Wannier90 v3.0 school, Virtual Edition 2020

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- **Is the symmetry-adapted procedure needed for the Gamma-only case?**
  In principle, to create localized functions, we need finite k-mesh. But, even in the Γ-only case, we can construct the symmetry-adapted unitary matrix to transform from Kohn-Sham gauge to symmetry-adapted Wannier gauge.
- **Can we perform the SAWF calculations for any crystalline compound?**
  Yes. As far as the crystals have a finite number of symmetry elements, we can create SAWF. Practically, you need to take care of preparing proper projections and energy window, which is compatible with symmetry.
- **Do the SAWF calculations take less computational time than the usual MLWF calculations?**
  I have never seriously checked the computational time. But SAWF should not increase the computational time much. Basically, what we do additionally are to symmetrize the unitary matrix in wannier90 and to compute D and $\tilde{d}$ matrices in pw2wannier90. These do not take too much time.

Is the spread of SAWFs smaller than usual MLWFs? I.e. are they more localised?

No. The total spread of SAWFs is the same as or bigger than that of MLWFs. This is because we restrict the form of U(**k**) (see page 6 of lecture PDF). But if we focus on a specific orbital, then the individual spread of SAWF can be smaller than that of MLWF. See the comparison between pages 17 and 18 in the lecture PDF.

- **Does the D matrix depend on the initial guess of the WFs?**
  Yes. D matrix shows how the symmetry-adapted Wannier-gauge Bloch functions are transformed by symmetry-operations. So if the initial guess is different, the transformation is also different.
- **If the initial projections are not fit to the local site-symmetry, will Wannier90 give an error?**
  Yes, it gives an error. Sometimes the error occurs because the symmetrize_eps is too strict (in my personal view, symmetrize_eps can be up to ~ 1.0E-5). If you still get an error with increasing symmetrize_eps up to 1.0E-5, you need to reconsider initial projections and energy window.
- **When or why should be the SAWF calculations performed? Could you please explain the purpose of SAWF?**
  One of the purposes of constructing Wannier functions is to obtain realistic tight-binding Hamiltonian. The symmetry of the tight-binding Hamiltonian is important in calculating topological properties, and to perform many-body calculations such as dynamical

mean-field calculations. In such cases, SAWFs are helpful because the tight-binding Hamiltonian will keep symmetry.

- **Is it possible to automatically generate Wannier functions (e.g. with SCDM-k) with enforced symmetry (SAWF) or there is a fundamental issue preventing this?**
  At least, we need the information on symmetry of the all Kohn-Sham wave functions produced by nscf calculations. For another possible difficulty, see the following comment by Valerio Vitale: “We also need to compute the D matrix, which we compute from initial projections, however with automatic projections we do not know the character of these function and we do not know how to construct the D matrix”.
- **Does SAWF work for lower-dimensional materials (2D for example)?**
  Yes. But sometimes putting the vacuum layer lowers the site-symmetry, and it might become impossible to make exactly atom-centered Wannier functions. See page 20 of the lecture PDF.
- **Can we use SAWF in strong-SOC cases?**
  If we introduce SOC, then we need to perform noncollinear calculations. In the case of noncollinear calculations, SAWFs can not be constructed at the moment.
- **Is it due to numerical or physical reasons that the symmetrized spread minimum is larger than the "global" minimum?**
  This is because we put symmetry constraints when minimising the total spread wrt the degrees of freedom in U(**k**). Then the total spread of SAWFs is larger or the same than that of MLWFs. See page 6 of the lecture PDF.
- **Does SAWF work without performing the disentanglement of bands?**
  SAWFs work both for isolated bands and entangled bands. In the former case, we do not perform disentanglement.
- **Are there any difficulties about implementation of SAWF in the disentanglement step? Especially when you already have constraints on U(k). Can we just symmetrize U(k) in the disentangle step?**
  SAWFs also work for entangled bands. For theoretical background, please have a look at the original paper by Rei Sakuma.
- **Suppose that I am trying to symmetrise a tight-binding model. First, I construct a D(g,k) matrix for its basis. The next step would be to construct the d matrix, which in this case is, in principle, the same. However, my code works only if I assume $\psi_{i\bar{k}}(\bar{r}) = \sum_j D_{ji}(g,\bar{k})\psi_{j\bar{k}}(\bar{r})$, instead of $\psi_{i\bar{k}} = \sum_j D_{ji}\psi_{jR\bar{k}}(\bar{r})$ (paper). Is it a bug? (The point is that SAWF code does not give me an error).**
  To answer this question, I need more detailed information.
- **Can you comment on the difference between SAWFs and minimizing constraining wannier centres (SLWFs)?**
  Answer by Valerio Vitale: When constraining the centres of the WFs you introduce a different kind of constraints in the minimisation of the spread functional. In the original paper by Wang *et al.* [*PRB **90**, 165125, (2014)*], it is stated that, at least for the few systems they have tested it on, the constraints on the centres automatically force the

resulting function to transform as eigenfunction of the local site-symmetry group. However, there is no formal mathematical proof of this.
One major difference between SAWFs and centre-constrained WFs is that you cannot constrain the centres of all your WFs, since the sum of the centres is invariant (modulo a lattice vector). So you can only constrain the centres of a subset of your WFs.

- **Can you use SAWF with collinear magnetism?**
  I have never tried, but in principle, it should work for the collinear calculations. We can make SAWFs for up and down spins separately. If you want to construct SAWFs for collinear calculations, please check your calculations carefully.
- **What is known about the reality of WF? Are SAWFs usually real, even though they are not a global minimum of the spread functional?**
  Yes, SAWFs are also real. It is explained in the original paper by Rei Sakuma, so please have a look at the paper.
- **Should we consider applying TR-symmetry by default for TR-symmetric systems?**
  For the moment, we do not consider TR-symmetry. But it might be a good idea also to consider TR-symmetry.