Computational Methods Assignment 2

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1 Exercise 1

1.1 Part a

Taking $k_b = 8.62 \times 10^{-5}$ eV K^{-1}, $\hbar = 0.276$ nm $\sqrt{eV\, m_e}$ where m_e is the mass of an electron, and $\mu = 1$ eV the average energy density of the electron gas, $\epsilon = \int_0^\infty d\omega d(\omega) f(\omega)$ where $f(\omega) = \left(e^{\omega - \mu/k_B T} + 1\right)^{-1}$, and $d(\omega) = \left(m_e^{3/2}\sqrt{\omega}\right)\left(\sqrt{2}\pi^2\hbar^3\right)^{-1}$, was found using functions and plotted for temperatures in the range $T \in [0\,K, 10000\,K]$. The graph of ϵ against T is shown in figure 1. Plotting from $T = 0$ K did cause jupyter to give warnings about runtime, roundoff, and overflow errors, however it still runs successfully.

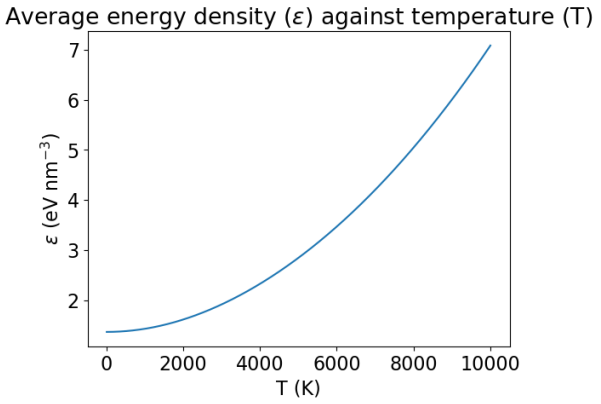


Figure 1: The average energy density for a constant chemical potential $\mu = 1$ eV against temperatures from 0 K to 10000 K.

1.2 Part b

On the same plot ϵ was plotted for a state with a fixed electron density $\rho = 2.27$ nm^{-3} where ρ is given by $\rho = \int_0^\infty d\omega d(\omega) f(\omega)$, and $d(\omega)$ and $f(\omega)$ are as above.

The density is kept constant by changing the value of μ at each temperature. The appropriate value for μ is found by starting with $\mu = 0$ eV and finding the value of ρ for this value of μ. If this is below the desired value of $\rho = 2.27$ nm^{-3} at this temperature μ is increased by a value $d\mu$ initially equal to 0.1 eV. When the density surpasses the desired value of 2.27 nm^{-3} μ is decreased to the last value which was below this value, e.g. if $\rho(\mu = 0.9\,eV) = 2.4$ nm^{-3} and $\rho(\mu = 0.8\,eV) = 2.2$ nm^{-3} then μ is decreased by $d\mu$ to 0.8 eV.

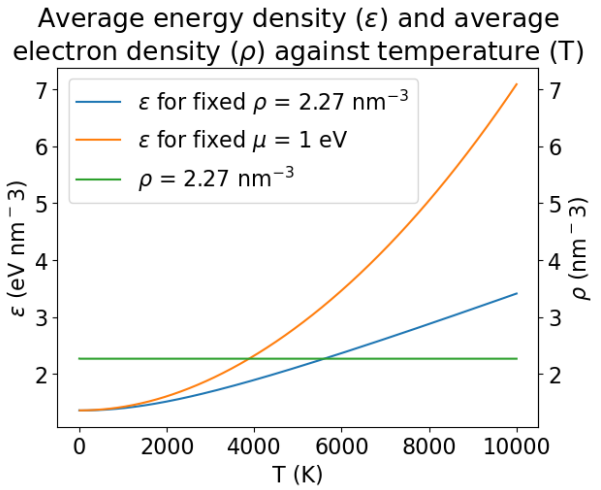


Figure 2: The average energy density for a constant density $\rho = 2.27$ nm^{-3} as well as ϵ for a chemical potential $\mu = 1$ eV (left axis), and the constant $\rho = 2.27$ nm^{-3} (right axis) against temperatures from 0 K to 10000 K.

The value of $d\mu$ is then decreased and this process is repeated until $d\mu$ becomes lower than 10^{-5} eV. When this state is reached it is checked to see which of the values of μ gives a value closer to the desired $\rho = 2.27$ nm^{-3}, the value which is just above it, or the value just below it. The appropriate value of μ is then saved. At each stage it is also checked if $\rho(\mu) = 2.27$ nm^{-3} and if it is then that value of μ is saved.

The graph of ϵ for constant ρ across the range of temperatures is plotted on the same axes as the function of ϵ calculated in Part a above for constant μ,

along with the computed $\rho = 2.27\ \text{nm}^{-3}$. This is shown in figure 2. The same warnings as above appeared again, but again the program ran without error.

Another potential method is to check whether the value of ρ higher or lower than $2.27\ \text{nm}^{-3}$ is closer to this value and acting accordingly, decreasing or increasing μ by $d\mu$. However it is currently 10:50 am on Wednesday as I write this and I have not been able to get it to work correctly so I have decided to leave it as it is.

2 Exercise 2

2.1 Part a

The Hamiltonian for the Aubry-Andre-Harper (AAH) model was defined with a function. It was decide to use $\hbar\lambda$ as units so $u = 2\hbar\lambda$. Then, for each value of $\alpha \in [1, 1/2, 1/3]$ a 500×500 Hamiltonian was defined.

The eigenvalues and vectors were calculated for the Hamiltonian, and then sorted in increasing order. The eigenvalues were then plotted for each value of α, these are shown together in figure 3.

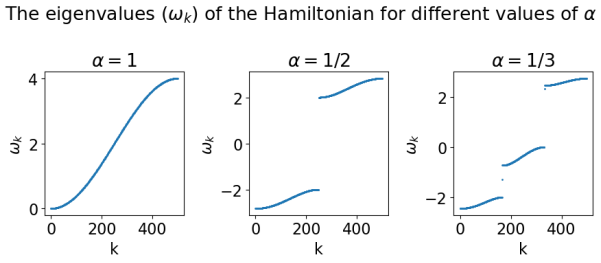


Figure 3: The eigenvalues of the AAH model Hamiltonians for $\alpha \in [1, 1/2, 1/3]$.

A histogram of the density of states, $\nu(\omega)$, was also plotted for each value of α and can be seen in figure 4. Because of the chosen units the width of each bin $\delta\omega$ was equal to $1/10$.

2.2 Part b

The value of α was set to $\varphi = (1+\sqrt{5})/2$, the golden ratio. A function was defined to find the inverse participation ratio (IPR) for a given eigenstate, k (I_k), and then one to find the mean of these values, $\overline{I}$ for all values of $k \in [0, L-1]$ for a given Hamiltonian which is an $L \times L$ matrix. This was found and plotted for values of $u = [0.0, 5.0]$ for a matrix with $L = 500$.

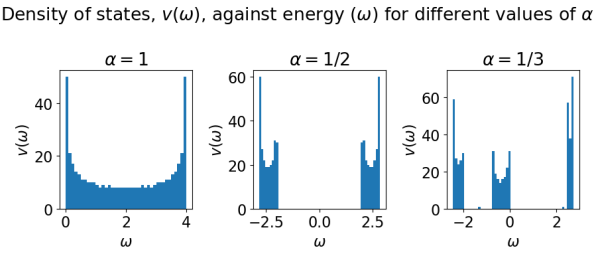


Figure 4: The density of states of the AAH model Hamiltonians for $\alpha \in [1, 1/2, 1/3]$.

A plot was made of u against $\overline{I}$ and can be seen in figure 5.

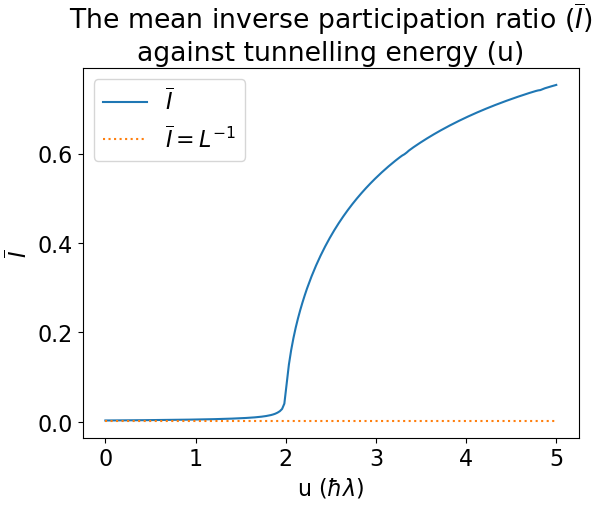


Figure 5: The mean inverse participation ratio for $u = [0.0, 5.0]$. The value of u_c can be seen to be approximately equal to 2 $\hbar\lambda$.

The critical disorder strength u_c was found by finding the point at which the graph begins to increase dramatically. This was done by finding the forward difference between consecutive calculated values of $\overline{I}$ and finding the maximum of these. This gives a value of $u_c = 2.01$. The value of $\overline{I}$ is consistently above $L^{-1} = 1/500$ before this, however it is at this point that $\overline{I}$ really begins to take off and approach 1.

The spatial probability distribution for an eigenstate in the extended phase ($u = 1\ \hbar\lambda$) and for an eigenstate in the localised phase ($u = 5\hbar\lambda$) were plotted and can be seen in figure 6. The same random eigenstate was chosen for each value of u, and were plotted on separate axes to account for the difference in scale between the probability distributions of the two states. Apart from a few smaller probability

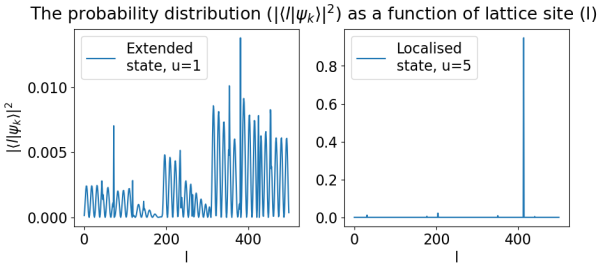


Figure 6: The probability distributions for the 461^{st} eigenstate for the localised and extended distributions, $u = 5$ and $u = 1$ respectively.

peaks across the distribution it can be seen clearly that the eigenstates are highly localised in the second graph in figure 6, which is not the case for the extended regime, as seen in the first graph in the same figure, as was expected.

3 Exercise 3

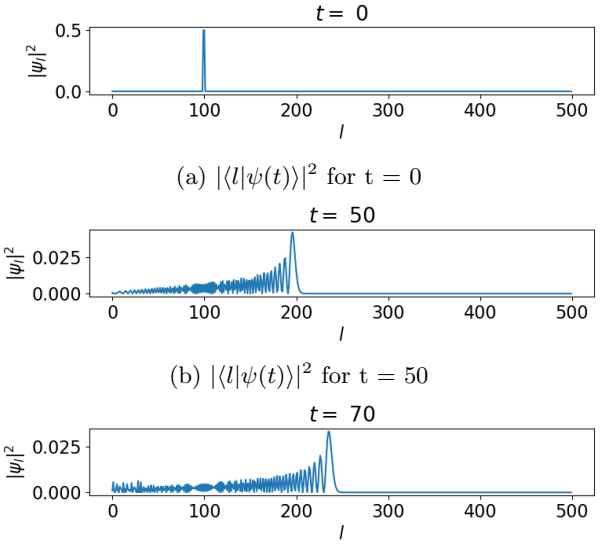
A function was defined to generate the Hamiltonian with the impurity, λ and $\hbar$ are both set equal to 1. The Hamiltonian with an impurity at the centre was defined, and the initial condition $|\psi(0)\rangle = (|99\rangle + i|100\rangle)/\sqrt{2}$. The ODE was then solved for a range of times, and the behaviour of the electron can be seen from the generated graphs, a selection of which can be found in figures 7 to 11.

Before the electron interacts with the impurity the electron's probability distribution $|\langle l|\psi(t)\rangle|^2$ spreads out to either side of the initial starting condition, with a higher amplitude arising towards the central impurity, and a lower amplitude developing away from the centre towards the edge of the lattice, see the graphs in figure 7.

When the part of the electron's probability distribution travelling to the right reaches the impurity, the probability of finding the electron at the impurity increases to be much higher than the probability of finding it anywhere else, see the graphs in figure 8.

It then mostly gets reflected back towards the direction it came from, however there is a small chance that it can tunnel through the impurity and so a small component of $|\langle l|\psi(t)\rangle|^2$ continues propagating towards the right, while a larger component propagates towards the left, interfering with the already present $|\langle l|\psi(t)\rangle|^2$, see the graphs in figure 9.

At about the same time as the electron reaches the impurity it also reaches the left of the lattice and reflects as well, see figures 7b, 7c and 8a. Later, the



(a) $|\langle l|\psi(t)\rangle|^2$ for t = 0

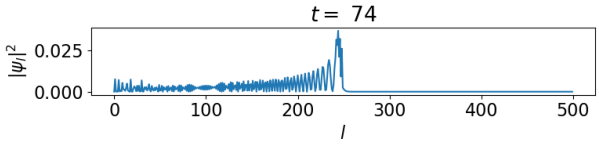
(b) $|\langle l|\psi(t)\rangle|^2$ for t = 50

(c) $|\langle l|\psi(t)\rangle|^2$ for t = 70

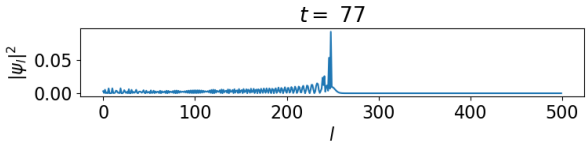
Figure 7: A selection of the spatial probability densities from before the electron reaches the impurity.

portion beyond the impurity also reaches the edge of the lattice and also reflects, see the graphs in figure 10.

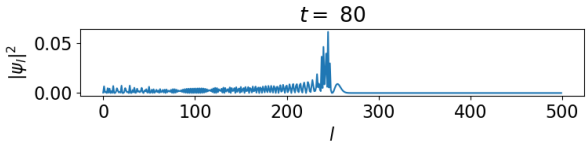
Finally, a long time after the electron has interacted with the impurity both sides have what appear to be highly irregular, likely due to much interference, time-varying function of $|\langle l|\psi(t)\rangle|^2$, with the left-hand side (where the electron started initially) at a much higher amplitude than the right (in general), see the graphs in figure 11.



(a) $|\langle l|\psi(t)\rangle|^2$ for t = 74

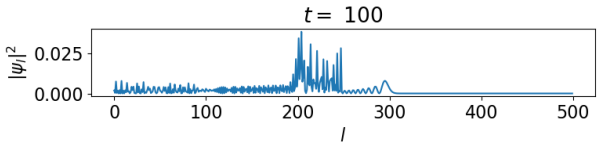


(b) $|\langle l|\psi(t)\rangle|^2$ for t = 77

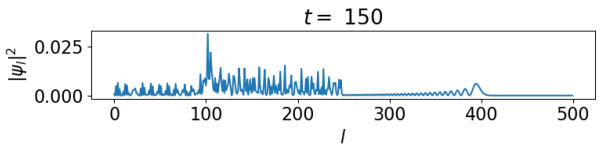


(c) $|\langle l|\psi(t)\rangle|^2$ for t = 80

Figure 8: A selection of the spatial probability densities as the electron reaches the impurity and interacts with it. Note the higher amplitude in figure 8b at the centre of the lattice, at the site of the impurity

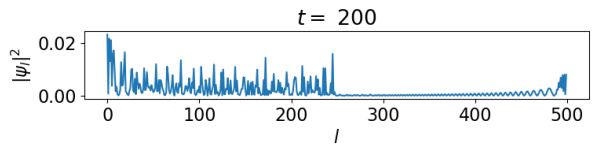


(a) $|\langle l|\psi(t)\rangle|^2$ for t = 100

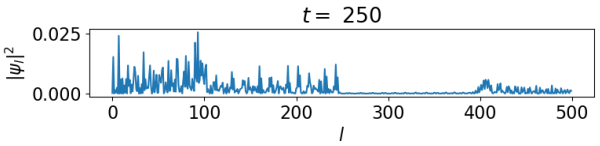


(b) $|\langle l|\psi(t)\rangle|^2$ for t = 150

Figure 9: A selection of the spatial probability densities after the electron has reached and interacted with the impurity. Note the reflection to the left, and small transmitted amplitude.

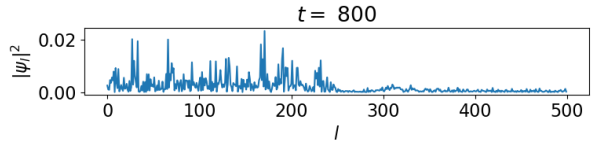


(a) $|\langle l|\psi(t)\rangle|^2$ for t = 200

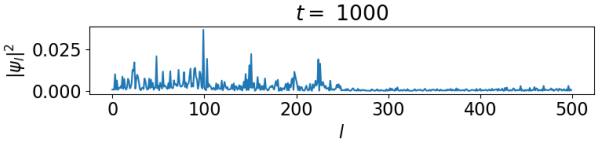


(b) $|\langle l|\psi(t)\rangle|^2$ for t = 250

Figure 10: A selection of the spatial probability densities while and after the electron's probability density reflects from the rightmost edge of the box.



(a) $|\langle l|\psi(t)\rangle|^2$ for t = 800



(b) $|\langle l|\psi(t)\rangle|^2$ for t = 1000

Figure 11: A selection of the spatial probability densities a long time after the electron interacts with the impurity. Note the higher amplitude of the probability density function on the left of the impurity, electron's initial side, than on the right.