem

- Local basis set: GTO (Gaussian program, NWCHEM, ORCA, CP2K, etc), ETO and numerical basis (fhi-aims, SIESTA, OPENMX, etc), muffin-tin orbitals (LMTO, RPSt, ..)
- Plane wave basis (QE, VASP, ABINIT, JDFTx, etc)
- Real-space based: finite-difference (Octopus, GPAW, PARSEC), finite-element (HelFEM,)
- Mixed and augmented basis set: FLAPW (Wien2k, ELK, exciting, fleur), PW + AO (Tombo)

Motivation: FLAPW in zoo of electronic structure methods

Approximation to exchange-correlation functional

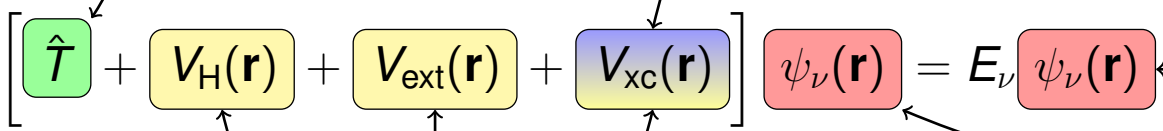
- local density approximation (LDA)
- generalized gradient approximation (GGA)
- LDA+U
- hybrid functionals
- EXX+RPA
- ...

Relativity

- non-relativistic
- scalar-relativistic
- fully relativistic

Representation of wave functions

- linear combinations of atomic orbitals (LCAO)
  - Gaussian orbitals
  - numerical orbitals
- plane waves (PW)
- real-space grid
- non-linear methods
  - KKR
  - augmented plane waves (APW)
- linearized methods
  - LMTO
  - linearized augmented plane waves (LAPW)



Contributions to potential

- pseudopotential
- all electron

Representation of potential

- spherical approximation
- full potential

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PWDFT.jl

- One of my many attempts to implement a Kohn-Sham DFT solver (other attempts can be found in `https://github.com/f-fathurrahman`).
- Using plane wave basis set and pseudopotentials (currently only GTH pseudopotentials are supported)
- LDA VWN + GGA PBE
- SCF (with density or potential mixing) and direct-minimization (for semiconductor)
- Force calculation is implemented but not tested yet

Topics related to improving PWDFT.jl

There are many topics:

- Documentation, testing, code clean up, visualization
- Adding and testing new Kohn-Sham solvers: Chebyshev-filtered subspace iteration, direct-minimization for metals, new mixing schemes
- Parallelization: multithreading, MPI and GPU (using CUDA)
- Implementing geometry optimization and molecular dynamics
- Implement calculation of stress tensor
- New physics: implement exact-exchange, meta GGA functionals, and vdW-DF
- Implement USPP and PAW

Machine learning related

Goals: replacing time-consuming quantum mechanical calculation with faster calculation via learning from training data.

- force-field related
- lsl

General tips + workflows

read softwares (need Fortran (both modern and F77), C/C++, Python, MATLAB, ...)

learn how they work

think + read books + how to improve

rewrite them using your own language, add features ...