Contents

1 Overview

This document is meant to log my progress in the investigation of mechanical modes in crystals of hard regular polygon particles. The system consists of $N = n^2 \times n_{\text{unit}}$ particles, where n is some integer and n_{unit} is the number of particles in the unit cell. The system is initialized in its densest known packing and then the crystal vectors are enlarged by constant factors to achieve a prescribed packing fraction. The motion of particles is decomposed into $n \times n$ distinct Fourier modes. There are $3n_{\text{unit}}$ relevant fields to investigate. The first $2n_{\text{unit}}$ are phonon fields signified by $\tilde{\mathbf{u}} = (\tilde{u}_x, \tilde{u}_y)$ (if the number of particles per unit cell is greater than 1, then these fields are further indexed *i.e.* $\tilde{\mathbf{u}}^{\alpha,\beta,\gamma\cdots}$. The remaining n_{unit} fields are libron fields, signified by $\tilde{\theta}^{\alpha,\beta,\gamma\cdots}$. In the case of hexagons, $n_{\text{unit}} = 1$, and in the case of many other polygons including pentagons studied here, $n_{\text{unit}} = 2$.

The various control parameters in a simulation are n the number of unit cells along one side of the box, ϕ the packing fraction, s the number of simulation steps, and the polygon shape. The densest packing, and thus the crystal lattice vectors, are determined by the polygon. The real space lattice vectors given by $\mathbf{a}_1, \mathbf{a}_2$ are usually meant to be in the densest packing, $\phi_{\max}$. When the system is relaxed to a smaller packing fraction, the lattice vectors are presumed to be $\mathbf{a}_i(\phi) = \mathbf{a}_i\sqrt{\phi_{\max}/\phi}$. The reciprocal lattice vectors $\mathbf{G}_i$ are constructed from these real space lattice vectors, and the unit cell of the reciprocal lattice forms the Brillouin zone within which $\mathbf{k}$ vectors are sampled. The relevant $\mathbf{k}$ vectors to sample are $n_1\mathbf{G}_1/n + n_2\mathbf{G}_2/n$, where n_i are integers. This way, the same number of Fourier modes are sampled as there are degrees of freedom in the real space system.

The Fourier modes are analyzed by considering their correlation functions. In Monte Carlo, dynamical information is not available, so collective degrees of freedom need to be analyzed from correlation functions by way of a kind of generalized law of equipartition. We assume that this hard particle system which is controlled exclusively by entropic interactions can be approximated by a harmonic Hamiltonian:

$$\mathcal{H} = \frac{1}{2m}p_i\delta_{ij}p_j + \frac{1}{2I}L_i\delta_{ij}L_j + \frac{1}{2}x_iK_{ij}x_j. \tag{1}$$

The first term is the translational kinetic energy and the second term is the rotational kinetic energy. The last term is a harmonic coupling by a $3N \times 3N$ matrix, and x_i represent both the particle positions and particle orientations. In thermal equilibrium, it is provable that

$$\langle x_ix_j\rangle = k_BTK^{-1}_{ij}. \tag{2}$$

The matrix K_{ij} is partially diagonalized by the Fourier transform with respect to the lattice vectors $\mathbf{a}_{1,2}(\phi)$, so we find that

$$\left\langle \tilde{x}^*_{\mu,\mathbf{k}} \tilde{x}_{\nu,\mathbf{k}} \right\rangle = C_{\mu\nu,\mathbf{k}} = k_B T K^{-1}_{\mu\nu,\mathbf{k}}. \tag{3}$$

This decomposes the large $3N \times 3N$ matrix K_{ij} into a block diagonal $n^2 \times n^2$ matrix whose diagonal elements are $3n_{\text{unit}} \times 3n_{\text{unit}}$ matrices $K_{\mu\nu}$. The modes $\tilde{x}_\mu$ can represent either $\tilde{\mathbf{u}}_x^{\alpha,\beta\cdots}$, $\tilde{\mathbf{u}}_y^{\alpha,\beta\cdots}$ or $\tilde{\theta}^{\alpha,\beta\cdots}$. The ultimate output of the analysis is the matrix $K_{\mu\nu,\mathbf{k}}$, which is obtained by computing every correlation function of all modes of the same wave vector and inverting the resulting matrix $C_{\mu\nu,\mathbf{k}}$. The elements of $\mathbf{K_k}$ are the squares of the phonon and libron dispersion relations, *i.e.* they furnish $\omega^2(\mathbf{k})$ for all $\mathbf{k}$ sampled in the Brillouin zone and for all collective modes $\tilde{\mathbf{u}}^{\alpha,\beta\cdots}$ and $\tilde{\theta}^{\alpha,\beta\cdots}$.

The matrices $\mathbf{K_k}$ depend on the packing fraction ϕ, the number of particles N, and the number of Monte Carlo sweeps taken s. If s is too small, then there is not a sufficient number of statistically independent Monte Carlo frames to compute the elements of the correlation matrix $\mathbf{C}$. The effect of s will be explored in Section 2.

In principle, the matrix $\mathbf{C}$ should be independent of N (or equivalently n), but having larger N helps resolve $\mathbf{C}$ as a function of $\mathbf{k}$, the wavevector, as the Brillouin zone is more densely populated. The effect of N will be explored in Section 3.

The matrix $\mathbf{C}$ is most markedly affected by changes in the packing fraction. Because some polygon crystals melt into various phases (hexatic, rotator, or plain fluid), particular elements of $\mathbf{C}$ should simply vanish across these transitions, which I will show leads to flat dispersion relations. That is, particular elements of $\mathbf{K_k}$ become independent of $\mathbf{k}$.