

Dear Editors,

We would like to thank both referees for their recommendation to publish our paper in PRB. Below, you will find the questions and comments of the referees together with our reply. We also made some revisions in our manuscript. A list containing all revisions can be found below. With these alterations, we are confident that our manuscript can now be published in PRB.

reply to the first referee

It seems to me that the ideas considered in the manuscript are quite heavily based on reference [24], perhaps more so than is readily understood without actually reading that reference. I think it would make sense to cite reference [24] and mention that they considered discontinuities of the trace of the correlation matrix already immediately after equation (30). Also the Chern number example considered in section VI C is very similar if not the same as the example considered in [24]. This could also be mentioned immediately in the beginning of section VI C so the reader can e.g. look at the picture of the cylinder geometry in that reference and otherwise compare.

It is not correct to say that the ideas and results in this manuscript are heavily based on reference [24]. Only VI is heavily related to [24], specially the connection of the trace of the correlation matrix with the topology of the system. The main results of our manuscript are contained in section V. Eq. (30) connects these results with the trace index of ref [24], but only for Chern insulators, and not for the other systems that we also consider.

However, we agree that we should mention ref [24] already below eq. (30). We have done so in the revised manuscript. We also mention the connection to [24] in the beginning of section VI and comment on what is already known and what is new in our manuscript.

1) I assume that N_A in eqn. (29) is just the total number operator for subsystem A (this should be mentioned), and $\langle P \rangle_0$ is just the expectation value of the number of particles in subsystem A in the ground state. This seems very simple, and somehow the flux insertion in the definition of the polarization feels like an unnecessary complication. Could you comment on this?

Yes, N_A is just the total number operator of particles in A and $\langle P \rangle_0$ is the expectation value of the number of particles in A. The flux insertion argument is needed to show that $\langle P \rangle_0$ is a geometric connection, and to related to the definition of $\langle P \rangle_0$ in equation(16). So while it is more complicated, we do not want to omit it.

2) In section VII possible extensions, such as weakly interacting systems, are discussed. Do you think an extension to finite temperature is possible? A geometric phase for mixed states based on Resta's definition of the polarization has recently been discussed [4].

Such an extension might indeed be possible, but it is not trivial to extend the results of [4] to our results. The issue is that we need the flux insertion to link the polarization, in the form of eq.(16), to the entanglement spectrum. Since (16) is not just an expectation value, we do not know how to properly generalise it for finite temperatures.

3) Regarding the extension to interacting systems, the authors mention the possibility that the single-particle correlation matrix encodes the topological information for some specific cases. A very similar

idea is the so-called topological Hamiltonian [5,6], where the topological information is contained in the zero-frequency Green's function. Noting that the correlation matrix is the zero-imaginary-time Green's function, there could be some connections between these ideas. Perhaps the authors want to mention this in their work.

That is an interesting questions. Unfortunately, we do not know whether an extension using the Green's function is really feasible. We have, however, mentioned this possible connection in the revised manuscript and added references [5] and [6] as suggested by the referee.

reply to the second referee

Before answering the referee, we would like to emphasise that it is important to distinguish between the ES and the EOS when discussing the results of our paper. The ES is strictly speaking computed from the reduced density matrix and always contains all the information about the state (whether one can extract it is another issue). In case of non-interacting systems, one can in principle compute the ES from the EOS by looking at all possible ways to fill single-particle energies with a certain number of particles. Even for relatively small systems however, this becomes unfeasible as the number of possible combinations grow too fast. That is why all our results are phrased in the EOS or the single-particle ES, both of which only grow linearly with system size.

(1) There is a statement in the paper that the entanglement occupancy spectrum ν_{si} is (a) 0 or 1 if the eigenstate is localized in the bulk; (b) away from 0 and 1 if the eigenstate is localized on the edge. I'm wondering if this is a numerical observation, or can be proven rigorously (or at least there is a strong argument)? This statement is crucial, as the (mod 1) definition of the main result Eq. (26) depends on it. (I failed to find an argument, except numerical observations, in Ref. 33 which was cited in this paper.)

This can be proven rigorously. We added an explanation in the second but last paragraph in section IV.

Let us here give a simplified argument using the dimerized limit of the SSH chain. For this limit, the EOS can be computed easily without the need of numerics.

In the topological phase, the eigenstates of the SSH chain can be written as $\frac{1}{\sqrt{2}} (|j, B\rangle \pm |j+1, A\rangle)$, where j denotes the unit cell index and A and B denote the sublattice sites. For a dimer in the interior of part A , the eigenstates are still eigenstates of the reduced density matrix, and the corresponding eigenvalue of the EOS is ± 1 if the eigenstate is occupied, 0 if it is not occupied. If the dimer, on the other hand, lies on the edge of A (say site j is in A , but site $j+1$ is in B), then the corresponding EOS eigenvalue will be $1/2$ since the EOS is completely oblivious to anything living in B . In a sense, one could say that the EOS is 'measuring' to how much of an occupied state is located in A .

(2) Below Eq. (27), it said that "if the degeneracy is four-fold or higher we must obtain the localized eigenstates". Could the authors give a procedure or algorithm on how to obtain the localized eigenstates in their numerical calculation?

We added an appendix detailing a procedure to count the number of localised eigenstates in each virtual edge, since that is the quantity that is needed. In summary, one can construct a projector into the subspace spanned by the degenerate eigenstates. Taking the trace on the left (right) half of A will give the number of localised eigenstates in each virtual edge. This will give a number exponentially close to an integer given that the eigenstates are exponentially localised on the edges.

(3) The paper also discussed 2D Chern insulator by viewing it as many 1D models parameterized by k_y . Is there a more intrinsic 2D relation between ES (say, of a disk subsystem) and the bulk topological invariants? It would be a more natural generalization of the 1D result of this paper.

The simplest relation between the EOS and a Chern insulator is obtained by bi-partitioning a torus into two cylinders. This exposes two chiral modes connecting the 0 and 1 'bands' of the EOS. This relation is already very well known, and gives the correct count of chiral edge modes for any Chern insulator and, thus, the bulk topological invariant. Using the EOS of the disk sounds simpler, as one would only have one edge. But it has the complication that one has no good quantum number to plot against (we are looking at lattice systems, so angular momentum does not work), which makes it much harder to interpret the results. One may easily determine that there are virtual edge modes in the EOS, but the number of modes and their chirality are hard to determine.

The aim of VI is rather to show how the polarization can be used to compute the Chern number in a simple way.

(4) I understand that the interaction effect is beyond the scope of this manuscript, but it is valuable if the authors can comment more on it. As far as I understand, the ES contains the information of edge state, which is related to the bulk topological invariants even with interactions. Therefore, it seems that the result of this paper could be generalized to interacting systems such as symmetry-protected topological phases. In the conclusion part of the paper, it said that "With interactions, the correlation matrix does not have the full information of the ground state". Do you mean that we should use the n -point correlation function to connect ES with bulk topological invariant?

Here it is important to distinguish between the ES and the EOS. The ES always contains the full information, but can only be computed for small systems. The question is whether the EOS or a suitable generalization contains some or all information about the system. This is a very interesting question that we do not have an answer to. It would already be an interesting result, if one could establish that the EOS retains at least some information even in presence of interactions. One should be able to reconstruct the full information from all the n -point functions, but this will be at least as hard as computing the ES. So in this context, it might be more useful to have a quantity that is very easy to compute and contains some information.

list of changes:

We have added an explanation on why the bulk modes in the EOS have eigenvalues close to 0 or 1, below equation (23).

We have added an appendix on how to count the number of localised states in each virtual edge of the EOS for the degenerate case, with a mention in the main text after equation (27).

After eq.(29) we have states what N_A is.

After eq.(30) we have explained the interpretation of the resulting polarisation in terms of N_A , and we have added a Reference to [24].

In the beginning of VI C we have added a reference to [24], stating the similarities with what we do in this section and what is new.

We have added two references as suggested by the first referee.