Absence of transport in certain disordered lattices

Consider a quantum particle described by a dimensionless Schroedinger equation ($\hbar = 1, m = \frac{1}{2}$, i is the imaginary unit)

$$i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + V(x)\psi \qquad (1)$$

in a 1d potential $V(x)$ made of equally spaced rectangular wells of two different widths. The particle could be an electron moving in a 1d crystal made of two different types of atoms (say, a doped semiconductor), or a photon moving in a stack of two different types of transparent material. If the potential has a regular pattern (e.g., narrow and wide wells intertwined), and the particle has sufficient energy, it will travel through the lattice at approximately constant speed. However, if we randomly rearrange the wells, the particle gets trapped and does not move, even though we have not changed the energies. This phenomenon, called localization, occurs in many problems in quantum physics and beyond. The following problem illustrates it.

Assume the following:

The initial condition:

$$\psi(x,0) = N\exp\left(-\frac{(x-x_0)^2}{2\sigma^2} + \frac{ivx}{2}\right) \qquad (2)$$

where N is a normalization factor (not given). This corresponds to a particle moving with speed v, the initial mean position x_0, and position uncertainty σ. Assume $v = 16$, $x_0 = 15$, $\sigma^2 = 5$.

Discretisation of H in space: divide space into equally spaced points such that $x = n\,dx$ and $n = 0,1,\dots,N-1$, where $N \equiv \frac{L}{dx}$. Equation (1) can be then represented as

$$i\frac{d\psi_n}{dt} = -\frac{\psi_{n+1} + \psi_{n-1} - 2\psi_n}{dx^2} + V_n\psi_n$$

or, in matrix notation,

$$i\frac{d\psi_n}{dt} = \sum_m H_{nm}\psi_m$$

The matrix H_{nm} has a special structure. What is it called?

Tasks to do:

Task	Points
1. Find numerically the first 101 lowest eigenvalues ("energies") of the discrete Hamiltonian matrix H, for $V = 0$ and $x = 0, \dots, L$, with $L = 100, dx = 1/8$ and with reflecting boundary conditions: $\psi_N \equiv \psi_{N-1}, \psi_{-1} \equiv \psi_0$ (here the index -1 denotes the element to the left of the element zero, not the element $N-1$ as in Python). Hint: The eigenvalues should be equal to $2\left(1-\cos\left(\frac{n\pi}{N}\right)\right)/dx^2$ where $n = 0,1,\dots,100$; the corresponding (non-normalized) eigenvectors are $\cos\left(\frac{n\pi x}{L}\right)$.	**25**
2. Select dx as a negative power of two ($dx = 2^{-n}$ for $n > 0$) such that the 101th eigenvalue differs from the $dx \to 0$ limiting value $\left(\frac{100\pi}{N}\right)^2/dx^2$ by less than 0.1%. Motivation: selecting a sufficiently small dx is required to obtain a good approximation to the original (continuous) equation (1) for subsequent tasks.	**10**
3. Solve equation (1) with the initial condition (2) for $V(x) = 0$, on a domain $x = 0 \dots 100$, for $t_{max} = 4$ and dx from task 2. Plot $\lvert\psi(x,t)\rvert^2$ for $t = 0,\ t_{max}$ and determine its mean given by $\int_0^{100}\lvert\psi(x)\rvert^2 x\,dx$. The mean should be between 78	**25**

and 80. Hint: use the procedure for creating the Hamiltonian matrix from tasks 1, 2. This will reduce the amount of coding required.	
4. Now repeat task (3) for a potential made up of regularly spaced wells such that $V = 70$ for $\|x - i\| < 0.25$ where $i = 0,1, \dots ,100$, and $V = 0$ elsewhere. Plot the potential. Determine the mean of $\|\psi(x,t)\|^2$ as before, with accuracy +/- 1. Make sure that dx and dt are sufficiently small to achieve this accuracy!	**10**
5. Calculate the probability P of the particle moving through the point $x = \frac{L}{2}$ by integrating the probability current $(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx})(x = L/2)$ over time, for $t = 0 \dots 4$. The probability can deviate from the true value by no more than ± 0.01. Hint: the correct value is between 0.5 and 1.	**10**
6. Plot the probability P as a function of particle energy $E = 0 \dots 100$, for at least 100 equally-spaced values from this range. All P values should be within ± 0.01 of the true values. Use the formula $E = \frac{1}{4} v^2$ to convert between energy and velocity (valid for Eqs. (1,2)). Bonus question: can you explain why the plot looks like this?	**10**
7. Assume again the initial condition (2) with $v = 16$, and consider a disordered potential in which $V = 70$ for $\|x - i\| < b_i$ where $i = 0,1, \dots ,100$, and b_i is a random variable uniformly distributed on [0.125,0.375]. Find the mean probability P by averaging over 100 realizations of the random potential. The result must be within ± 0.02 of the correct value. Plot the histogram of P. Comment on the value of P compared with task 5.	**10**

The mark for the checkpoint is the sum of points for all tasks. What will be marked: (i) numerical correctness, (ii) efficiency i.e. how long it takes to execute the code (it shouldn’t take more than a few minutes), (iii) coding style.

The Jupyter notebook provides the most comprehensive set of instructions for the task. In the case of discrepancy between this document and the Jupyter notebook, please follow instructions as specified in the Jupyter notebook.