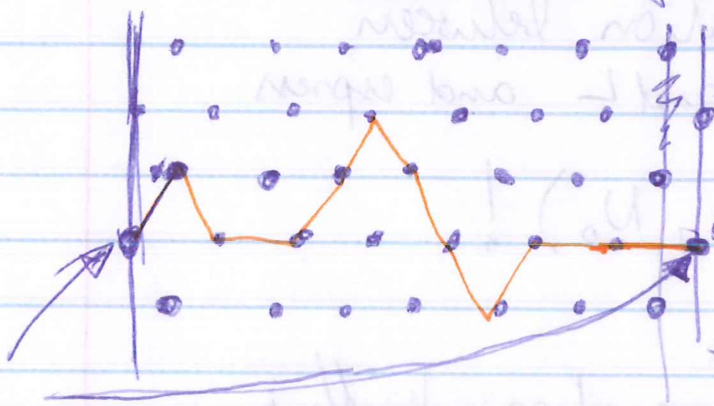
2D model of a liquid



* hexagon lattice
* end points distance L apart
* no overhanging waves

Same hight

* Energy of the surface is determined by its length only ("surface tension")

* aim: calculate the length of the surface as a function of temperature.

$N_0 \hat{=}$ # of horizontal elements
$N_+ \hat{=}$ # of elements with positive slope (from left to right)
$N_- \hat{=}$ # of elements with negative slope

$\Rightarrow$ Energy is defined as:

$$E = \varepsilon (N_+ + N_- + N_0 - L)$$

so that "calm see" $\Leftrightarrow$ $E = 0$

(a) find a relation between N_0, N_+, N_- and L and express

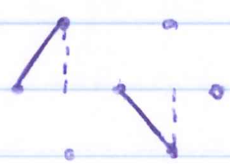
$$E(\varepsilon, L, N_0)\,!$$

- since end points are at same high:

$$N_+ = N_-$$

- since projection onto the horizontal line has to give L, we have (due to the hexagonal geometry)

$$\text{eq. (1)} \qquad N_0 + \frac{N_+ + N_-}{2} = L$$



if we denote the lattice spacing by l, then a rising/falling slope contributes $\frac{l}{2}$ in the projection!

$$(1) \Rightarrow N_+ + N_- = 2(L - N_0)$$

$\rightarrow$ back into E:

$$E = \varepsilon(2(L - N_0) + N_0 - L) = \varepsilon(L - N_0)$$

$$\boxed{E = \varepsilon (L - N_0)}$$

(b) Show that the microcanonical partition function

$$g(E) \triangleq \# \text{ of possible states with energy } E$$

is given by

eq. (2) $$g(E) = \frac{(2L - N_0)!}{N_0! \, \left((L-N_0)! \right)^2}$$

• obviously we have:

$$g(E) = \frac{(N_0 + N_+ + N_-)!}{N_+! \, N_-! \, N_0!}$$

with $\boxed{N_+ = N_- = L - N_0}$

and $\boxed{N_0 + N_+ + N_- = 2L - N_0}$

relation (2) follows!

(c) calculate the entropy

$$S(E) = k_B \ln g(E)$$

using Stirlings approximation

$$\ln N! \cong N(\ln N - 1) \simeq N \ln N$$

$$\rightarrow \frac{1}{k_B} S(E) \cong \ln \frac{(2L-N_0)!}{N_0!\,((L-N_0)!)^2}$$

$$= \ln(2L-N_0)! - \ln N_0! - 2\ln(L-N_0)!$$

- substitute $E = (L - N_0)\cdot\varepsilon \rightarrow N_0 = L - \frac{E}{\varepsilon}$

$$\Rightarrow \frac{1}{k_B} S(E) = \ln\left(L + \frac{E}{\varepsilon}\right)! - \ln\left(L - \frac{E}{\varepsilon}\right)! - 2\ln\left(\frac{E}{\varepsilon}\right)!$$

$$\boxed{\frac{1}{k_B} S(E) \simeq \left(L + \frac{E}{\varepsilon}\right)\ln\left(L + \frac{E}{\varepsilon}\right) - \left(L - \frac{E}{\varepsilon}\right)\ln\left(L - \frac{E}{\varepsilon}\right) - 2\frac{E}{\varepsilon}\ln\frac{E}{\varepsilon}}$$

#

(d) calculate the temperature

$$\frac{1}{T} = \frac{\partial S}{\partial E}$$

$$= \frac{k_B}{\varepsilon}\left[\ln\left(L - \frac{E}{\varepsilon}\right) + \ln\left(L + \frac{E}{\varepsilon}\right) - 2\ln\left(\frac{E}{\varepsilon}\right)\right]$$

$$\boxed{\frac{1}{T} = \frac{k_B}{\varepsilon}\ln\left(\frac{L^2\varepsilon^2 - E^2}{E^2}\right)} \quad \text{eq}(3)$$

$$\Leftrightarrow e^{\frac{\varepsilon}{k_B T}} = \frac{L^2\varepsilon^2 - E^2}{E^2}$$

(e) Solve eq. (3) for E and calculate the temperature dependence of the length of the surface $l(T)$ taking into account that:

$$l(T) = N_0 + N_+ + N_- = 2L - N_0 = L + \frac{E}{\varepsilon}$$

solving eq. (3) for E yields:

$$E = \frac{L\varepsilon}{\sqrt{e^{\varepsilon/k_B T}+1}}$$

$\Rightarrow$ total length of the surface is now

$$l(T) = L + \frac{E}{\varepsilon} = L\left(1 + \frac{1}{\sqrt{e^{\varepsilon/k_B T}+1}}\right)$$

what are the limits for

$$k_B T \ll \varepsilon \rightarrow l(T) \simeq L$$

(little thermal fluctuations)

$$k_B T \gg \varepsilon \rightarrow l(T) \simeq L\left(1 + \frac{1}{\sqrt{2}}\right)$$