Exact diagonalization Report

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1 One dimension

Throughout our report we will use natural units: $\hbar = m = \omega = 1$

Our project concerns the tight binding model. The lattice Hamiltonian in 1D is given by:

$$H = -t \sum_n |n+1\rangle \langle n| + |n\rangle \langle n+1| + V_n |n\rangle \langle n| \tag{1}$$

For $t = 1$ and $N = 5$ the Hamiltonian is:

$$\underbrace{\begin{bmatrix} V_1 & 1 & 0 & 0 & 0 \\ 1 & V_2 & 1 & 0 & 0 \\ 0 & 1 & V_3 & 1 & 0 \\ 0 & 0 & 1 & V_4 & 1 \\ 0 & 0 & 0 & 1 & V_5 \end{bmatrix}}_{\text{Closed boundaries}} \quad \underbrace{\begin{bmatrix} V_1 & 1 & 0 & 0 & 1 \\ 1 & V_2 & 1 & 0 & 0 \\ 0 & 1 & V_3 & 1 & 0 \\ 0 & 0 & 1 & V_4 & 1 \\ 1 & 0 & 0 & 1 & V_5 \end{bmatrix}}_{\text{Periodic boundaries}}$$

We can take the continuum limit of our Hamiltonian in order to connect out lattice properties with physical constants.

$$\lim_{a \to 0} \langle n \,|\, H \,|\, \psi \rangle = H\psi(x) = (-t)a^2 \frac{d^2\psi(x)}{dx^2} + (-2t)\psi(x) + V(x)\psi(x)$$

Where a is the lattice constant. Comparing with the Schrodinger equation we get:

$$t = \frac{1}{2a^2}, \quad V_{grid} = V(x) + 2t$$

After calling the diagonalization routine, we need to make sure the results are correct. We will first check the orthonormality of our eigenvectors by checking $Z^T Z = I$. Due to roundoff erros, our result will never be exactly zero, therefore we check the element of $S = Z^T Z - I$ with the highest absolute value S_{max}. Using the same method we also check the eigenvalue equation $HZ = EZ$ For $N = 50$ and the harmonic oscilator potential $V = \frac{1}{2}x^2$ the first 5 eigenvalues were:

$$E_0 = 0.49869 \quad E_1 = 1.4934 \quad E_2 = 2.48295 \quad E_3 = 3.46714 \quad E_4 = 4.44597$$

Which match the exact values $E_n = (n + \frac{1}{2})$ quite well. The time evolution step will be inversly proportional to the probabilty t.

$$\Delta\tau = \frac{1}{t}$$

. By diagonalizing we are changing from the position basis to the energy basis. This allows us to find the time evolution of the wavefunction

$$\psi(x,t) = \sum_n a_n \psi_n(x) e^{-iE_n t} = \sum_n \langle \psi_0 \,|\, \psi_n \rangle \psi_n(x) e^{-iE_n t} = \sum_n \langle \Big(\sum_i c_i |x_i\rangle \Big) |\psi_n\rangle \psi_n(x) e^{-iE_n t}$$
$$= \sum_{i,m} c_i \langle x_i \,|\, \psi_n \rangle \psi_n e^{-iE_n t}$$

Where c_i is the normalized initial probability amplitude and $\langle x_i \,|\, \psi_n \rangle$ is the ith element of the nth energy eigenvector.

For the initial probability we will use a moving particle wavefunction which is equal up to normalization:

$$\psi_j \simeq \sum_k e^{-\lambda(k-k_0)^2} e^{-ik(j-j_0)}$$

Where k is the quantized wavevector $k = \frac{2\pi}{N} m$ where m is an integer. Chossing $l = 20 \quad k_0 = \frac{2\pi}{N} 5$ we get the following initial probability amplitude distribution:

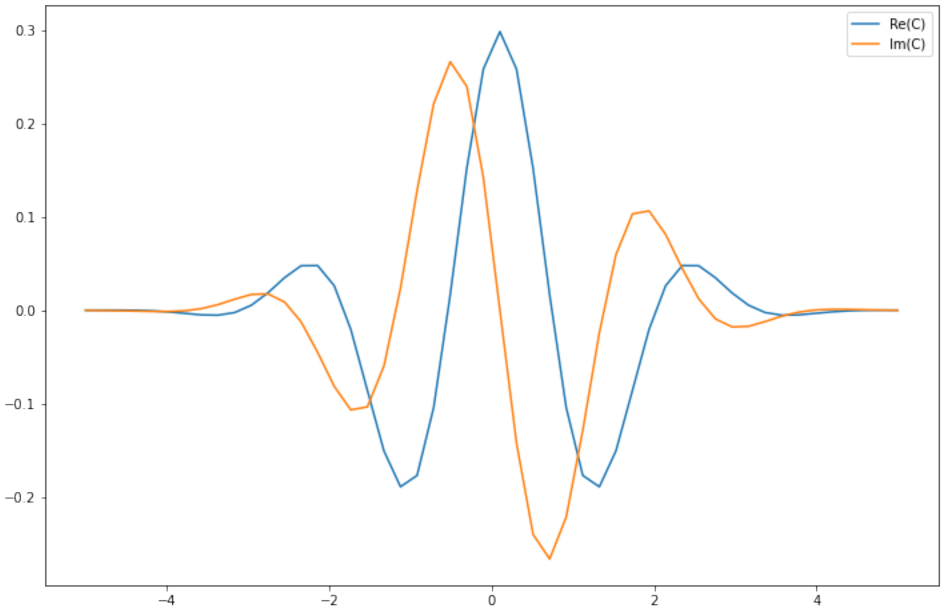

Figure 1: Initial probability amplitudes

The results of the previous were:

The first figure corresponds to a harmonic oscilator potential with closed boundaries, the second coresponds to a free particle with open boundaries and the third corresponds to a free particle with closed boundaries.

2 Two dimensions

The problem for 2 dimensions is largely the same, the only difficulty is encountered when constructing the Hamiltonian matrix. We label each point of the 2D grid with an integer and get the following hamiltonians:

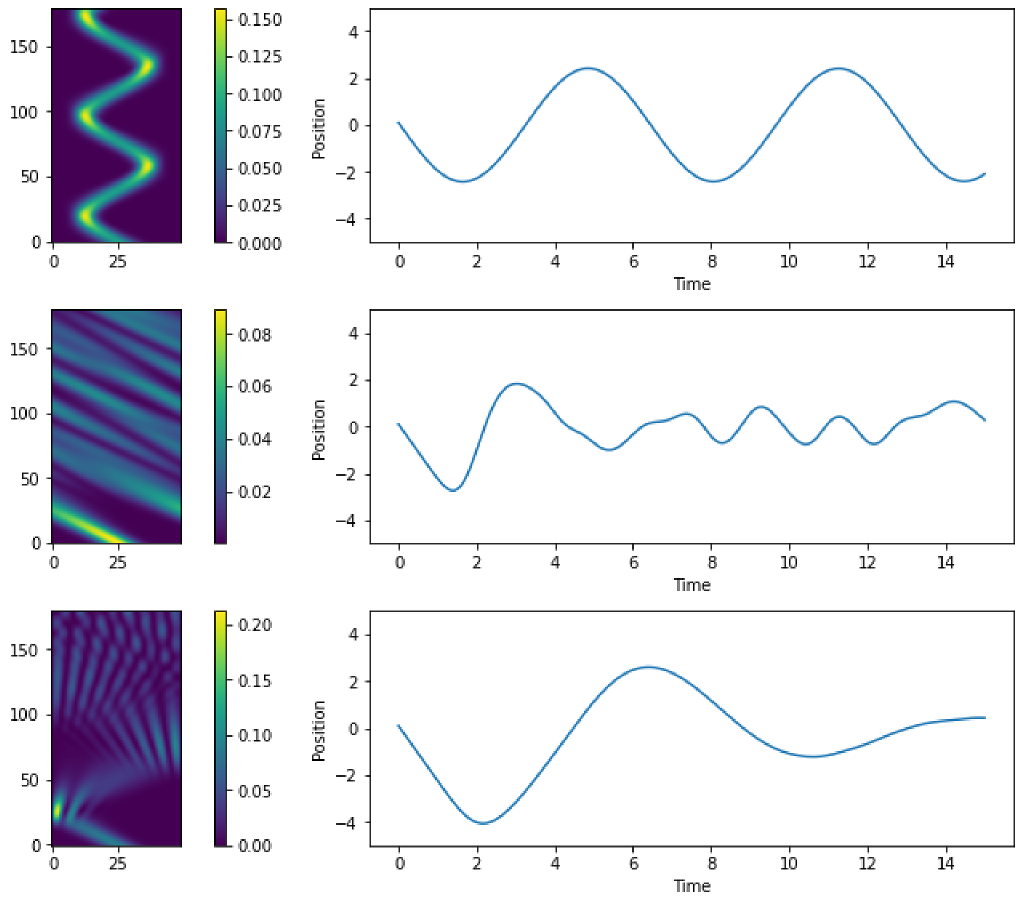

Figure 2: 1D Results

$$\underbrace{\begin{bmatrix} V_1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & V_2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & V_3 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & V_4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & V_5 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & V_6 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & V_7 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & V_8 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & V_9 \end{bmatrix}}_{\text{Closed boundary}} \quad \underbrace{\begin{bmatrix} V_1 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & V2 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & V_3 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & V_4 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & V_5 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & V_6 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & V_7 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & V_8 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & V_9 \end{bmatrix}}_{\text{Periodic boundary}}$$

Taking the same continium limit as the 1D case we can show:

$$t = \frac{1}{2a^2}, \quad V_{grid} = V(x) + 4t$$

Lets test the hamiltonian with the 2D isotropic harmonic oscilator potential:

$$V(x, y) = \frac{1}{2}\left(x^2 + y^2\right) = \frac{1}{2}r^2$$

For a 30×30 grid of points, the 10 first eigenvalues are:

$$\begin{array}{lllll} E_0 = 0.992 & E_1 = 1.977 & E_2 = 1.977 & E_3 = 2.946 & E_4 = 2.946 \\ E_5 = 2.962 & E_6 = 3.900 & E_7 = 3.900 & E_8 = 3.931 & E_9 = 3.931 \end{array}$$

Which match the exact values $E_n = n + 1$ with degeneracy $n + 1$, quite well.

For a gaussian inital probability amplitude

$$C \simeq e^{-\frac{x^2+y^2}{2}}$$

and closed boundaries, the time evolution gives:

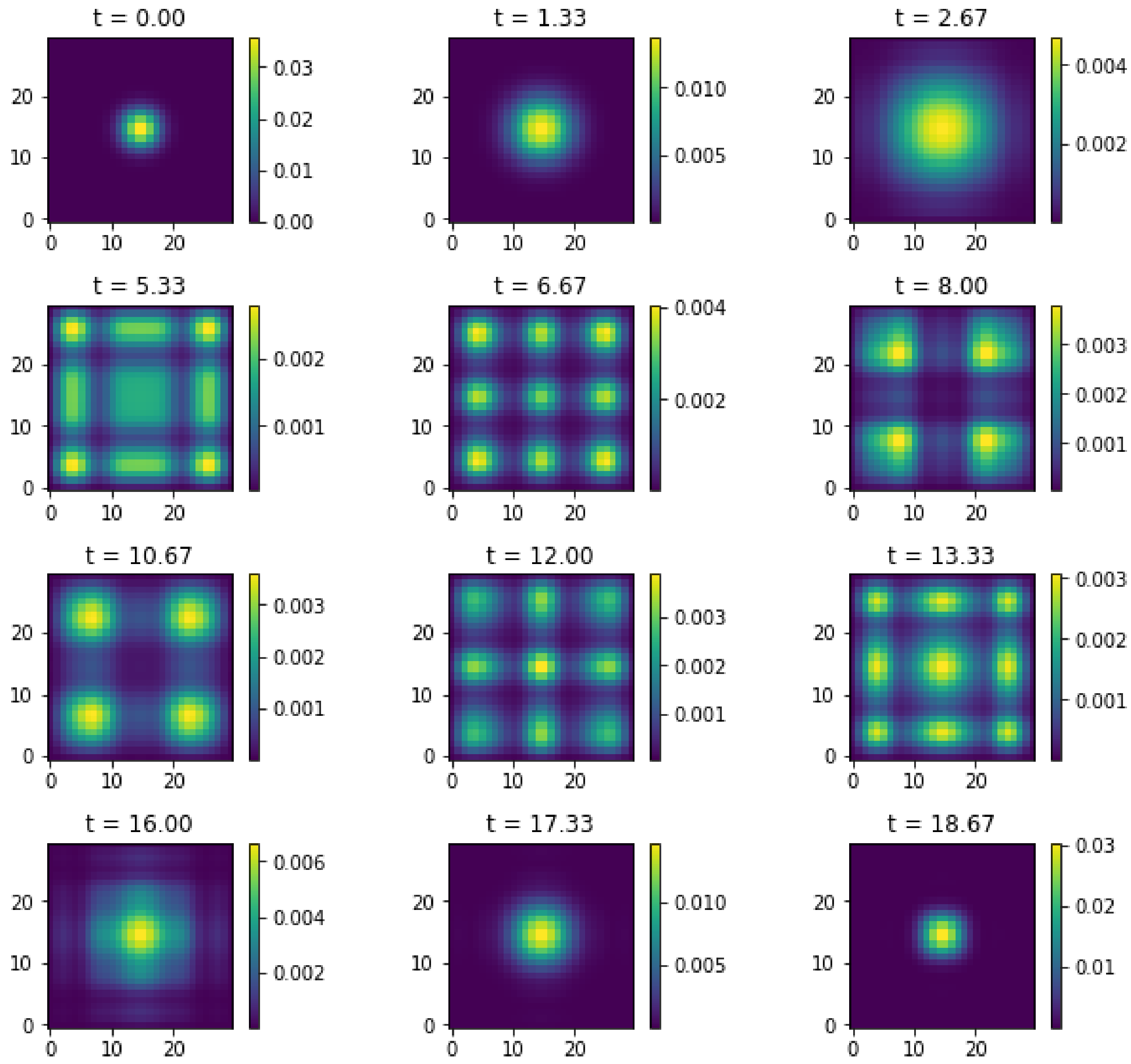

Figure 3: V = 0

We can see that the gaussian

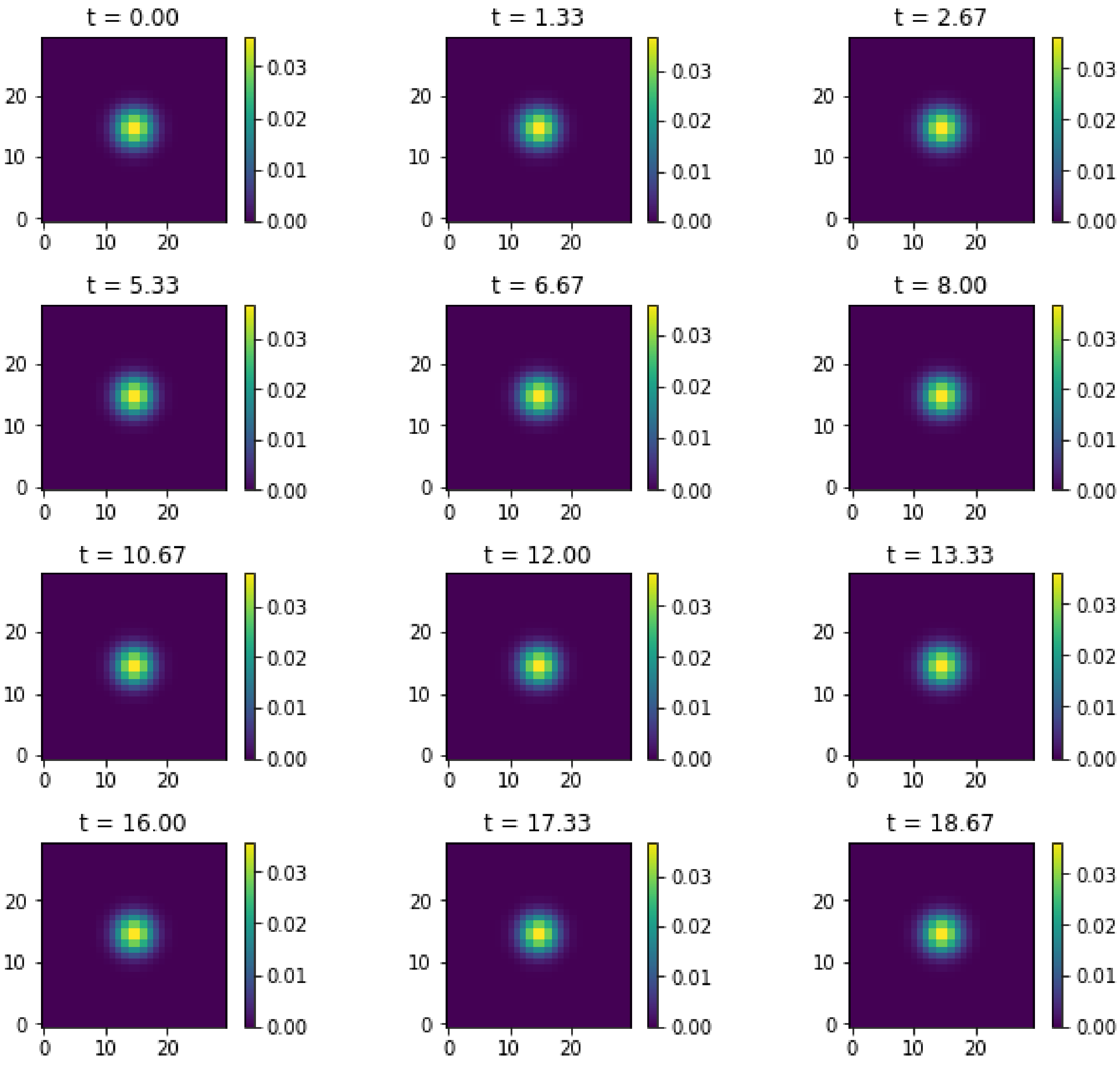

Figure 4: V $= \frac{1}{2}(x^2 + y^2)$