20: Disentanglement restricted inside spherical regions of k space

$LaVO_3$

- Outline: *Obtain disentangled MLWFs for strained $LaVO_3$.*
- Directory: `examples/example20/`
- Input Files
  - `LaVO3.scf` *The* PWSCF *input file for ground state calculation*
  - `LaVO3.nscf` *The* PWSCF *input file to obtain Bloch states on a uniform grid*
  - `LaVO3.pw2wan` *Input file for* `pw2wannier90`
  - `LaVO3.win` *The* `wannier90` *input file*

1. Run PWSCF to obtain the ground state of $LaVO_3$.
   `pw.x < LaVO3.scf > scf.out`
2. Run PWSCF to obtain the Bloch states on a uniform k-point grid.
   `pw.x < LaVO3.nscf > nscf.out`
3. Run `wannier90` to generate a list of the required overlaps (written into the `LaVO3.nnkp` file).
   `wannier90.x -pp LaVO3`
4. Run `pw2wannier90` to compute the overlap between Bloch states and the projections for the starting guess (written in the `LaVO3.mmn` and `LaVO3.amn` files).
   `pw2wannier90.x < LaVO3.pw2wan > pw2wan.out`
5. Run `wannier90` to compute the MLWFs.
   `wannier90.x LaVO3`

Inspect the output file `LaVO3.wout`. In the initial summary, you will see that the disentanglement was performed only within one sphere of radius 0.2 arount the point $A = (0.5, 0.5, 0.5)$ in reciprocal space:

```
|  Number of spheres in k-space              :                1             |
|   center n.   1 :     0.500   0.500   0.500,    radius   =   0.200         |
```

Compare the band structure that Wannier90 produced with the one obtained using Quantum ESPRESSO. You should get something similar to Fig. 9. Notice how the t_{2g}-bands are entangled with other bands at A and the Wannier-interpolated band structure deviates from the Bloch bands only in a small region around that k-point. It is important to keep in mind that all symmetry equivalent k-points within the first Brillouin zone must be written explicitly in the list of sphere centers. For instance, the A point in the simple tetragonal lattice of this example is non-degenerate, while the X point has degeneracy two, hence one must specify both $(1/2, 0, 0)$ and $(0, 1/2, 0)$ (see the $SrMnO_3$ example here below).

Further ideas

- Try to obtain the Wannier functions using the standard disentanglement procedure (without spheres, `dis_spheres_num = 0`). You will notice that the Wannier-interpolated band structure

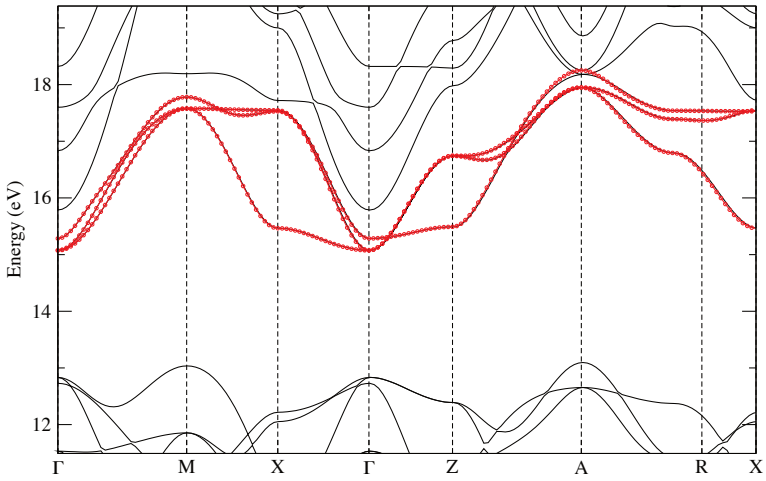

Figure 9: Band structure of epitaxially-strained (tetragonal) $LaVO_3$. Black: Bloch bands; red circles: Wannier-interpolated band structure. The disentanglement was performed only for k-points within a sphere of radius 0.2 Å^{-1} centered in A.

now shows deviations also in regions of k-space far away from A, where disentanglement is actually not necessary. If you disable the disentanglement completely, instead, the Wannierisation procedure does not converge.

- In order to illustrate all possible cases, it is instructive to apply this method to $SrMnO_3$, where the t_{2g} bands are entangled with the above-lying e_g bands, and also with the deeper O-2p states. In the $SrMnO_3$ subfolder, you can find input files for building three different sets of Wannier functions: only t_{2g} states, only e_g states, or all V-3d-derived states ($t_{2g} + e_g$). In each case one needs to specify different disentanglement spheres, according to which region(s) in k-space show entanglement of the targeted bands. Also the index `dis_sphere_first_wan` needs to be adapted to the new disentanglement window, which here contains also states below the lowest-lying Wannier function (at variance with the $LaVO_3$ case).

References

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