PWDFT.jl Developer's Note

Fadjar Fathurrahman

PWDFT.jl uses Hartree atomic units.

1 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.

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.

`Zvals` is set when constructing `PWHamiltonian`.

Equation

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

2 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
```

3 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`.