Supplementary Material

Appendix 1: The Bose-Hubbard dimer

We will start with the easiest case, a dimer with 2 excitations on it. This model will shed some light on our path to two particle interaction, making it easier to understand future models.

One of the main changes between this and the 1 excitation dimer is the basis in which we are working. In the two excitation limit we have a 3 element basis of the form $\mathfrak{B} = \{|2,0\rangle, |1,1\rangle, |0,2\rangle\}$. Where the kets represent the two particles on the first site, one particle at each site or the two particles on the second site. We have taken into account that the particles are indistinguishable so, we can't assign a label to each one and distinguish between a-b and b-a, for this reason there are only three kets in the basis.

In this Basis the Hamiltonian reads:

$$H = \begin{pmatrix} 2\omega_0 + U & \sqrt{2}J & 0 \\ \sqrt{2}J & 2\omega_0 & \sqrt{2}J \\ 0 & \sqrt{2}J & 2\omega_0 + U \end{pmatrix} \tag{34}$$

Since it is a 3×3 matrix, its eigenvalues and eigenvectors can be computed analytically. The energies of the dimer are:

$$E_0 = \frac{U}{2} + 2\omega_0 - \sqrt{\frac{U^2}{4} + 4J^2} \quad E_1 = 2\omega_0 + U$$
$$E_2 = \frac{U}{2} + 2\omega_0 + \sqrt{\frac{U^2}{4} + 4J^2} \tag{35}$$

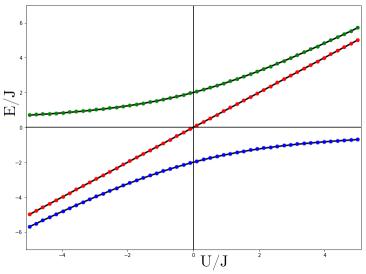

Figure 20: Numerical and analytical energies

In Fig. 20 we see a perfect match of the energies obtained numerically with the energies obtained from direct diagonalization of the matrix. The eigenvectors are:

$$|\psi_0\rangle = \sqrt{\frac{J^2}{\frac{U^2}{4} + 4J^2 + \frac{U}{2}\sqrt{\frac{U^2}{4} + 4J^2}}} \begin{pmatrix} 1 \\ \frac{-\frac{U}{2} - \sqrt{\frac{U^2}{4} + 4J^2}}{\sqrt{2}J} \\ 1 \end{pmatrix} = \alpha_0 \begin{pmatrix} 1 \\ \gamma_0 \\ 1 \end{pmatrix}$$
$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \qquad |\psi_2\rangle = \sqrt{\frac{J^2}{\frac{U^2}{4} + 4J^2 - \frac{U}{2}\sqrt{\frac{U^2}{4} + 4J^2}}} \begin{pmatrix} 1 \\ \frac{-\frac{U}{2} + \sqrt{\frac{U^2}{4} + 4J^2}}{\sqrt{2}J} \\ 1 \end{pmatrix} = \alpha_2 \begin{pmatrix} 1 \\ \gamma_2 \\ 1 \end{pmatrix} \tag{36}$$

It is interesting to see that when $U \to \infty$ the eigenvectors are:

$$\lim_{U\to\infty} |\psi_0\rangle \approx |11\rangle \quad \lim_{U\to\infty} |\psi_1\rangle = \frac{1}{\sqrt{2}}(|20\rangle - |02\rangle) \quad \lim_{U\to\infty} |\psi_2\rangle \approx \frac{1}{\sqrt{2}}(|20\rangle + |02\rangle) \tag{37}$$

So $|\psi_0\rangle$ corresponds to one excitation in each site and $|\psi_1\rangle$, $|\psi_2\rangle$ are antisymmetric and symmetric combinations of the doubly occupied kets, respectively. It is also insightful to see the states in the $U \to -\infty$ limit.

$$\lim_{U\to-\infty} |\psi_0\rangle \approx \frac{1}{\sqrt{2}}(|20\rangle + |02\rangle) \quad \lim_{U\to-\infty} |\psi_1\rangle = \frac{1}{\sqrt{2}}(|20\rangle - |02\rangle) \quad \lim_{U\to-\infty} |\psi_2\rangle \approx |11\rangle \tag{38}$$

So, we see that for attractive interactions $|\psi_0\rangle$ and $|\psi_2\rangle$ switch their roles and the lowest energy state is the symmetric combination of the doubly occupied kets.

Appendix 2: Bethe ansatz for the Bose Hubbard model with a finite chain

In this appendix we will use another notation different to the main text m, n now are j, k, $K\ k\ k_1\ k_2$ are respectively $P\ p\ p_1\ p_2$. We assume that the eigenfunction of this Hamiltonian is of the form

$$|\phi\rangle = \sum_{j,k} \phi_{jk} b_j^\dagger b_k^\dagger |0\rangle \tag{39}$$

This is because $[\mathcal{H}, \sum_j \hat{n}_j] = 0$. The ϕ_{jk} term is the one that carries all the information of the wavefunction. Its square is the probability of finding one of the particles at site j and the other one at k having the wavefunction $|\phi\rangle$. Due to the particles being bosons it obeys $\phi_{jk} = \phi_{kj}$. We want to write the Schrödinger equation as a recurrence relation between these coefficients. We apply the Hamiltonian to our ket though we only use the term j of its sum

$$\mathcal{H}_j |\phi\rangle = -J \sum_{j,k} \Big[\phi_{j+1,k} b_j^\dagger b_k^\dagger |0\rangle + \phi_{j,k} b_{j+1}^\dagger b_k^\dagger |0\rangle + \phi_{j,k+1} b_j^\dagger b_k^\dagger |0\rangle + \phi_{j,k} b_j^\dagger b_{k+1}^\dagger |0\rangle\Big] + U \sum_{j,k} \phi_{jk} \delta_{jk} b_j^\dagger b_k^\dagger |0\rangle \tag{40}$$

We now want only the terms which contain $b_j^\dagger b_k^\dagger |0\rangle$. Applying them to the Schrödinger equation we get

$$-J(\phi_{j+1,k} + \phi_{j-1,k} + \phi_{j,k+1} + \phi_{j,k-1}) + U\delta_{jk}\phi_{jk} = E\phi_{jk} \tag{41}$$

The Bethe Ansatz method consists on supposing for ϕ_{jk} a sort of plane wave ansatz given by

$$\phi_{jk} = (a_{12} e^{i(p_1 j + p_2 k)} + a_{21} e^{i(p_1 k + p_2 j)})\theta(j-k) + (a_{12} e^{i(p_1 k + p_2 j)} + a_{21} e^{i(p_1 j + p_2 k)})\theta(k-j) \tag{42}$$

Where $\theta(x)$ is the step function which obeys $\theta(0) = 1/2$. What this equation means is that when particle at site j is to the left of particle at site k $\theta(j-k) = 1, \theta(k-j) = 0$ a_{12} is the weight of the wavefunction that j has momentum p_1 and k has momentum p_2 and a_{21} the weight on the wavefunction of the particle at j having momentum p_2 and k having momentum p_1. When j is at the right of k it's exactly the contrary. This expression can be rewritten in a more intuitive form defining the centre of mass coordinate and momentum X, P and the relative x, p as

$$X = \frac{j+k}{2} \quad x = j - k \quad P = p_1 + p_2 \quad p = \frac{p_1 - p_2}{2} \tag{43}$$

With a little bit of algebra we can show that

$$p_1 j + p_2 k = PX + p|x| \quad p_1 k + p_2 j = PX - p|x| \tag{44}$$

So the Bethe Ansatz expressed in this coordinates is

$$\phi_{jk} = e^{iPX}\left(a_{12} e^{ip|x|} + a_{21} e^{-ip|x|}\right) \tag{45}$$

We substitute this in (41). Let's assume that $j > k$. If the particles are closer than in the ϕ_{jk} state $|x| = |x_{jk}| - 1$, this is the case for $\phi_{j-1,k}$ and $\phi_{j,k+1}$. If the particles are further apart than in ϕ_{jk} $|x| = |x_{jk}| + 1$, this is the case in $\phi_{j+1,k}$ and $\phi_{j,k-1}$. If the centre of mass is to the right of the c.o.m. of ϕ_{jk} $X = X_{jk} + \frac{1}{2}$, this is the case in $\phi_{j+1,k}$ and $\phi_{j,k+1}$. If the c.o.m. is to the left $X = X_{jk} - \frac{1}{2}$ and this if the case in $\phi_{j-1,k}, \phi_{j,k-1}$. Knowing this the recurrence relation obtained from the Hamiltonian is:

$$\begin{aligned} -J[&e^{iPX} e^{+iP/2}(a_{12} e^{ip|x|} e^{+ip} + a_{21} e^{-ip|x|} e^{-ip}) + e^{iPX} e^{-iP/2}(a_{12} e^{ip|x|} e^{-ip} + a_{21} e^{-ip|x|} e^{+ip}) + \\ &+ e^{iPX} e^{+iP/2}(a_{12} e^{ip|x|} e^{-ip} + a_{21} e^{-ip|x|} e^{+ip}) + e^{iPX} e^{-iP/2}(a_{12} e^{ip|x|} e^{+ip} + a_{21} e^{-ip|x|} e^{-ip})] + \\ &+ U\delta_{x0} e^{iPX}\left(a_{12} e^{ip|x|} + a_{21} e^{-ip|x|}\right) = E e^{iPX}\left(a_{12} e^{ip|x|} + a_{21} e^{-ip|x|}\right) \end{aligned} \tag{46}$$

In the hopping part of the expression we see that term 1-4 and 2-3 have the same parenthesis so it can be taken as a common factor and we obtain:

$$-J\left[e^{iPX}2\cos\frac{P}{2}(a_{12}e^{ip|x|}e^{+ip}+a_{21}e^{-ip|x|}e^{-ip})+e^{iPX}2\cos\frac{P}{2}(a_{12}e^{ip|x|}e^{-ip}+a_{21}e^{-ip|x|}e^{+ip})\right]+$$
$$+U\delta_{x0}e^{iPX}\left(a_{12}e^{ip|x|}+a_{21}e^{-ip|x|}\right)=Ee^{iPX}\left(a_{12}e^{ip|x|}+a_{21}e^{-ip|x|}\right) \quad (47)$$

$$-Je^{iPX}4\cos\frac{P}{2}\left(a_{12}e^{ip|x|}\cos p+a_{21}e^{-ip|x|}\cos p\right)+U\delta_{x0}e^{iPX}\left(a_{12}e^{ip|x|}+a_{21}e^{-ip|x|}\right)=$$
$$=Ee^{iPX}\left(a_{12}e^{ip|x|}+a_{21}e^{-ip|x|}\right) \quad (48)$$

For the off-diagonal terms the term in U vanishes so from this expression the energy of this states is

$$E=-4J\cos\frac{P}{2}\cos p \quad (49)$$

A similar expression can be obtained with $p_{1,2}$ and it is $-2J(\cos p_1+\cos p_2)$. We will take that the expression (26) describes the energy of both the scattering states $j\neq k$ and the doublons $j=k$. From this we can obtain a second expression, which relates a_{12} and a_{21} and which will allow us to obtain numerically the momentums of the states. All the wavefunctions for $j=k$ involved in the recurrence relation are

$$\phi_{jj}=e^{iPX}(a_{12}+a_{21})\quad \phi_{j,j+1}=e^{iPX}(a_{12}e^{ip}+a_{21}e^{-ip})e^{iP/2}\quad \phi_{j-1,j}=e^{iPX}(a_{12}e^{ip}+a_{21}e^{-ip})e^{-iP/2}$$
$$\phi_{j,j-1}=e^{iPX}(a_{12}e^{ip}+a_{21}e^{-ip})e^{-iP/2}\quad \phi_{j+1,j}=e^{iPX}(a_{12}e^{ip}+a_{21}e^{-ip})e^{iP/2} \quad (50)$$

Substituting this in the Hamiltonian and the expression for the energy obtained before we get

$$-J(a_{12}e^{ip}+a_{21}e^{-ip})\cancel{e^{iPX}}4\cos\frac{P}{2}+U\cancel{e^{iPX}}(a_{12}+a_{21})=-4J\cos\frac{P}{2}\cos p(a_{12}+a_{21})\cancel{e^{iPX}} \quad (51)$$

$$a_{12}\left(-4Je^{ip}\cos\frac{P}{2}+4J\cos\frac{P}{2}\cos p+U\right)=a_{21}\left(-4J\cos\frac{P}{2}\cos p+4J\cos\frac{P}{2}e^{-ip}-U\right) \quad (52)$$

$$\xrightarrow{e^{ix}=\cos x+i\sin x} a_{12}\left(\cancel{-4J\cos\frac{P}{2}\cos p}-4iJ\cos\frac{P}{2}\sin p+\cancel{4J\cos\frac{P}{2}\cos p}+U\right)=$$
$$a_{21}\left(\cancel{-4J\cos\frac{P}{2}\cos p}-4iJ\cos\frac{P}{2}\sin p+\cancel{4J\cos\frac{P}{2}\cos p}-U\right) \quad (53)$$

We define the ratio of the coefficients as a function $y(P,p)$ and we obtain that it is

$$y(P,p)=\frac{a_{21}}{a_{12}}=-\frac{U-4iJ\cos\frac{P}{2}\sin p}{U+4iJ\cos\frac{P}{2}\sin p} \quad (54)$$

We note that, as long as $p\in\mathbb{R}$, $|y(P,p)|=1$ so we can express it just as a pure phase shift. This is true for scattering states but doublons have complex p. Assuming periodic boundary conditions $\phi_{j,1}=\phi_{j,L+1}$ we can obtain the values of P and note that they are quantized.

$$\phi_{j1}=a_{12}e^{iP(j+1)/2}(e^{ip(j-1)}+y(P,p)e^{-ip(j-1)})=a_{12}e^{iP(j+L+1)/2}(e^{ip(L+1-j)}+y(P,p)e^{-ip(L+1-j)}) \quad (55)$$

So P has to obey:

$$e^{iP(j+L+1)/2}=e^{iP(j+1)/2}\Rightarrow e^{iPL}=1\Rightarrow PL=2\pi n \quad (56)$$

$$P_n = \frac{2\pi n}{L} \tag{57}$$

Where $n \in \{1, 2, \ldots, L\}$. Knowing this, as P is in the equation (55) in the form $e^{iPL/2}$ we have an extra term $e^{i\pi n} = (-1)^n$. Setting the parentheses equal we obtain

$$\begin{aligned} e^{ip(j-1)} + y(P_n, p)e^{-ip(j-1)} = (-1)^n(e^{ip(L+1-j)} + y(P_n, p)e^{-ip(L+1-j)}) = \\ = (-1)^n e^{ipL}e^{-ip(j-1)} + (-1)^n e^{-ipL}y(P_n, p)e^{ip(j-1)} \end{aligned} \tag{58}$$

So, for this equation to hold we obtain the condition

$$(-1)^n e^{ipL} = y(P_n, p) \tag{59}$$

We have to solve this equation numerically.

Appendix 3: Analytical solution for the Bose Hubbard model with an infinite chain

We start from (41) and introduce an Ansatz of the form:

$$\psi_{j,k} = e^{iKR}\psi_K(r_i) \tag{60}$$

Where $i = j-k$ and $r = di$ is the relative coordinate where d is the lattice constant, that we usually take to be 1. K is the centre of mass quasi-momentum and k the relative quasimomentum. Substituting in the equation we obtain

$$\begin{aligned} -J\left(e^{iK(R-d/2)}\psi_K(r_{i-1}) + e^{iK(R+d/2)}\psi_K(r_{i+1}) + e^{iK(R-d/2)}\psi_K(r_{i+1}) + e^{iK(R+d/2)}\psi_K(r_{i-1})\right) + \\ U\delta_{r0}e^{iKR}\psi_K(r_i) = Ee^{iKR}\psi_K(r_i) \end{aligned} \tag{61}$$

$$-J\left(2\cos\frac{Kd}{2}\psi_K(r_{i-1}) + 2\cos\frac{Kd}{2}\psi_K(r_{i+1})\right) + U\delta_{r0}\psi_K(r_i) = E\psi_K(r_i) \tag{62}$$

We can define $J_K = 2J\cos\frac{Kd}{2}$ and we obtain a recurrence relation analogous (for $r \neq 0$) to the 1D tight-binding model.

$$-J_K(\psi_K(r_{i-1}) + \psi_K(r_{i+1})) + U\delta_{r0}\psi_K(r_i) = E_K\psi_K(r_i) \tag{63}$$

Scattering states

We can consider that the 2 particles in a scattering state are asymptotically free. So the energy of all the state is just the sum of the two energies. We consider that the two particles have momenta $q_1 = K/2 + k$ $q_2 = K/2 - k$ and substituting a plane wave solution $\psi_K(r) = e^{\pm ikr}$ and $U = 0$ in (63) we obtain

$$E^{\text{Scatt}}_{K,k} = E_{q_1} + E_{q_2} = -4J\cos\frac{Kd}{2}\cos kd = -2J_K\cos kd \tag{64}$$

This is the result we used in (29) substituting the maximum and minimum values that $\cos kd$ can have. We also see in the plot that the density of states in the scattering band is not constant. We can also obtain an expression for this.

$$\rho(E, K) = \frac{L}{2\pi}\frac{\partial k}{\partial E} \tag{65}$$

$$-\frac{E}{2J_K} = \cos kd \Rightarrow k(E) = d^{-1}\arccos\frac{-E}{2J_K} \Rightarrow \frac{\partial k}{\partial E} = d^{-1}\frac{-1}{\sqrt{1-(E/2J_K)^2}}\frac{-1}{2J_K} \tag{66}$$

$$\rho(E,K) = \frac{L}{2\pi d}\frac{1}{\sqrt{4J_K^2 - E^2}} = \frac{L}{2\pi d}\frac{1}{\sqrt{(4J\cos Kd/2)^2 - E^2}} \tag{67}$$

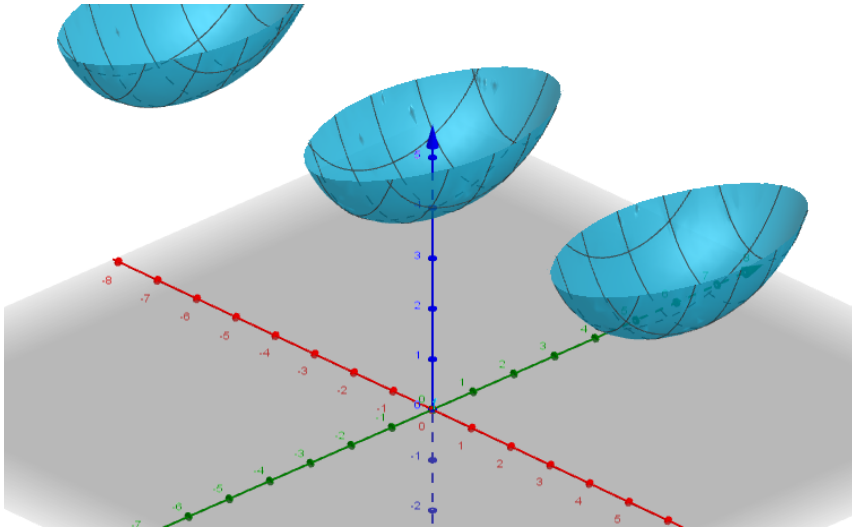

Figure 21: Density of states as a function of K and E for the $N \to \infty$ limit of the Bose Hubbard model.

We can obtain the wavefunction of the scattering states assuming an Ansatz of the form

$$\psi_{K,k}(r_i) = A\sin kd|i| + C\cos kdi \tag{68}$$

With the initial condition $\psi(r_0) = C$. Substituting the expression for the energy and this Ansatz in (63) in $i = 0$ we obtain

$$-J_K(\psi_{K,k}(1)+\psi_{K,k}(-1)) = (E-U)\psi_{K,k}(0) \Rightarrow -2J_K(A\sin kd+\cancel{C\cos kd}) = (\cancel{-2J_K\cos kd}-U)C \tag{69}$$

$$A = C\frac{U}{2J_K\sin kd} \tag{70}$$

And substituting this relation between A and C in the ansatz we obtain an expression for the wavefunction of the scattering states.

$$\psi_{K,k}(r_i) = C\cos kr_i + C\frac{U}{2J_K\sin kd}\sin k|r_i| = e^{ik|r_i|}e^{i\delta_{K,k}} + e^{-ik|r_i|}e^{-i\delta_{K,k}} \tag{71}$$

Where $\delta_{K,k}$ is a phase shift made by the interaction which is given by

$$\tan\delta_{K,k} = -\frac{U}{2J_K\sin kd} \tag{72}$$

In the limit $U \to 0$ this gives us the trivial two non-interacting boson solution $\cos kr_i$ and in the limit $U/J_K \to \infty$ this gives us a 'fermionized' solution that is $\sin k|r_i|$, which makes sense because in that limit we are doing the same as in the Pauli exclusion principle.

Doublons

For the doublons we use an exponential ansatz of the form

$$\psi_K(r_i) = C\alpha_K^{|i|} \tag{73}$$

Where C is a normalization factor. Substituting this ansatz on (63) both for $i = 0$ and $i \neq 0$ we obtain

$$\begin{cases} -2J_K\alpha_K + U = E_K^{Doubl} \\ -J_K(\alpha_K^{|i|-1} + \alpha_K^{|i|+1}) = E_K^{Doubl}\alpha_K^{|i|} \end{cases} \tag{74}$$

If we set $i = 1$ in the second equation and substitute we obtain

$$-J_K(1+\alpha_K^2) = -2J_K\alpha_K^2 + U\alpha_K \Rightarrow J_K\alpha_K^2 - U\alpha_k - J_K = 0 \tag{75}$$

Whose solution is, defining $\mathcal{U}_K = U/2J_K$

$$\alpha_K = \mathcal{U}_K \pm \sqrt{\mathcal{U}_K^2 + 1} \tag{76}$$

For the state to be normalizable $|\alpha_K| < 1$. Taking this into account for **attractive interactions** we obtain

$$\alpha_K = \sqrt{\mathcal{U}_K^2 + 1} - |\mathcal{U}_K| \quad E_K^{Doubl} = -\sqrt{U^2 + 4J_K^2} \tag{77}$$

$$\psi_K(r_i) = \frac{\sqrt{|\mathcal{U}_K|}}{\sqrt[4]{\mathcal{U}_K^2 + 1}} \left(\sqrt{\mathcal{U}_K^2 + 1} - |\mathcal{U}_K|\right)^{|i|} \tag{78}$$

And for **repulsive interactions**:

$$\alpha_K = \mathcal{U}_K - \sqrt{\mathcal{U}_K^2 + 1} \quad E_K^{Doubl} = \sqrt{U^2 + 4J_K^2} \tag{79}$$

This expression for the energy is the one we used in (29). Its wavefunction is:

$$\psi_K(r_i) = \frac{\sqrt{|\mathcal{U}_K|}}{\sqrt[4]{\mathcal{U}_K^2 + 1}} \left(\mathcal{U}_K - \sqrt{\mathcal{U}_K^2 + 1}\right)^{|i|} \tag{80}$$

Appendix 4: Non-Interacting Bosons in the SSH model

In this appendix we show that some of the excitations in the 2 particle SSH model can be understood looking at the system with two particles without interaction. One class of states nicely seen in the non interacting limit is the bulk-edge states. There are three classes of states in this system:

- **Bulk-Bulk states**: The two particles are in the bulk of the material.
- **Bulk-Edge states**: One of the particles is in the bulk of the material while the other one is localized at one of the edges.
- **Edge-Edge states:** The two particles are localized at the ends of the chain.

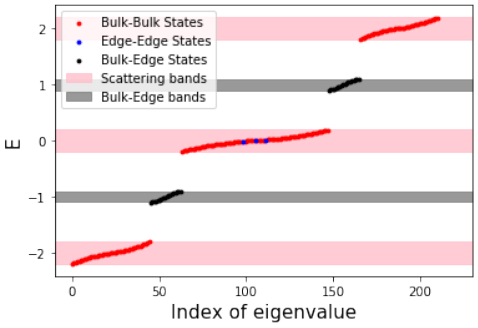

Figure 22: Energy plot for $J_1 = 0.1$, $\omega_0 = 0$ and $J_2 = 1$

We have three bulk-bulk energy bands, with two bulk-edge bands with energies in between them. We also see that there are three edge-edge states with zero energy. We can see the form of the edge-edge states in Figure 23.

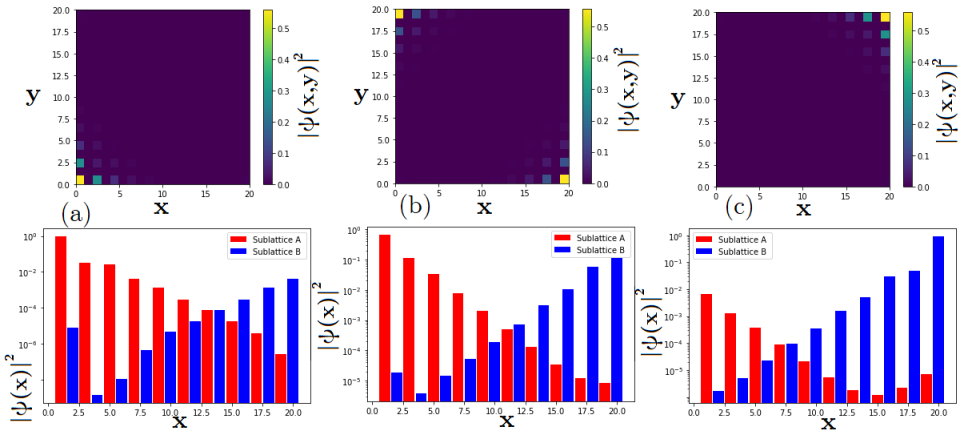

Figure 23: Edge states of non interacting bosons for $J_1 = 0.5$ $J_2 = 1$

We can see that (a) and (c) are mostly localized at one of the edges while (b) is localized on both of them. This is made by the little perturbation added to ω_0 that breaks chiral symmetry, making the edges slightly different.

It is also interesting to see the form of the bulk-edge states, like the one shown at the right. We see that either x or y is localized in one edge.

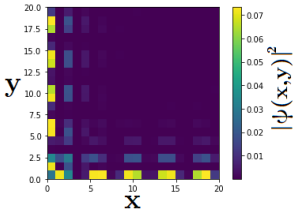

Figure 24: 2D plot of a bulk-edge state.

In figure 22 we showed some energy bands, which can be obtained from the expression of the bands in the 1 particle model. Its expressions for the bulk-bulk bands are$-2J_2 - 2J_1 \leq E \leq -2J_2 + 2J_1$; $-2J_1 \leq E \leq 2J_1$; $2J_2 - 2J_1 \leq E \leq 2J_2 + 2J_1$.

The bulk-edge bands have the same bands as the 1-particle SSH model $-J_2 - J_1 \leq E \leq -J_2 + J_1$; $J_2 - J_1 \leq E \leq J_2 + J_1$. All the differences between the states can be seen in the PR plots.

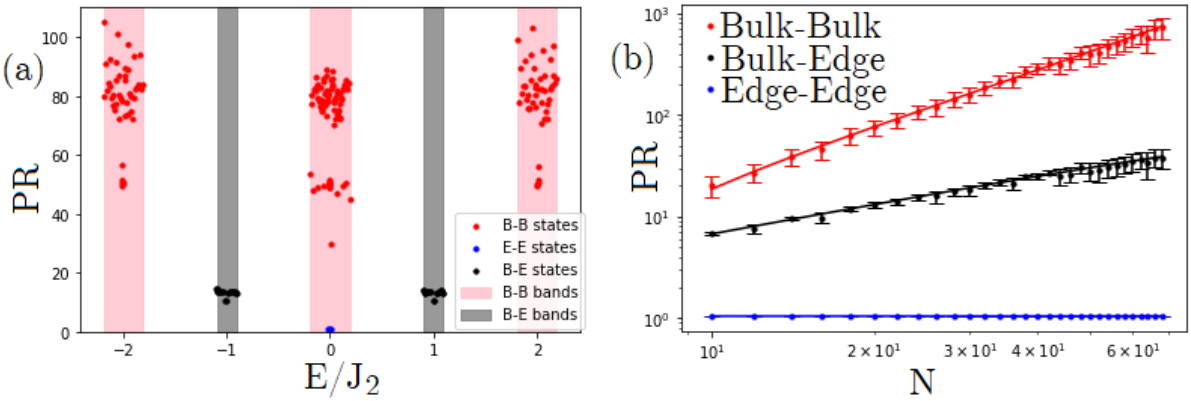

Figure 25: (a) PR of the states as a function of their energy for $N = 20$ $\omega_0 = 2$ $J_1 = 0.5$ $J_2 = 1$.(b) PR as a function of N for $\omega_0 = 2$ $J_1 = 0.1$ $J_2 = 1$.

In (a) we see that the three classes of states have different PR. Bulk-bulk states have the biggest

PR and Edge-edge states the lowest. We can see the scaling with N in the plot (b). We see that bulk-bulk states scale quadratically, bulk-edge states scale linearly and edge-edge states stay constant. This is the behaviour expected for each class of states.

In the trivial phase the only class of states seen is the bulk-bulk states. Their energy bands can also be obtained from the energy bands of the 1 particle SSH model and are given by: $-2J_2 - 2J_1 \leq E \leq -2J_1 + 2J_2$; $-2J_2 \leq E \leq 2J_2$; $2J_1 - 2J_2 \leq E \leq 2J_2 + 2J_1$.

The fact that we only see bulk-bulk states suggests that both the edge-edge and bulk-edge states are topological in nature.

In the next section we will work with interacting bosons in the SSH model, this means that we will see states like the doublons shown in the Bose-Hubbard model, and we will see that they can exhibit topological properties.

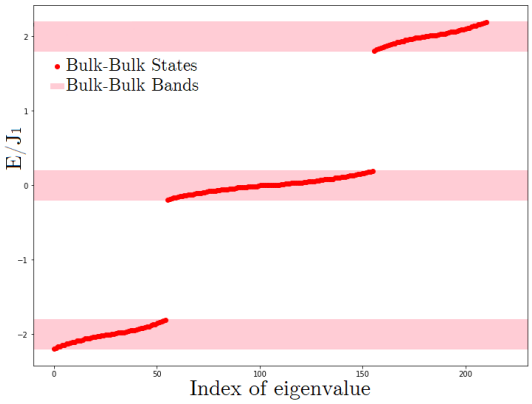

Figure 26: Energy plot of the 2 particle SSH model in the trivial phase with parameters $J_1 = 1$ $J_2 = 0.1$ $\omega_0 = 0$.

Appendix 5: Further numerical study of the weakly dimerized limit

A5.1: Weakly dimerized limit with large ω_0

When we set a very big ω_0 we obtain the plot at the right. We see that around $U/J_2 \sim 4$ the Scattering Edge state starts to be the second most localized, then the third and for $U/J_2 \sim 6$ there are three more localized states in the doublon bands. This does not mean that we don't have a Scattering Edge state for $U/J_2 > 6$ or that we have three edge doublons. What happens is that the edge doublons and bulk doublons become very localized, not because $J_{1,2}$ is strong but because of the large values of ω_0 and U. This localization causes the edge doublon to be the state with lowest PR and causes some bulk doublons to be more localized than the scattering edge state. Even though the 2nd and 3rd lowest PR now fall on the symmetric band the edge doublon (triangles) is still on the antisymmetric band. In this section we have shown another path to localization of the edge states which relies on the on-site potential ω_0 and the particle-particle repulsion rather on the nearest neighbour couplings J_1, J_2.

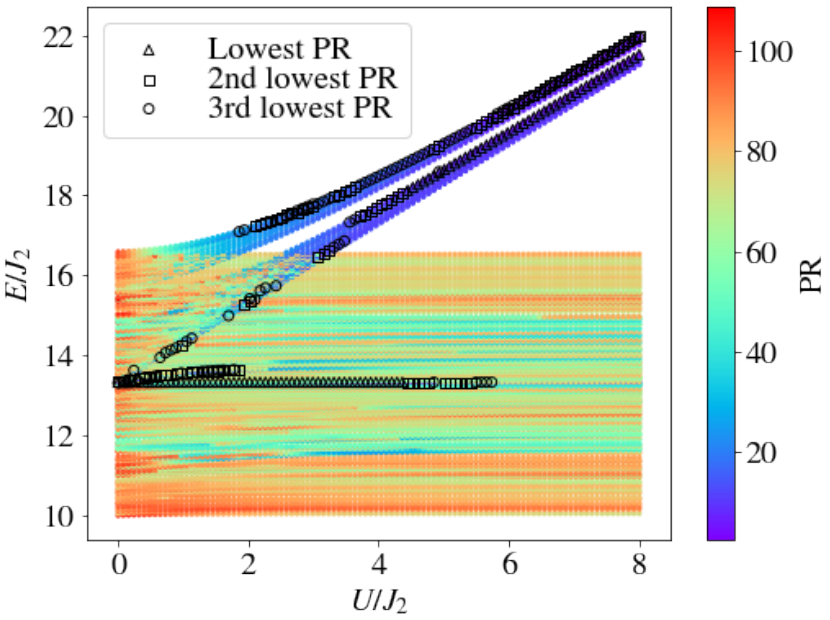

Figure 27: Evolution of the energies of the system as a function of U. Parameters: $N = 20$, $J_1 = 1$, $J_2 = 1.5$ and $\omega_0 = 10$.

A5.2: Absolute plots of localization on the weakly dimerized limit

In this section we show the absolute plots of the min(PR) for both phases rather than their difference. This lets us distinguish which phase suffers more the effects of the perturbation.

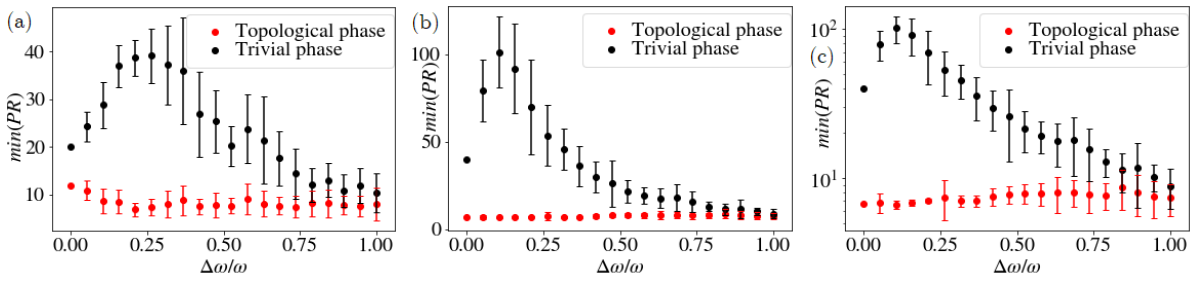

Figure 28: Plots of the minimun of PR in each phase for the weakly dimerized limit for $U = 0.05J_2$. Same parameters as Fig. 18 (a)$N = 20$. (b)$N = 40$. (c)$N = 40$ in logarithmic scale.

In these plots we see clearly that the perturbation affects more the minimum PR of the trivial phase. This is reasonable because the topological phase already has localization. For small values of $\Delta\omega$ the trivial phase first delocalizes (increases its min(PR)) and around $\Delta\omega/\omega \sim 0.25$ for $N = 20$ it starts to localize. In (b) we see clearly that this also happens for a longer chain although it starts localizing before. In (c) we see that the decaying to the trivial localized phase fits correctly to an exponential after the first peak, i.e. it is linear in logarithmic scale.

Appendix 6: Bethe ansatz for the Su-Schrieffer-Heeger model with an infinite chain

The Hamiltonian for the SSH model in the 2 excitation limit reads

$$\mathcal{H} = -J_1 \sum_m (\hat{b}^\dagger_{A,m}\hat{b}_{B,m} + \hat{b}^\dagger_{B,m}\hat{b}_{A,m}) - J_2 \sum_m (\hat{b}^\dagger_{A,m+1}\hat{b}_{B,m} + \hat{b}^\dagger_{B,m}\hat{b}_{A,m+1}) + \\ + \frac{U}{2}\sum_m (\hat{n}_{A,m}(\hat{n}_{A,m}-1) + \hat{n}_{B,m}(\hat{n}_{B,m}-1)) \quad (81)$$

Where A & B refer to the two sublattices because we have two elements on the basis. We assume that our wavefunction is of the form

$$|\psi\rangle = \sum_{\alpha,\gamma=A,B}\sum_{m,n} \beta^{\alpha\gamma}_{mn}\hat{b}^\dagger_{\alpha,m}\hat{b}^\dagger_{\gamma,n}|0\rangle \quad (82)$$

Applying the m-th term of the Hamiltonian to the wavefunction the Schrödinger equation reads

$$\mathcal{H}_m|\psi\rangle = -J_1 \sum_{\alpha,\gamma,m,n} \{\beta^{B\gamma}_{mn}\hat{b}^\dagger_{A,m}\hat{b}^\dagger_{\gamma,n}|0\rangle + \beta^{A\gamma}_{mn}\hat{b}^\dagger_{B,m}\hat{b}^\dagger_{\gamma,n}|0\rangle + \beta^{\alpha B}_{mn}\hat{b}^\dagger_{\alpha,m}\hat{b}^\dagger_{A,n}|0\rangle + \beta^{\alpha A}_{mn}\hat{b}^\dagger_{\alpha,m}\hat{b}^\dagger_{B,n}|0\rangle\} \\ - J_2 \sum_{\alpha,\gamma,m,n} \{\beta^{B\gamma}_{mn}\hat{b}^\dagger_{A,m+1}\hat{b}^\dagger_{\gamma,n}|0\rangle + \beta^{A\gamma}_{m+1n}\hat{b}^\dagger_{B,m}\hat{b}^\dagger_{\gamma,n}|0\rangle + \beta^{\alpha B}_{mn}\hat{b}^\dagger_{\alpha,m}\hat{b}^\dagger_{A,n+1}|0\rangle + \beta^{\alpha A}_{mn+1}\hat{b}^\dagger_{\alpha,m}\hat{b}^\dagger_{B,n}|0\rangle\} \\ + U\sum_{\alpha,\gamma,m,n}\delta_{\alpha,\gamma}\delta_{m,n}\beta^{\alpha\gamma}_{mn}\hat{b}^\dagger_{\alpha,m}\hat{b}^\dagger_{\gamma,n}|0\rangle = \varepsilon\sum_{\alpha,\gamma,m,n}\beta^{\alpha\gamma}_{mn}\hat{b}^\dagger_{\alpha,m}\hat{b}^\dagger_{\gamma,n}|0\rangle \quad (83)$$

Taking the terms in $\hat{b}^\dagger_{A,m}\hat{b}^\dagger_{A,n}|0\rangle$ and the others in AB, BA & BB we can obtain four recurrence

relations.

$$\begin{cases} -J_1(\beta^{BA}_{mn}+\beta^{AB}_{m,n})-J_2(\beta^{BA}_{m-1,n}+\beta^{AB}_{m,n-1})=(\varepsilon-U\delta_{mn})\beta^{AA}_{m,n} \\ -J_1(\beta^{BB}_{m,n}+\beta^{AA}_{m,n})-J_2(\beta^{BB}_{m-1,n}+\beta^{AA}_{m,n+1})=\varepsilon\beta^{AB}_{m,n} \\ -J_1(\beta^{BB}_{m,n}+\beta^{AA}_{m,n})-J_2(\beta^{BB}_{m,n-1}+\beta^{AA}_{m+1,n})=\varepsilon\beta^{BA}_{m,n} \\ -J_1(\beta^{BA}_{mn}+\beta^{AB}_{m,n})-J_2(\beta^{BA}_{m,n+1}+\beta^{AB}_{m+1,n})=(\varepsilon-U\delta_{mn})\beta^{BB}_{m,n} \end{cases} \tag{84}$$

These four equations describe all the possible ways of getting to a given state $\beta^{\alpha\gamma}_{m,n}$ via intra-cell hopping (J_1) or via inter-cell hopping (J_2). We have written four equations and it may seem like two of them are redundant because of bosonic symmetry and it is true, the third equation can be obtained from the second via this symmetry, nonetheless when writing an Ansatz for this equations we will only take the intracell coordinate AA, AB, BA & BB to mark the states and $\beta^{AB}\neq\beta^{BA}$, what is true is $\beta^{AB}_{m,n}=\beta^{BA}_{nm}$, this is the reason why we write the four equations.

Scattering Bands

Once we have the recurrence relations we can substitute an Ansatz and derive from there the dispersion relation. The Ansatz is of the form

$$\beta^{\alpha\gamma}_{m,n}=C^{\alpha\gamma}e^{i(k_1(m+\delta_{\alpha,B}/2)+k_2(n+\delta_{\gamma,B}/2))} \tag{85}$$

This is a similar way to write the ansatz as in the paper by Gorlach et al, the only thing is that they do not use the sublattices A,B, I find this use more physically meaningful and this is why I use it. We have to keep in mind that with this definition we're assuming a lattice parameter of $a=1/$ between A-B and 1 between A-A, and with this we will obtain a similar results to them. Substituting this Ansatz we obtain

$$\begin{cases} -J_1(C^{BA}e^{ik_1/2}+C^{AB}e^{ik_2/2})-J_2(C^{BA}e^{-ik_1/2}+C^{AB}e^{-ik_2/2})=\varepsilon C^{AA} \\ -J_1(C^{AA}+C^{BB}e^{ik_1/2}e^{ik_2/2})-J_2(C^{AA}e^{ik_2/2}+C^{BB}e^{-ik_1/2}e^{ik_2/2})=\varepsilon C^{AB}e^{ik_2/2} \\ -J_1(C^{AA}+C^{BB}e^{ik_1/2}e^{ik_2/2})-J_2(C^{AA}e^{ik_1}+C^{BB}e^{ik_1/2}e^{-ik_2/2})=\varepsilon C^{BA}e^{ik_1/2} \\ -J_1(C^{BA}e^{ik_1/2}+C^{AB}e^{ik_2/2})-J_2(C^{BA}e^{ik_1/2}e^{ik_2}+C^{AB}e^{ik_1}e^{ik_2/2})=\varepsilon C^{BB}e^{ik_1/2}e^{ik_2/2} \end{cases} \tag{86}$$

We can simplify the exponentials with ε and we know that for an homogeneous system to have a non-trivial solution its determinant has to vanish. The determinant to solve is

$$\begin{vmatrix} -\varepsilon & -J_1e^{ik_2/2}-J_2e^{-ik_2/2} & -J_1e^{ik_1/2}-J_2e^{-ik_1/2} & 0 \\ -J_1e^{-ik_2/2}-J_2e^{ik_2/2} & -\varepsilon & 0 & -J_1e^{ik_1/2}-J_2e^{-ik_1/2} \\ -J_1e^{-ik_1/2}-J_2e^{ik_1/2} & 0 & -\varepsilon & -J_1e^{ik_2/2}-J_2e^{-ik_2/2} \\ 0 & -J_1e^{-ik_1/2}-J_2e^{ik_1/2} & -J_1e^{-ik_2/2}-J_2e^{ik_2/2} & -\varepsilon \end{vmatrix}=0 \tag{87}$$

We see that the matrix is hermitian, as it should be. We define the following variables which will simplify the following calculations.

$$J_{k_i}=J_1e^{ik_i/2}+J_2e^{-ik_i/2} \qquad J^*_{k_i}=J_1e^{-ik_i/2}+J_2e^{ik_i/2} \tag{88}$$

In terms of this variables the expression of the determinant is much easier:

$$\begin{vmatrix} -\varepsilon & -J_{k_2} & -J_{k_1} & 0 \\ -J^*_{k_2} & -\varepsilon & 0 & -J_{k_1} \\ -J^*_{k_1} & 0 & -\varepsilon & -J_{k_2} \\ 0 & -J^*_{k_1} & -J^*_{k_2} & -\varepsilon \end{vmatrix}=0 \tag{89}$$

$$\Rightarrow\ \varepsilon^4-2\varepsilon^2(|J_{k_1}|^2+|J_{k_2}|^2)+|J_{k_1}|^4+|J_{k_2}|^4-2|J_{k_1}|^2|J_{k_2}|^2=0 \tag{90}$$

The following identities will be useful

$$|J_{k_i}|^2 = J_1^2 + J_2^2 + 2J_1J_2\cos k_i \tag{91}$$

$$|J_{k_i}|^2|J_{k_j}|^2 = J_1^4 + J_2^4 + 2J_1^2J_2^2 + 4J_1^2J_2^2\cos k_i\cos k_j + 2J_1J_2(J_1^2+J_2^2)(\cos k_i + \cos k_j) \tag{92}$$

$$\Rightarrow \varepsilon^4 - 4\varepsilon^2(J_1^2 + J_2^2 + J_1J_2(\cos k_1 + \cos k_2)) + 4J_1^2J_2^2(\cos k_2 - \cos k_1)^2 = 0 \tag{93}$$

So, we obtain an expression for the energy in terms of k_1 and k_2. This expression is analogous to (S5) in the paper by Gorlach taking into account that our lattice parameter is half of theirs. We can obtain the energies, which are given by the expression

$$\varepsilon = \pm\Bigg[2(J_1^2 + J_2^2 + J_1J_2(\cos k_1 + \cos k_2)) \pm 2\sqrt{J_1^4 + J_2^4 + 2J_1^2J_2^2(1 + 2\cos k_1\cos k_2) + 2J_1J_2(J_1^2+J_2^2)(\cos k_1 + \cos k_2)}\Bigg]^{1/2} \tag{94}$$

This expression gives us four bands, two of which overlap. Using the identity $\sqrt{p} + \sqrt{q} = \sqrt{p + q + 2\sqrt{pq}}$ these energy bands can be rewritten in the more familiar form:

$$\varepsilon = \pm\sqrt{J_1^2 + J_2^2 + 2J_1J_2\cos k_1} \pm \sqrt{J_1^2 + J_2^2 + 2J_1J_2\cos k_2} \tag{95}$$

Which is just the sum of two contributions of the form (9) of the energies of the 1 particle SSH. This is the result we would expect, just the sum of the energies, because the scattering bands are with independent particles. We have obtained similar results(energy is the sum of the energies) for the Bose-Hubbard model, even though this is true, the wavefunction is not the product of independent wavefunctions and in it U does play a role.