III. REPLY TO REFEREE 3

- *"The authors investigate the spectral properties of lattices with position-dependent hopping amplitudes and on-site potentials. They find the integral expression Eq. (2) for the single-particle density of states (DOS) and discuss the inverse problem of constructing the hopping amplitudes in a lattice model yielding a given DOS. The analytic results are compared to and validated by numerics obtained by exact diagonalization of the hopping model on the lattice.*
I have a number of questions and concerns:"

We thank the referee for their report and comments which have helped us to improve the clarity and accessibility of our paper. In the following we address all the points raised by the referee.

- *1. "The first sentence of the Introduction ("The density of states (DOS) is a key physical quantity in condensed matter physics - ...") is too general. The single-particle DOS is central only for single-particle physics, or equivalently non-interacting systems. When interactions are present, even the notion itself would need refining. In particular, the reference to "strongly correlated ... phenomena" at the end of the first paragraph of the Introduction is overstretching things in my opinion."*

We thank the referee for pointing out that the main applicability of single-particle physics is to non-interacting systems. We agree, and we therefore reformulated the introduction to avoid being overly generic.

We would still like to insist however, that the notion of a DOS is not limited solely to non-interacting cases, and can still be useful also in weakly-interacting or uncorrelated, yet interacting situations. The Moire superlattices mentioned at the end of the first paragraph are related to our work because of the appearance of flat bands causing divergences in the DOS at the single-particle level. We do agree that the inclusion of the interactions that dominate the full, many-particle physics of these materials is beyond the scope of the current manuscript.

- *"The "PWFs" of Eq. (4) first reminded me of the "projector augmented waves" [P. E. Blöchl, Phys. Rev. B 50, 17953 (1994)] that are famous in the ab-initio context. However, on closer inspection, I have some more basic problems: Eq. (4) appears to define periodic functions. In particular, there is no damping at the boundaries, as suggested by the "partial Wannier" sketch of Fig. 1(a). This raises the question about boundary terms, e.g., in Eq. (6) at the boundaries of Hintra. A related question is: isn't $B(x)$ in Eq. (10) and the following line simply proportional to $\delta_{x,0}$?"*

We thank the referee for suggesting a possible connection to Projector Augmented Waves. Although it is, in principle, possible to add damping to the definition of our PWFs, it is unnecessary and generally leads to unwanted complications. To see this, notice that first of all, the basis defined by Eq. (4) is already orthogonal as the states with different m_c have exactly zero spatial overlap, while those with equal m_c (inside the same piece) but different quasi-momenta ϑ are orthogonal for the same reasons that plane waves with different momenta are orthogonal.

Secondly, in the case of "projector augmented waves" a distinction is made between two regions of space: the inside and the outside of spheres centered on the nuclei, and the projection is applied only within the spheres. In contrast, in the PWF formulation of the current manuscript, there are no physical boundaries anywhere, and the amplitude of PWFs on the ends of each small chain should not be different from those within the small chains. Consequently, there is no distinction between "boundary" and "bulk" terms, as can be seen for example in Eq. (6).

About $\mathcal{B}(x)$, the comment of the referee helped us realize there was a typo in the original manuscript, with a missing prefactor n_s inside the sum. This is fixed in the revised manuscript, and the correct expression, stemming from the corresponding forms in Eqs. (7) and (8), is not proportional to $\delta_{x,0}$. We are grateful to the referee for pointing out this issue.

- *"The mapping of a DOS to a hopping model also appears in dynamical mean-field theory (DMFT) when solved with the numerical renormalisation group, see, e.g., Kenneth G. Wilson, Rev. Mod. Phys. 47, 773 (1975) and Ralf Bulla, Theo A. Costi, and Thomas Pruschke, Rev. Mod. Phys. 80, 395 (2008). Consequently, I believe that the essence of chapter 5 of the present manuscript is well-known. The semi-circular density of states Eq. (36) is a classic in DMFT although I have to admit that many related publications glance over the explicit expressions for the related Wilson chain."*

We thank the referee for pointing out a relation of our work to results in DMFT. Indeed a type of hopping model which is in the class of systems that we consider appears in the context of numerical RG methods, and especially in the famous Kondo problem. We accordingly include a discussion of such specific incarnations of the generic problem that we consider in the revised manuscript.

But we should insist that, to the best of our knowledge, neither our motivation, nor the generality of our approach, nor our central and explicit findings such as the DOS formula and the inverse relation (Eqs. (2) and (21-22)) are present in the DMFT literature or any other previous study. This is in particular supported by the review mentioned by the referee [Bulla et al. in RMP (2008)], which states that "Analytical solutions for the recursion relations have so far been given only for a few special cases". In contrast, we provide a rigorous and general picture for the mapping between DOS and hopping models.

In addition, the purpose of our construction is quite different from that in the RG studies, where the tight-binding model is constructed such that it gives a special form for the hybridization function $\Delta(\omega)$ of the Kondo model. Considering the special cases of a constant $\Delta(\omega)$ (which corresponds to a constant DOS of conduction electrons in the Kondo Hamiltonian), an exponential dependence for the hoppings has been obtained. In contrast, in our case an exponentially varying t_n does not lead to a constant DOS. We point this out explicitly in the revised manuscript.

Finally, within the context of the current manuscript, the semicircular DOS is just one example among many others. We highlight it in the manuscript as part of the numerical justification of our approach.

- *"The main concerns have been listed in the report. Further details are:*
  1- Four lines below Eq. (30): a periodic function $\varepsilon(k)$ cannot be "completely monotonic". I believe that this can be remedied by considering different regions of k, but the authors should be more precise.
  2- Fig. 3 has no panel labels. This is inconsistent with the last paragraph of page 12.
  3- Fix excessive lower-casing in titles of references, in particular "I" in [11] and names in [13,17,19,24]."

We thank the referee for bringing these points to our attention. We fixed them in the revised manuscript.