Homework 1

2. d)

Let us first consider the case for the cubic lattice. Due to isotropy and homogeneity of this lattice, we only need to consider the average time spent at $\vec{r} = (||\vec{r}||, 0, 0)$.

In[123]:=
```
r = 0;
NIntegrate[ E^(i q1 r) / ((2 π)^3 (1 - 1/3 (Cos[q1] + Cos[q2] + Cos[q3]))),
 {q1, -π, π}, {q2, -π, π}, {q3, -π, π}]
```

Out[124]=
```
1.51639
```

For the body centered cubic lattice we have the following result

In[125]:=
```
r = 0;
NIntegrate[ E^(i q1 r) / ((2 π)^3 (1 - 1/4 (Cos[q1] + Cos[q2] + Cos[q3] + Cos[q1 + q2 + q3]))),
 {q1, -π, π}, {q2, -π, π}, {q3, -π, π}]
```

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

NIntegrate: The global error of the strategy GlobalAdaptive has increased more than 2000 times. The global error is expected to decrease monotonically after a number of integrand evaluations. Suspect one of the following: the working precision is insufficient for the specified precision goal; the integrand is highly oscillatory or it is not a (piecewise) smooth function; or the true value of the integral is 0. Increasing the value of the GlobalAdaptive option MaxErrorIncreases might lead to a convergent numerical integration. NIntegrate obtained 1.393012028544957` and 0.00003620724288534162` for the integral and error estimates.

Out[126]=
```
1.39301
```

Using the correct result after Alexandre's suggestion we obtain a new result

In[145]:=
```
a = 2;
r = 0;
a1 = a/2 {-1, 1, 1};
a2 = a/2 {1, -1, 1};
a3 = a/2 {1, 1, -1};
NIntegrate[E^(i q1 r) / ((2 π)^3
    (1 - 1/4 TrigExpand[Cos[{q1, q2, q3}.a1] + Cos[{q1, q2, q3}.a2] + Cos[{q1, q2, q3}.a3] +
        Cos[{q1, q2, q3}.(a1 + a2 + a3)]])), {q1, -π, π}, {q2, -π, π}, {q3, -π, π}]
```

NIntegrate: Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

NIntegrate: The global error of the strategy GlobalAdaptive has increased more than 2000 times. The global error is expected to decrease monotonically after a number of integrand evaluations. Suspect one of the following: the working precision is insufficient for the specified precision goal; the integrand is highly oscillatory or it is not a (piecewise) smooth function; or the true value of the integral is 0. Increasing the value of the GlobalAdaptive option MaxErrorIncreases might lead to a convergent numerical integration. NIntegrate obtained 1.448630930282385` and 0.2551354288221919` for the integral and error estimates.

Out[150]=
```
1.44863
```