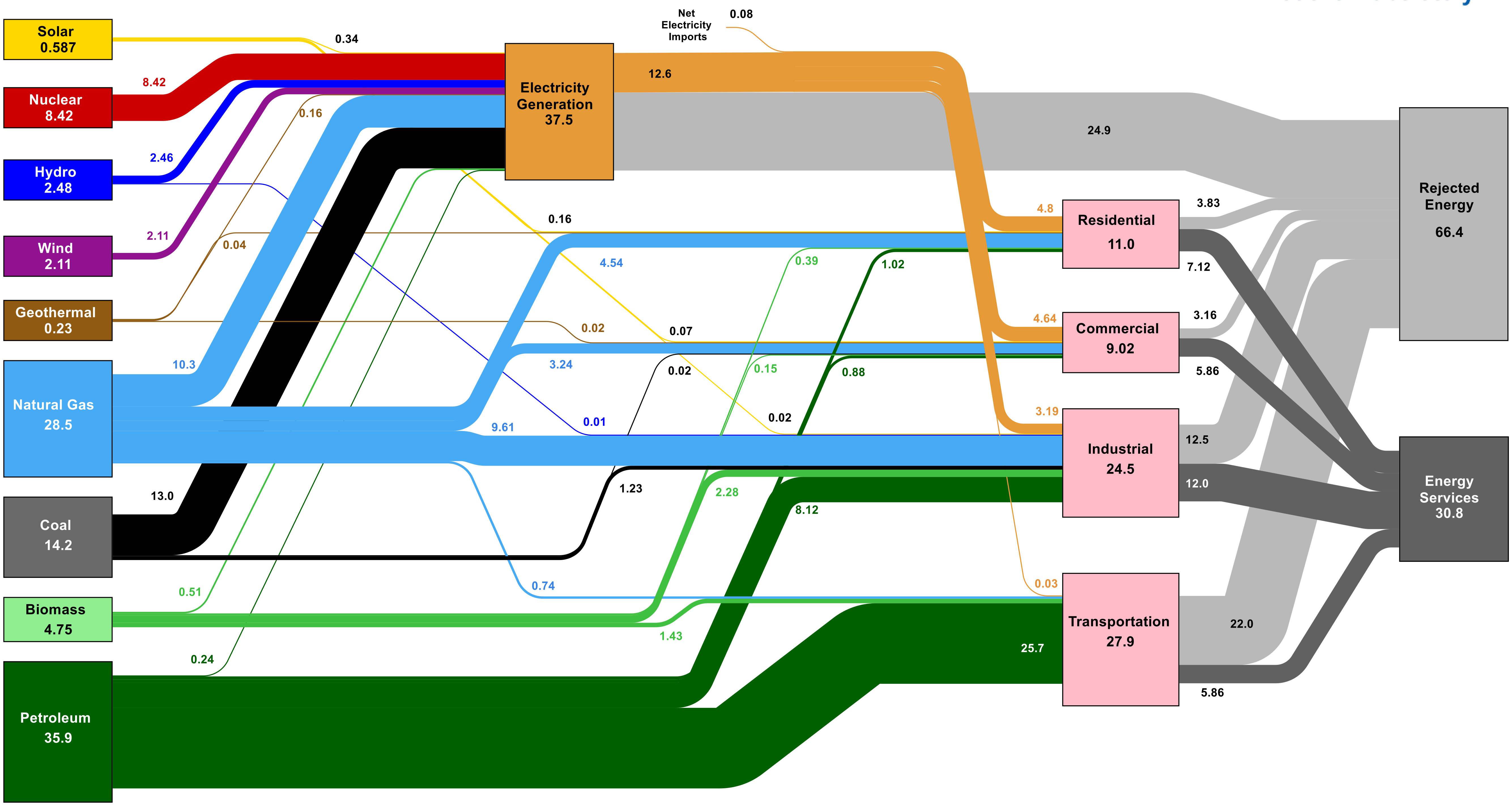
Phonons in Thermoelectric Devices
or
Anderson Localization in Random Multilayer Thin Films: a Phonon Story

Anthony Frachioni for Professor Jak Chakhalian for Solid State I

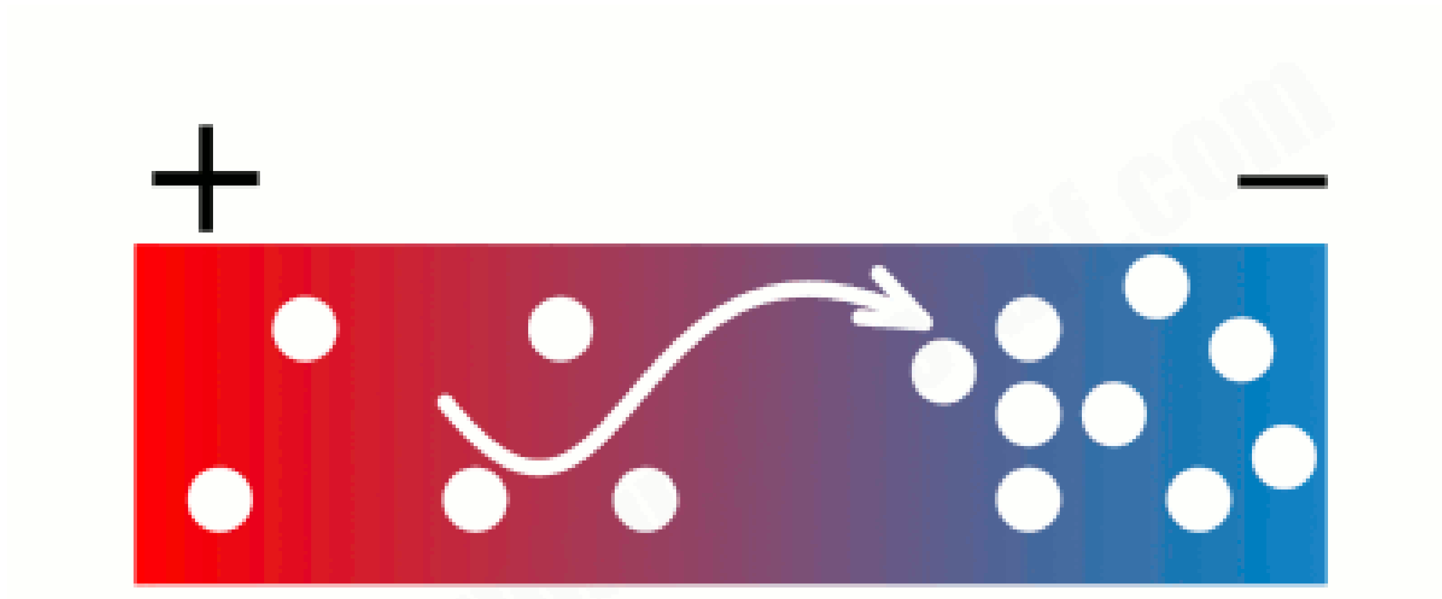
Fall 2017

Estimated U.S. Energy Consumption in 2016: 97.3 Quads



Source: LLNL March, 2017. Data is based on DOE/EIA MER (2016). If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. This chart was revised in 2017 to reflect changes made in mid-2016 to the Energy Information Administration's analysis methodology and reporting. The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 65% for the residential sector, 65% for the commercial sector, 21% for the transportation sector, and 49% for the industrial sector which was updated in 2017 to reflect DOE's analysis of manufacturing. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

Seebeck Effect



$$ZT = \frac{S^2 \sigma T}{\kappa_{\mathrm{ph}} + \kappa_{\mathrm{el}}}$$

$$
\begin{aligned}
U &= \frac{k}{2}\sum_i \left((u_{i-1} - u_i)^2 + (u_i - u_{i+1})^2 \right) \\
&= \frac{k}{2}\sum_i 2u_i^2 + u_{i+1}^2 + u_{i-1}^2 - 2u_i u_{i+1} - 2u_i u_{i-1}
\end{aligned}
$$

$$
\begin{aligned}
m_i \ddot{u}_i &= -\frac{\partial U}{\partial u_i} \\
&= -\frac{k}{2}\left(4u_i - 2\left(u_{i+1} + u_{i-1}\right)\right)
\end{aligned}
$$

With the ansatz $u_i(t) = A_i e^{ikia - \omega t}$,

$$
-m_i \omega^2 u_i = k\left(2u_i - u_{i+1} - u_{i-1}\right)
$$

$$-m_i \omega^2 u_i = k\left(2u_i - u_{i+1} - u_{i-1}\right)$$

if we set $m_i = M \forall i$,

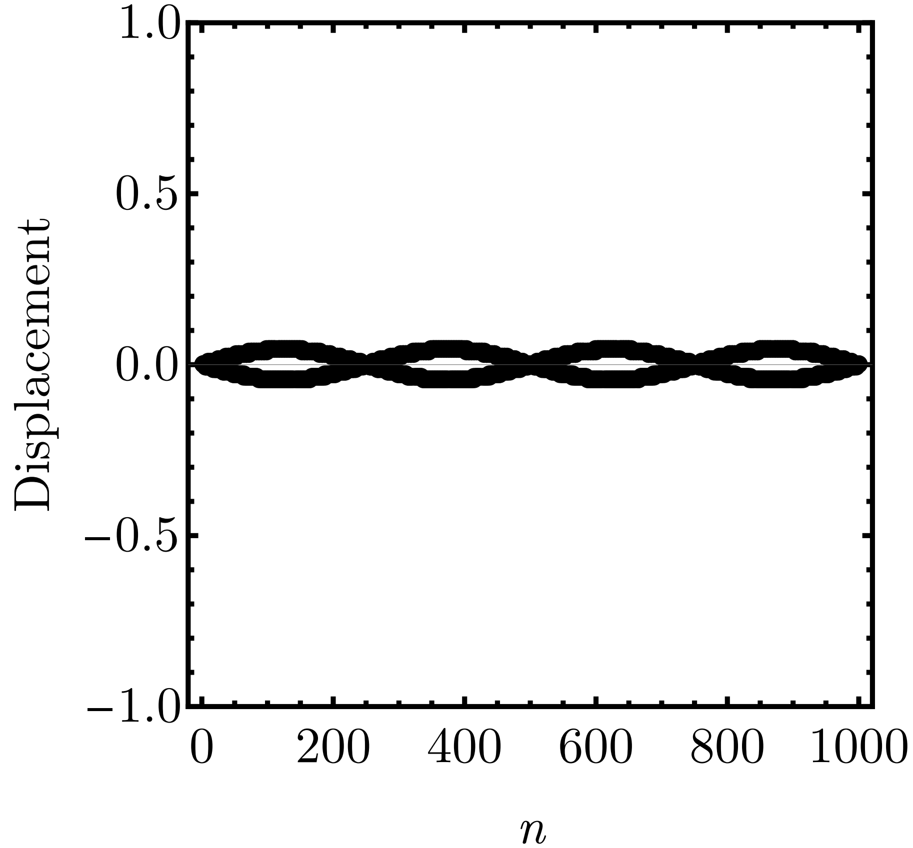
$$\begin{aligned}
-M\omega^2 e^{i(kna-\omega t)} &= -k\left(2 - e^{-ika} - e^{ika}\right) e^i(kna - \omega t) \\
&= -2k(1-\cos ka)e^{i(kna-\omega t)}.
\end{aligned}$$

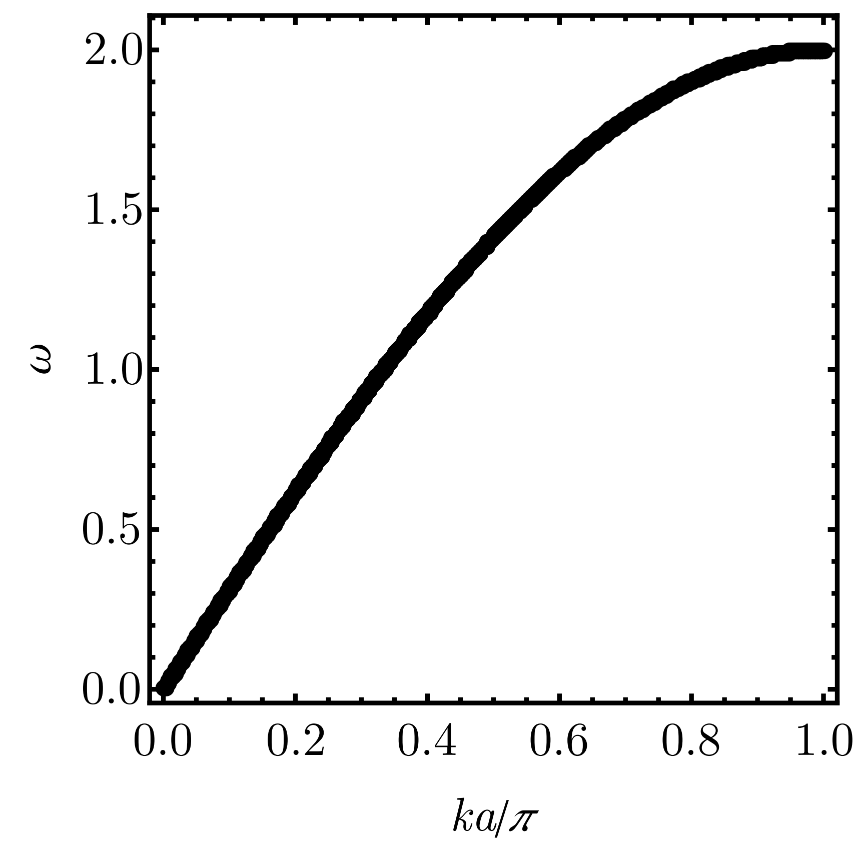
This furnishes

$$\begin{aligned}
\omega(k) &= \sqrt{\frac{2k(1-\cos ka)}{M}} \\
&= 2\sqrt{\frac{k}{M}}\left|\sin\frac{1}{2}ka\right|
\end{aligned}$$

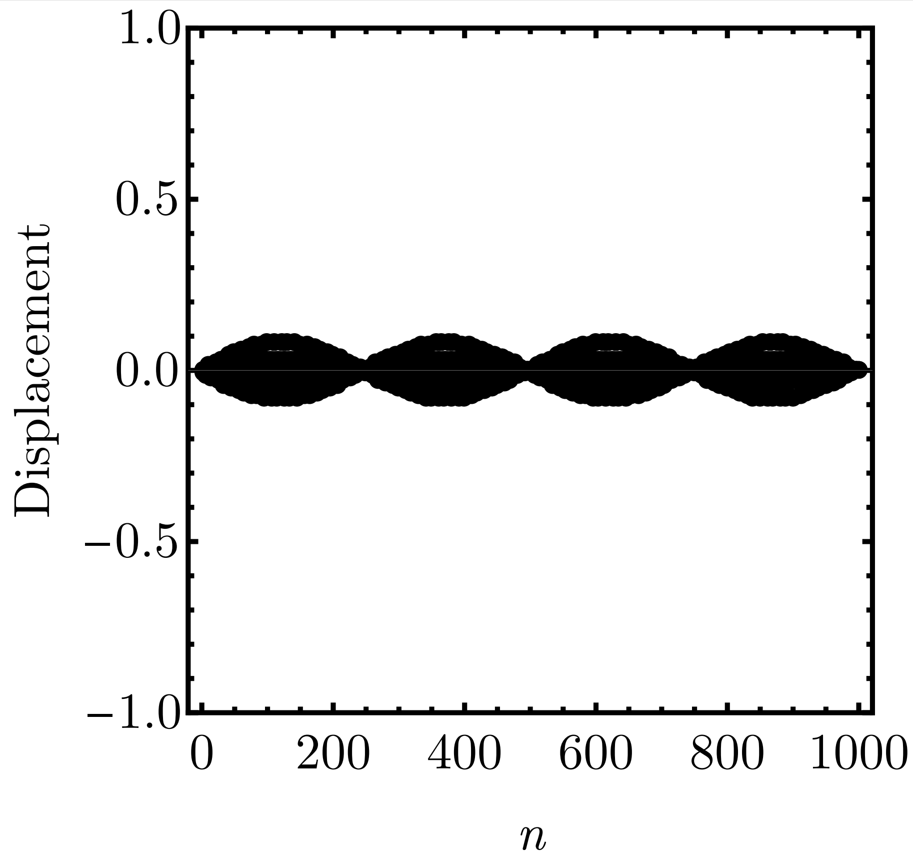
1D Solid

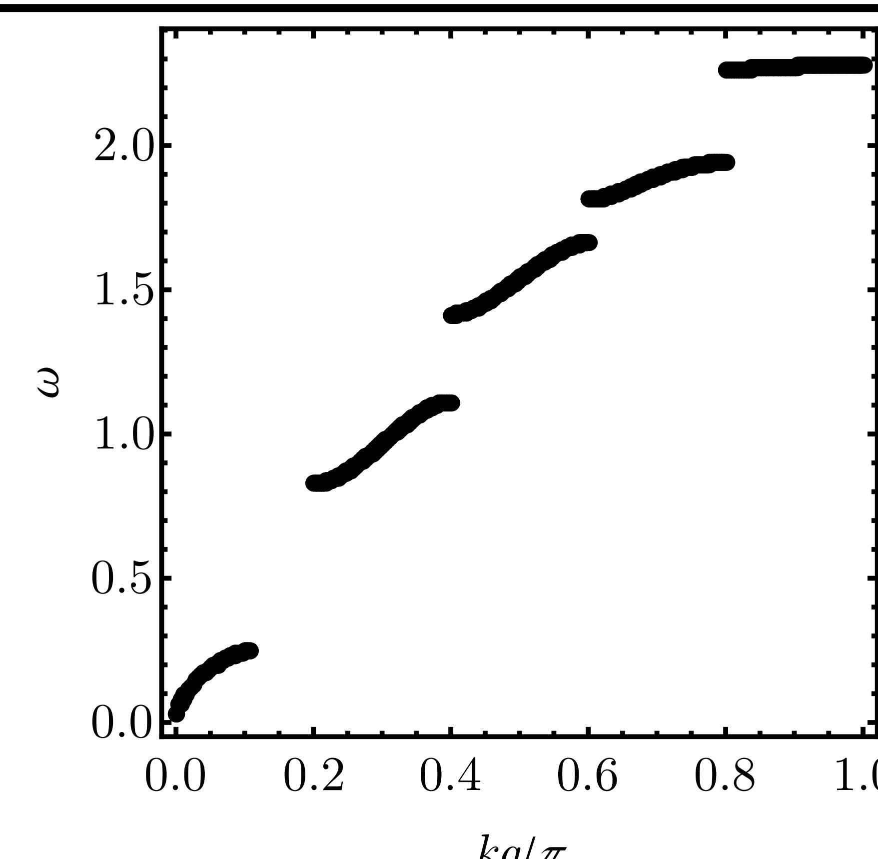
Uniform Masses



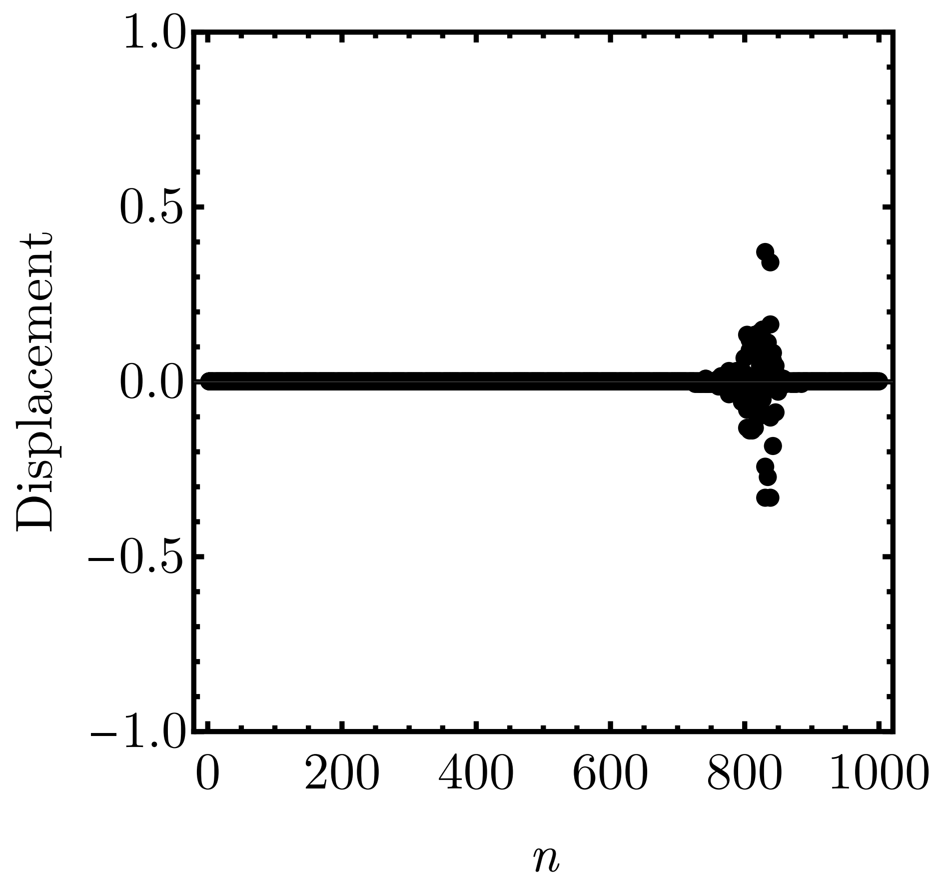


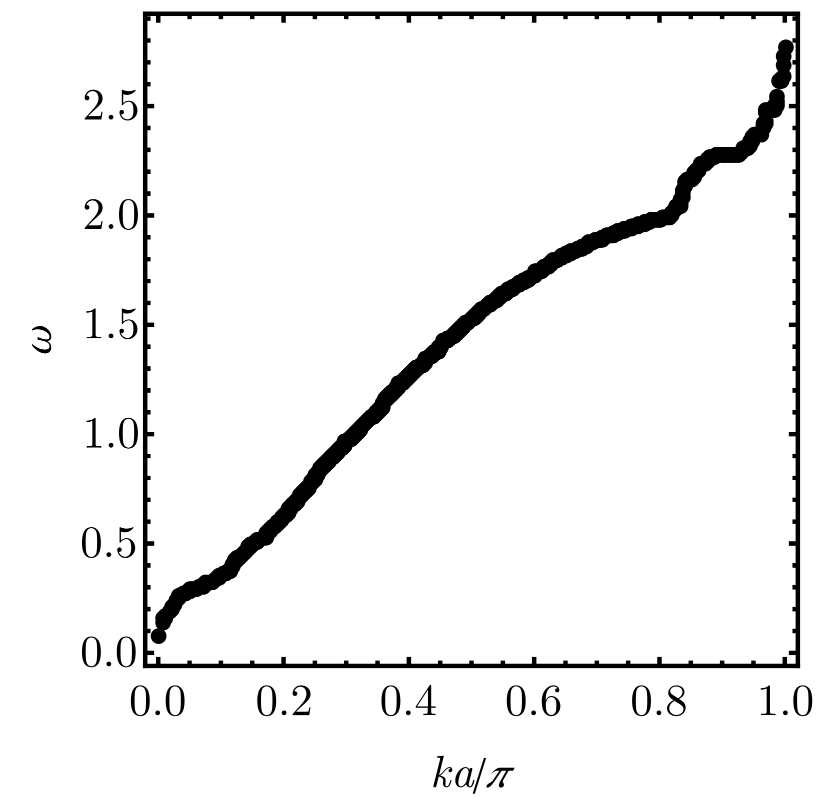
Periodic Superlattice

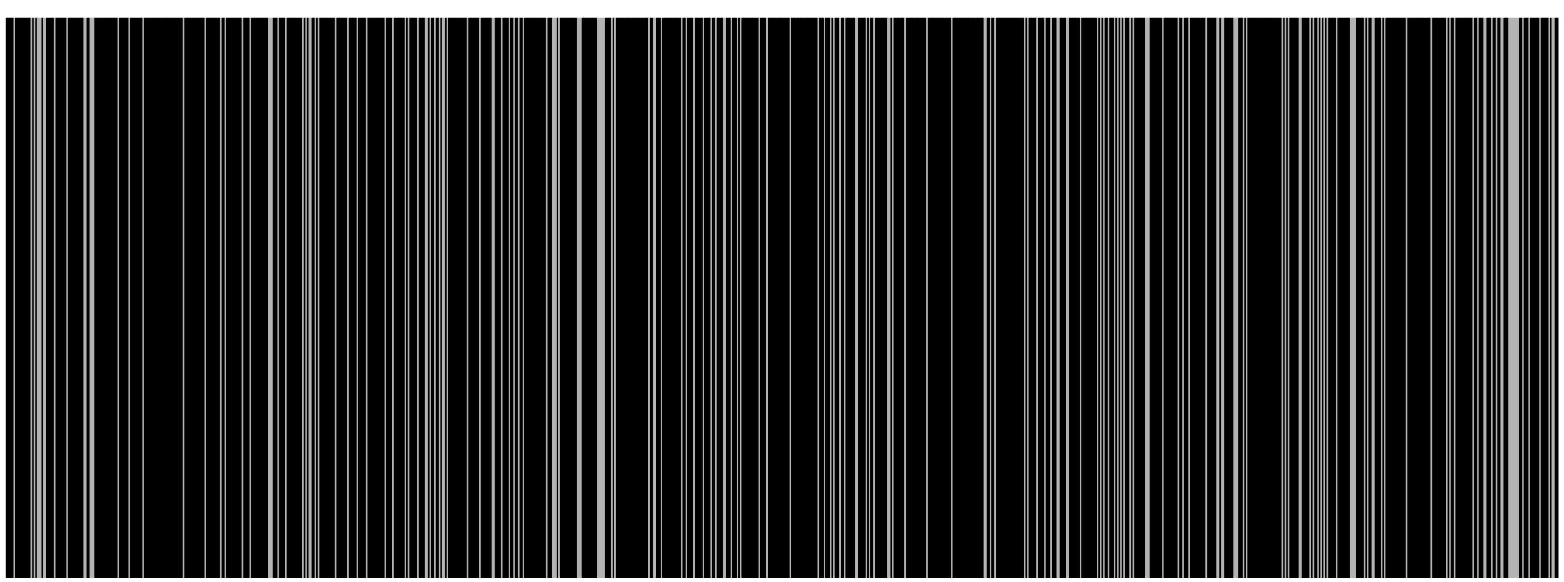


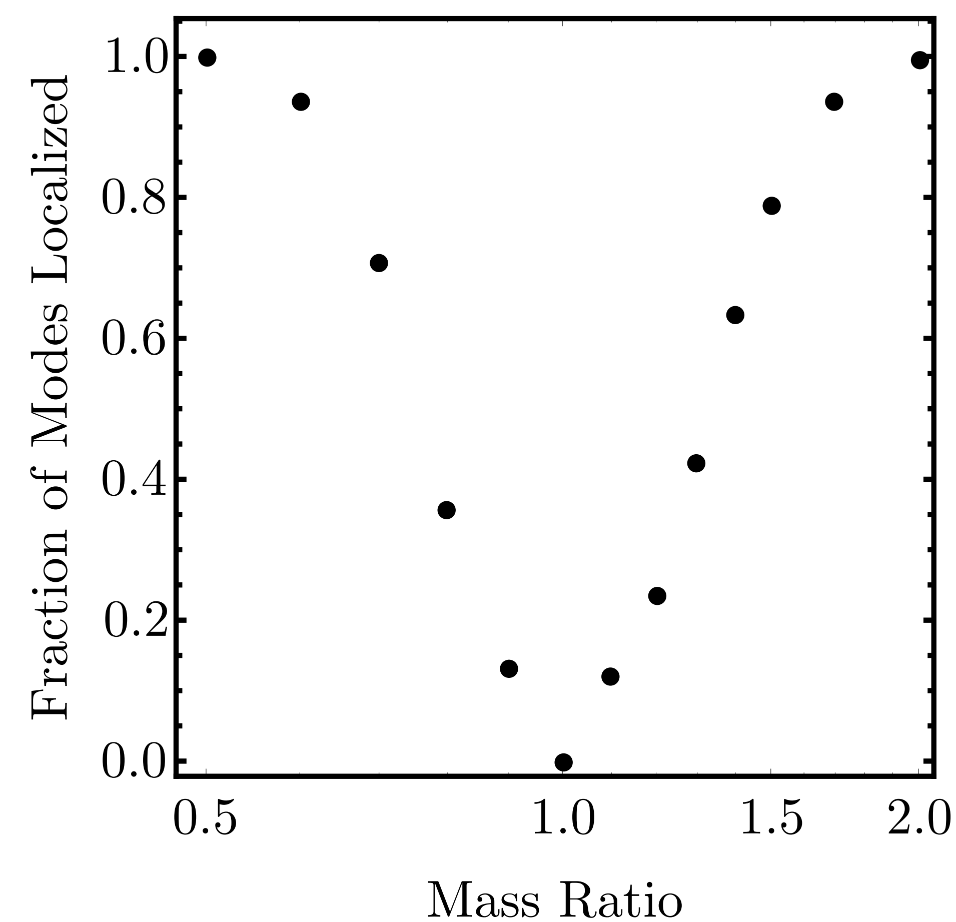


1D Solid with random disorder









3D Solid by Molecular Dynamics