

I. REPLY TO REFEREE 1

- *“The authors derive an integral formula for the density of states (DOS) of a generic noninteracting tight-binding model with position-dependent hoppings $t(x)$ and on-site energies $\mu(x)$. Their focus is on the simpler case of 1D tight-binding models with a single orbital per site, but they also provide a generalization to higher dimensions and multiorbital models. Their approach utilizes a hybrid Bloch-Wannier basis which diagonalizes the Hamiltonian for smooth hoppings in the limit of an infinite lattice. The authors then use their result to solve the inverse problem, namely, how to construct the function $t(x)$ (assuming $\mu(x) = 0$) that gives rise to a given DOS. Finally, they also consider the inverse problem but for translationally invariant tight-binding models with longer-range hopping.*

This is an interesting study which employs clever mathematical tricks to solve a rather general problem in condensed matter physics (one could say more generally, in quantum mechanics) that, to my knowledge, has only been treated purely numerically in the prior literature. It should be of interest to a fairly wide audience of researchers in the quantum simulation/designer Hamiltonian communities. The paper is well written, clearly organized, and technically sound as far as I can tell. If the authors can address my questions below, I would be happy to recommend the manuscript for publication.”

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 raised points and questions.

- 1. *“The integral over position in Eqs. (2) and (18) is reminiscent of taking the trace of the imaginary part of the retarded single-particle Green’s function in the position basis, which is a standard way of computing the DOS. Is it possible to derive those equations using Green’s function methods?”*

It is indeed possible to re-formulate our method in terms of Green’s functions. We can begin by writing the Green’s function in the partial Wannier basis and then apply perturbation theory to that, which yields

$$G_{m_c, \vartheta; m'_c, \vartheta'} = G_{m_c, \vartheta}^0 \delta_{m_c m'_c} \delta_{\vartheta \vartheta'} + G_{m_c, \vartheta}^0 \langle m_c, \vartheta | \mathcal{H}_1 | m'_c, \vartheta' \rangle G_{m'_c, \vartheta'}^0 + \dots \quad (1)$$

The lowest order Green’s function is diagonal in the PWF basis where $G_{m_c, \vartheta}^0 = (\omega + i0^+ - E_{m_c, \vartheta}^{(0)})^{-1}$. Therefore, using the basic relation of DOS in terms of Green’s function i.e.

$$D(\omega) = \Im \text{Tr} \hat{G} = \Im \sum_{m_c, \vartheta} G_{m_c, \vartheta; m_c, \vartheta} \quad (2)$$

in the lowest order, the Eqs. (2) or equivalently (18) of the main text can be obtained again.

- 2. *“I find the discussion of van Hove singularities on p. 9 a bit confusing. The authors write that “simple 1D TB models typically have van Hove singularities at the band edges as $D(\omega) \propto \sqrt{\omega_{max}^2 - \omega^2}$, yet it remains finite and differentiable, otherwise.” The simplest 1D TB model I can think of, with uniform hopping $-t$, has van Hove singularities of the *inverse* square root form at the band edges with $\omega_{max} = 2t$. These are integrable but still divergent. Given the reference to the Wigner semicircle law in the following section, I think the authors may have in mind random TB models, but if so, this should be mentioned explicitly. Also in that same paragraph, when referring to the logarithmic behavior at an ordinary van Hove singularity, it is again not clear if the authors are referring to band-edge or band-center singularities, since both are discussed earlier in the paragraph.”*

Following the suggestion of the referee, we refined the discussion of van Hove singularities in the main text, and improved its clarity by explicitly distinguishing where we concentrate on band-center or band-edge singularities. We also thank the referee for pointing out the missing inverse in the 1D density of states.

Regarding the semicircular distribution, we agree that this refers to random matrices, as stated explicitly in the main text: “... emerge in $n \times n$ symmetric random matrices with independent and identically distributed entries”. In the revised manuscript, we also explicitly mention “the random TB model”. Please notice however, that we show here that the semicircular distribution can also arise in a position-dependent TB model with hopping profile $t(x) = \sqrt{x}$.

- 3. *“In Sec. 4, the authors use nondegenerate perturbation theory to compute finite-size corrections due to H_1^{intra} and H_1^{inter} . Naively, H_1^{intra} will couple degenerate “Bloch” states at $\vartheta = \pi$ and $\vartheta' = -\pi$, for example, as in the standard nearly-free-electron problem. Shouldn’t one use degenerate perturbation theory for those terms?”*

We thank the referee for pointing out this potential point of confusion. Our formulation in the current manuscript departs from the tight-binding model, which is the opposite starting point for the band theory as compared to the nearly-free-electron picture. The degeneracies at the boundaries of the Brillouin zone mentioned by the referee are not generically present in tight-binding models. They could appear due to some symmetry constraint, and one should treat those cases with a bit more caution, as suggested by the referee. In the main text, we assume a band structure with well-separated bands and without any symmetry-enforced or accidental degeneracies, in which we can rely on the non-degenerate perturbative treatment.

- 4. *“For all the numerical examples of DOS chosen, there is no gap in the spectrum. Does the smoothness requirement for $t(x)$ and $\mu(x)$ necessarily imply a gapless spectrum? For example, the simplest 1D TB model that has a gap is the SSH model, but the function $t(x)$ would not be smooth in this case. Conversely, is it possible to solve the inverse problem for a gapped DOS by the authors’ method?”*

As pointed out by the referee, we considered only single-band models in our numerical examples. However, as we explicitly elaborate on in Sec. 7, our approach can be extended straightforwardly to multi-band cases. For the special example of the SSH model, treating the two sublattices as two orbitals would allow us to still consider it a uniform-hopping model. Then, by assuming smooth variations for the intra- and inter-cell hoppings, we can even consider generalized, position-dependent SSH models and apply the correspondence of DOS relation (Eq. 2).

The inverse problem can also still be solved for multi-band scenarios, by assuming the bands are isolated in energy and applying our formulas to each band separately. We would like to stress, however, that in the multi-band case the inverse problem is likely to have multiple solutions and the particular solution obtained with the method of Sec. 5 may not be the most natural or interesting solution.