PWDFT.jl Developer's Note

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PWDFT.jl uses Hartree atomic units.

1 Status

- **28 May 2018** The following features are working now:
  - LDA and GGA, spin-paired and spin polarized calculations
  - Calculation with k-points (for periodic solids). Monkhorst-Pack grid generation is done using spglib

  Band structure calculation is possible in principle as simply solving Schrodinger equation with converged Kohn-Sham potentials, however there is currently no tidy script or function to do that.

  Total energy result for isolated systems (atoms and molecules) agrees quite well with ABINIT and PWSCF results.

  Total energy result for periodic solid is quite different from ABINIT and PWSCF. I suspect that this is related to treatment of electrostatic terms in periodic system.

  SCF is quite shaky for several systems, however it is working in quite well in nonmetallic system.

2 Describing an atomic system

Because plane wave basis set is used, all atomic systems are assumed to be periodic. For isolated molecular systems, a periodic bounding box must be specified.

Currently, the definition of type Atoms is given below.

```
mutable struct Atoms
    Natoms::Int64
    Nspecies::Int64
    positions::Array{Float64,2}
    atm2species::Array{Int64,1}
    atsymbs::Array{String,1}
    SpeciesSymbols::Array{String,1}
    LatVecs::Array{Float64,2}
    Zvals::Array{Float64,1}
end
```

Information about LatVecs and Zvals are also available from PWGrid and PsPotGTH, respectively. They are included to reduce number of required arguments to several functions.

LatVecs represents lattice vectors a_1, a_2, dan a_3, stacked by column in 3×3 matrix.

`Zvals` is set when constructing `PWHamiltonian`. The default value is `zeros(Nspecies)`.

Currently, the following functions are provided to initialize an `Atoms`:

- Using dummy constructor:

  ```
  atoms = Atoms()
  ```

  It is important to set other fields of `atoms` accordingly.

- Using xyz-like structure

  ```
  atoms = init_atoms_xyz(filexyz; in_bohr=false, verbose=false)
  atoms = init_atoms_xyz_string(filexyz; in_bohr=false, verbose=false)
  ```

  In the first function, `filexyz` is a string representing path of the xyz file while in the second function `filexyz` represent directly the content of xyz file. Example:

  ```
  # Initialize using an existing xyz file
  atoms = init_atoms_xyz("H2O.xyz")
  # Initialize using 'inline' xyz file
  atoms = init_atoms_xyz(
  """
  2

  O   -0.8  0.0  0.0
  O    0.8  0.0  0.0
  """
  ```

Note that, for both way `LatVecs` must be set manually by:

```
atoms.LatVecs = 16*eye(3) # for example
```

Currently there is no warning or check being performed to make sure that `LatVecs` is defined properly. The default value is `zeros(3,3)`. So an error will happen if an instance of `PWGrid` is constucted because we will try to invert a zero matrix.

Equation

$$\frac{\alpha}{\beta} \tag{1}$$

3 Hamiltonian

`Hamiltonian` is the central object. It designed such that we can perform application or multiplication of Hamiltonian to wave function:

```
Hpsi = op_H(H, psi)
```

or (by 'overloading' `*`)

```
Hpsi = H*psi
```

4 k-points (Bloch wave vectors)

Monkhorst-Pack grid (used for Brillouin-zone integration)

$$\sum_{i=1,2,3} \frac{2n_i - N_i - 1}{2N_i} \mathbf{b}_i \tag{2}$$

where $n_i = 1, 2, ..., N_i$ size $= (N_1, N_2, N_3)$ and the $\mathbf{b}_i$'s are reciprocal lattice vectors.
Please see file `kpoint_grid.f90` in `PW/src`.