Wannier90 v3.0 school, Virtual Edition 2020

Speaker: Anil Damle

26 March 2020 - Questions and answers session

- **Does one need to sum over the BZ?**
    - We discuss k-point sampling in the latter part of the talk and address this question.
- **How do you pick the P columns to start with? Randomly?**
    - The column-pivoted QR algorithm is a “direct” method and non-iterative, so there is no need to specify an initial guess for the columns. The factorization is simply computed starting just from Ψ^* and that is the only necessary input. See https://www.netlib.org/lapack/lug/node42.html for a brief note on which version is implemented in LAPACK
- **How do you quantify "well conditioned" numerically? Does it mean that they are as orthonormal as possible?**
    - “Well conditioned” here means with respect to the two-norm condition number. So, for an $n \times k$ matrix A with $n \geq k$ we want the ratio $\sigma_1(A)/\sigma_k(A)$ to be as close to one as possible. The colloquialism “as orthonormal as possible” stems from the fact that if A has orthonormal columns it will have condition number equal to 1.
- **Can you comment on the difference between SCDM functions and Natural Orbitals?**
    - In general there is no specific connection. I am somewhat less familiar with natural orbitals and know that the term can be somewhat overloaded, so it is possible I have misinterpreted this question.
- **Is SCDM always a localised function? Are they maximally-localised?**
    - In some sense the SCDM orbitals are always localized, though there are some cases (such as topological insulators where this breaks down). However, they are not explicitly defined or constructed to try and minimize a MLWF like objective function. Therefore, while they are typically localized they are not necessarily a stationary point of the MLWF objective.
- **If we don’t need initial guess functions, how do we determine the number of WF?**
    - This depends, typically in the isolated case the number of Wannier Functions is equal to the number of bands of interest. In the entangled case things get a bit more complicated and this could be considered an input parameter. As discussed during Giovanni’s talk there can be good chemical/physical ways to determine the number of Wannier Functions desired in the entangled case.

- **How do you choose the template column as a basis for orthogonalization at k=Gamma? Do you try all combinations of columns and pick the one that is the most orthogonal (i.e. best well-conditioned)?**
    - We again use the column-pivoted QR factorization algorithm to achieve this task and avoid having to look at all possible subsets (a prohibitively expensive proposition). More generally, any so-called rank-revealing QR factorization will suffice.
- **Does the Ng grid on which the Psi's are defined need to be uniform? Can you just use Wyckoff positions?**
    - It does not, but some care must be taken to include the integration weights appropriately. We have tried some heuristics to pick columns but most break down because they do not account for similarity of certain columns. The projection steps that occur in the column-pivoted QR to "eliminate" columns similar to those we have already picked are quite important.
- **Does the SCDM method provide atom-centred WFs?**
    - Not necessarily, it depends on the system; they can be bond or atom centered as appropriate.
- **Why should we do a W90 optimization on top of the SCDM guess?**
    - At least in the isolated case, if one really cares about orbital spread with respect to the MLWF objective there is no harm in running W90 after the fact — the spread can only be further reduced. In the entangled case it is a bit trickier since there is not a one-to-one correspondence between minimizing spread and quality of things like band-interpolation (see Giovanni's talk for a more in-depth perspective on this).
- **From the plot in the slides, RMSE was lower for SCDM+w90, but it seemed visually that pure SCDM did a better job interpolating bands, especially near the edges? Is this true?**
    - For that case it is, but it is hard to generalize that quality more broadly; in Giovanni's talk there is a much broader analysis of spread vs. band interpolation quality that explores this point.
- **Also, in the case of Si, if you zoom on the CBM, the position of the CBM (in k-space) is very tricky to get with Wannier90. Does this improve with SCDM-k?**
    - Valerio Vitale's answer: When I looked at this, it seems that SCDM does not improve the situation
    - Anil: Valerio has looked at this and I have not, so I do not really have anything to add to his answer.
- **Does the SCDM method work with spin-orbit coupling?**
    - Yes, my understanding is that it does now.
- **How to do w90 optimization on top of SCDM? just restart=wannierise?**
    - The user guide and examples for W90 describe how to use a SCDM based initial guess with W90 by adding information to the .win and .pw2wan file (so that pw2wannier90 generates the SCDM initial guess).
- **In practice, how do you choose the best procedure for i.e. interpolation?**

    - This can be a bit tricky, in principle it is all close to Fourier Interpolation and there are many schemes with, formally, the same asymptotic behavior. However, the "grids" are small enough here that constants matter and the use of specialized interpolation schemes is valuable — I am not necessarily the best person to comment on all of the possible options. For the talk we use what is the default in W90.
- **Does the SCDM algorithm guarantee anything w.r.t. the symmetry of the Wannier functions? If not, can the output be symmetrized?**
    - Valerio Vitale's answer: Sometimes the SCDM functions are not as symmetric as MLWFs from projections, e.g. in copper you don't get a well separation between t2g and eg.
    - Anil: SCDM does not make any guarantees of symmetry. In principle there could be ways to symmetrize the method by respecting symmetries while selecting columns and doing the orthogonalization. However, we have not worked out details for this and it would certainly require more input information to encode the desired symmetries.
- **Is selecting columns of Psi^dagger rather than P formally equivalent, or is there an approximation there?**
    - Technically this can depend on the type of rank-revealing QR factorization used. With the column-pivoted QR (the one in LAPACK and what we use) they are equivalent. This is a consequence of the specifics of the CPQR algorithm and may or may not hold for other rank-revealing factorizations (I have not checked them all). However, the more important/key observation is that a good rank-revealing QR factorization of Ψ^* immediately implies that you have a good rank-revealing QR factorization of $P = \Psi\Psi^*$ (even if it is not quite the same as the one that would be computed if P was operated on directly). To see this observe that given a rank-revealing QR factorization of Ψ^* as $\Psi^*\Pi = Q[R_1\ R_2]$ we have that $P\Pi = (\Psi Q)[R_1\ R_2]$. Since ΨQ has orthonormal columns this is a (reduced) QR factorization of P and we see that the condition number of the columns of P that we select is $\kappa(R_1)$ the same as it is for the columns we selected of Ψ^*. So, if we found a well-conditioned set of columns of Ψ^* we have also found a well-conditioned set of columns of P.
- **Any comment on wannierise conduction bands for 2D materials? Do SCDM functions show the same issues as MLWFs, namely being centred in the vacuum region and be delocalised?**
    - I do not have much to say here, I have not personally explored 2D materials much. Though, some work does suggest that you could have SCDM based localized functions that are centered in vacuum and more delocalized when dealing with conduction bands.
- **Does the SCDM method work with other electronic structure codes (e.g. VASP)?**
    - I do not have a full accounting of where adding SCDM is in development, but to the best of my knowledge it has not yet been implemented in VASP.