In spectroscopy:

<https://www.wikiwand.com/en/Wavenumber#/In_spectroscopy>

The unit of “wavenumber” is  , so it has unit cm^{-1}.

Here is a useful website for this:

<https://www.powerstream.com/inverse-cm.htm>

(Note in this website:

300 cm-1 => 33 microns

20,000 cm-1 => 500 nm

Relationship between wavenumber and wavelength.)

in spectroscopy, frequency denoted by cm^{-1} is inverse of wavenumber \lambda

For angular velocity \omega:

ω = f \* 2 π \*c

For example wavenumber λ=500 nm. 1/λ = 2\*10^{7} m^{-1}

= 20,000 cm^{-1}

For room temperature T = 300 K.

kBT = ħω

ω = 3.927 \* 10^{13}

Then spectrscopy frequency f= ω / (2\*pi \* c) = 20837 m^{-1} = 200 cm^{-1}.

Also we can know the unit of time in our program:

cf =0.02997 \* dt \* 2π

c= 2.997 \* 10^{8}

if we let ħ==1 (or we let Hamiltonian rescale by ħ in our simulation).

Then ω= f (spectroscopy frequency, in unit of cm^{-1}) \* 2π\*c \* 100 (convert cm^{-1} to m^{-1})

= 2.997 \* 10^{10} \* 2π \* dt (/s) \*f (cm^{-1})

= 0.02997 \* 2π \* dt (/s) \* 10^{12} \*f (cm^{-1})

=0.02997 \* 2π \* dt (/ps) \* f (cm^{-1})

The unit of time is ps.

For Hamiltonian iħ d |phi>/dt = ħω |phi> (ħ cancel).

Thus our Hamiltonian V is in unit of ħ f (cm^{-1})

(As shown above, f could convert to ω by ω= f \* 2π \* c \* 100 ).

In our New\_parameter unit:

Our frequency : 114, 50.8 , 29.1, 47.6, 80.6, 30.3

They stand for (1140, 508, 291, 476, 806, 303).

in this unit, our time is 0.1 ps. (Unit of energy is 10 cm^{-1})

We could set them to right frequency f and also scale intra-detector coupling and inter-detector coupling in the same time.

How to compute recurrence time scale from density of states:

1 cm-1 ~ 3\*10^{-2} (ps)^{-1}

Thus for D(E) in unit of (cm) we have:

t = D(E) (cm) = D(E)/ (3\*10^{-2}) ps

= 0.03 \* D(E) ns

If we have D(E) = 2\*10^{3} as in Wolynes paper for example, then we have t = 60 ns (naphthalene).

In most of simulation, we have local density of states around 3 cm, thus we have t = 100 ps as recurrence time.

The vibrational time for f=1100 cm-1 is:

f= 3\*10^{8} m/s \* 1100 cm^{-1} = 3.3\*10^{13} /s

Thus t = 0.3 \* 10^{-13} s = 30 fs = 0.03 ps.

How to compute temperature T from the state \vec{n} we choose:

We assume we can arrive at equilibrium, then the average quanta in each state should be given by:

For boson field obey BE distribution:

1/(eβf - 1) = <n>

We have average energy: <E> = Σ <n i > fi = Σ fi/(eβfi - 1)   
Given initial state n\_{init}, E is given by initial state as

E = Σ n\_{init }f . Thus temperature is unique determined by initial state. (Use simple python script can compute temperature from initial state) ( There are one-to-one correspondence between energy E and temperature. )

Given f : frequency is known, we have a one-to-one relationship between initial state and temperature T.

MSS bound: Maldacena - Shenker- Stanford Bound:

λ L = 2πkBT/ħ

As when compute k\_{B} T in unit of cm^{-1}. If we want to transfer to unit of Kelvin, we have:

kB T (cm^{-1} ) \* c \* h = kB T (in unit of J)

Thus we have λ L = (2π) 2 \* c \* ( kB T (cm^{-1} ) )

As our time scale is ps, we transform λ L  to unit of (ps)-1

we have λ L = 1.183 \* kB T (cm^{-1} )

An example:

frequency = [1149.8, 509, 291.87, 474, 842.92, 332.9 ]  
  
mode\_number = [1,1,2,2,3,2 ]

kB T (cm^{-1} ) = 1136

Bound on λ L = 1343.