Packing fraction $\phi = \frac{N\pi(\sigma/2)^2}{H_d L}$.

$h = H_d - \sigma$ is the width available to the centres of the disks.

Three ranges for the width:

- $H_d < (1 + \sqrt{3}/2)\sigma$ – nearest-neighbour contacts only. (NN case).
- $(1 + \sqrt{3}/2)\sigma \leq H_d \leq 2\sigma$ – nearest and next-nearest neighbour contacts possible. (NNN case).
- $H_d > 2\sigma$ – disks can move past each other. This case cannot be solved with the transfer matrix approach.
The NN case case first. Figures for $H_d = (1 + \sqrt{3}/2) \sigma$.

Upper Figure: the jammed state of maximum density. $\phi_{\text{max}} = 0.8418$.

Lower Figure: a jammed state with a defect. $\Delta_a = \sigma - \sqrt{\sigma^2 - h^2}$ is the extra length associated with the defect. Note that it interrupts the zigzag structure.
Number of Jammed or Inherent States $S_c(\phi)$ for NN case

$$S_c(\phi) = \ln N_J(\phi) / N.$$
Philosophy of approach

- In theoretical physics we can basically solve exactly one-dimensional models or infinite dimensional models (i.e. mean-field theories).

- Mean-field theories for glasses and jamming e.g. RFOT and glass close-packing involve replica symmetry breaking ideas. The "transitions", e.g. at $\phi_d$, $\phi_K$, $\phi_{GCP}$ probably "avoided" transitions in three dimensions.

- Narrow channels are effectively one-dimensional systems, so only "avoided" transitions can be expected for them too.

- Results from our calculation support an old picture of glassy behaviour where the growth of the long-relaxation times is associated with structural changes in the system, e.g. Charles Frank – icosahedra, Paddy Royall and Williams, Gilles Tarjus etc..

- In our system we can identify the structural features responsible for the growing time scale. It is the growth of zig-zag order.
System can be regarded as a set of hard rods whose distance of closest approach on the $x$-axis is $\sigma(y_i, y_{i+1}) = [\sigma^2 - (y_i - y_{i+1})^2]^{1/2}$. The Helmholtz potential $A_L$ is

$$\exp(-\beta A_L) = \frac{1}{\Lambda^d N!} \int_{-h/2}^{h/2} \prod_i dy_i [L - \sum_{i=1}^{N} \sigma(y_i, y_{i+1})]^N$$

The sum is the total excluded volume of the hard rods. Define the Gibbs potential via

$$\exp(-\beta \Phi) = \int_0^\infty dL \exp(-\beta A_L) \exp(-\beta f L)$$

$f$ is the force on the confining piston which keeps the $N$ disks in a channel of length $L$.

$$\exp(-\beta \Phi) = \frac{1}{(\beta f)^{N+1} \Lambda^d N!} \int_{-h/2}^{h/2} \prod_i dy_i \exp \left( -\beta f \sum_{i=1}^{N} \sigma(y_i, y_{i+1}) \right).$$
NN Transfer Matrix

\[ \lambda_n u_n(y_1) = \int_{-h/2}^{h/2} e^{-\beta f \sigma(y_1, y)} u_n(y) \, dy. \]

As \( N \to \infty \)

\[ \beta \Phi \to -N \ln \left( \lambda_1 / \beta f \Lambda^2 \right). \]

\( \lambda_1 \) is the largest eigenvalue of the integral equation (i.e. transfer matrix). The equation of state is \( L = \partial \Phi / \partial f \).

The next largest eigenvalue \( \lambda_2 \) gives information on the correlation length.

\[ \xi = \frac{1}{\ln(\lambda_1 / |\lambda_2|)}. \]

It describes the decay of the zig-zag correlation:

\[ \langle y_i y_{i+s} \rangle \sim (-1)^s \exp(-s / \xi), \]
Numerically exact equation of state and zig-zag correlation length $\xi$. Red lines are the defect based theory which becomes exact at high densities.
Fluid – fcc crystal first order transition at $\phi_c \approx 0.49$. No genuine phase transitions in one-dimensional channels.

Onset of slow activated dynamics for hard spheres at $\phi > \phi_d = 0.58$. This is normally “explained” by mode-coupling theory. $\phi_d$ marks the onset of caging. There is a $\phi_d$ for the NN channel at $\approx 0.48$.

Random close packing density $\phi_{rcp} \approx 0.64$. A related feature exists for the NNN case of the narrow channel.

$\phi_J$ dependence on compression rate can be understood in the channel.

Numerical work for hard spheres becomes difficult for $\phi > 0.60$. A G-point $\phi_G$ where timescales diverge at finite pressure has been suggested (Berthier and Witten). $S_c$ is supposed to vanish at the Kauzmann density $\phi_K$. The Adam-Gibbs formula is supposed to relate $\tau_\alpha \sim \exp[A/S_c]$.

Do these features arise in narrow channels?
Understanding the equation of state and $\xi$ for the NN case at high densities

At high densities behaviour is controlled by defects. When disks are on opposite sides of the channel the excluded volume is

$$\sigma(1, 2) = \sqrt{\sigma^2 - (h - z_1 - z_2)^2} \approx \sqrt{\sigma^2 - h^2} + \frac{h}{\sqrt{\sigma^2 - h^2}}(z_1 + z_2).$$

($z_i$ denotes the distance of disk $i$ from its confining wall at $y = \pm h/2$).

When the disks are on the same side i.e. within a defect, it is

$$\sigma(1, 2) \approx \sigma + O \left[ \frac{(z_1 - z_2)^2}{\sigma} \right]; \text{ there is no term linear in } z_1 \text{ or } z_2.$$

For $M$ defects, the total excluded volume is

$$\sum_{i=1}^{N-1} \sigma(y_i, y_{i+1}) \approx (N-M) \sqrt{\sigma^2 - h^2} + M\sigma + \sum_{k=1}^{2M} \frac{h z_k}{\sqrt{\sigma^2 - h^2}} + \sum_{k=2M+1}^{N} \frac{2h z_k}{\sqrt{\sigma^2 - h^2}}.$$

We can insert this into the expression for $\exp(-\beta\Phi)$ and integrate the $z_i$ from 0 to $\infty$, with negligible error at large density.
\[ \exp(-\beta \Phi) = \frac{1}{(2\beta f \Lambda^2)^N} \sum_M W_M e^{-\beta f [(N-M)\sqrt{\sigma^2-h^2} + M\sigma]} \left( \frac{\sqrt{\sigma^2-h^2}}{\beta fh} \right)^N 2^{2M}, \]

where the combinatorial factor \( W_M \) is

\[ W_M = \frac{(N-M)!}{M! (N-2M)!}. \]

In the thermodynamic limit we can convert the sum over \( M \) to an integral over \( \theta \), where \( M = \theta N \). Then on using steepest descents, at large \( \beta f \sigma \)

\[ \theta \approx 4 \exp[-\beta f \Delta_a]. \]

\( \Delta_a = \sigma - \sqrt{\sigma^2-h^2} \) is the extra length of the system containing one defect over that of the state of maximum density.

- The work done in increasing the length against the applied force is then \( \Delta E = f \Delta_a \).
- The exponential is of the Boltzmann form \( \exp(-\beta \Delta E) \).
Good agreement with the simulations of Bowles and Saika-Voivod as $\phi \rightarrow \phi_{\text{max}}$. 
The equation of state is

$$\beta f = \frac{2N}{L - N[(1 - \theta)\sqrt{\sigma^2 - h^2} + \theta \sigma]}.$$ 

In the limit $\phi \to \phi_{\text{max}}, \theta \to 0$, so

$$\beta f \approx \frac{2N}{L(1 - \phi/\phi_{\text{max}})},$$

(cf Salsburg and Wood).

The correlation length

$$\xi \approx \frac{1}{8} \exp(\beta f \Delta_a).$$

Notice that $\xi$ is basically the distance between defects $1/\theta$ and grows exponentially rapidly as $\phi \to \phi_{\text{max}}$.

Summary: the static and thermodynamic properties of the NN model can be completely determined. Analysis in terms of defects is an excellent approximation at high densities.
The Structure Factor $S(k_x, k_y)$

Plots are of $\log S(k_x, k_y)$.

$\beta f \sigma = 3.5$, i.e. low density.  

$\beta f \sigma = 7.5$, a density close to $\phi_d$. 

![Graph 1](image1.png)  

![Graph 2](image2.png)
As the density is increased there is growing “crystalline” as well zig-zag order. Results for $\beta f\sigma = 20$. 
Onset of Activated Dynamics in the NN model

One can calculate using molecular dynamics the autocorrelation function

\[ F(t) = \frac{1}{N} \sum_{i=1}^{N} \frac{\langle y_i(0)y_i(t) \rangle}{\langle y_i^2 \rangle}. \]

For \( \phi > \phi_d \approx 0.48 \) (Bowles et al.) the time scales are long and activated.
\( \tau \) is the time for a single defect to move. Data from MD simulation of Bowles and Saika-Voivod, PRE 73, 011503 (2006). **Red line:** transition state theory i.e. activated dynamics.
For three dimensional systems it has been suggested that there is perhaps a growing length scale associated with the growing time scale as $\phi_d$ is approached. Only in mean-field type theories does it truly diverge.

\[ \xi \sim \frac{1}{1 - \phi/\phi_d} \]
The saddle point which has to be passed over to move the defect from (say) (3,4) to (4,5) in red. Extra length at the saddle point is $\Delta_b = \sqrt{4\sigma^2 - h^2} - \sigma - \sqrt{\sigma^2 - h^2}$. Then $1/\tau \sim \exp(-\beta f \Delta_b)$. 
Transition state theory for creating Pairs of Defects

The saddle point for the creation of a pair of defects requires an extra length \( \Delta_c = \sqrt{4\sigma^2 - h^2} + \sigma - 3\sqrt{\sigma^2 - h^2} \). Rate of pair defect creation \( 1/\tau_D \sim \exp(-\beta f \Delta_c) \).
• Defects are typically spaced by $\xi$ and are created and annihilate in pairs.

• When they have moved a distance $\xi$ by a diffusion like process they will typically annihilate.

• Time to annihilation $\tau_D$ is therefore $\sim D\xi^2$, where $D$ is the diffusion coefficient.

• $D \sim \tau_D/\xi^2 \sim 1/\tau$. $D$ is the rate $1/\tau$ for a defect to move a single place.

• Transition state estimates of $\tau_D$ and $\tau$ and the estimates of $\xi$ at large densities are all consistent.
The diameter of the disks is increased at a rate $\gamma = \sigma^{-1} d\sigma/dt$ in the molecular dynamics simulation until the system jams at a packing fraction $\phi_J$.

( Ashwin, Yamchi and Bowles, PRL 110, 145701 (2013)).
- The slower the compression rate, the higher the final jammed density $\phi_J$.
- If there are $M$ defects in the jammed state

$$\phi_J = \frac{N \pi \sigma^2}{4H_d[M\sigma + (N - M)\sqrt{\sigma^2 - h^2}]} = \frac{\pi \sigma^2}{4H_d[\theta \sigma + (1 - \theta)\sqrt{\sigma^2 - h^2}]}.$$  

- The Kibble-Zurek hypothesis: the system will fall out of equilibrium when the rate of compression exceeds the rate at which defects can annihilate, $1/\tau_D$.
- At this point $\theta$ is frozen in and is not changed by the last stages of the LS compression.
- By equating $1/\tau_D(\theta)$ to $\gamma$ we obtain the red line for $\phi_J$ versus $\gamma$.  

The structure factor $S(k_x, k_y)$ of the NN model in the vicinity of $\phi_d$ changes rapidly as a function of $\phi$.

The structure factor of real glasses and hard spheres hardly alters near $\phi_d$. Glasses with very similar structure factors can have very different dynamics (Berthier and Tarjus).

Maybe for them the important changes in the structure causing the change to activated dynamics shows up only in higher correlation functions, reflecting bond angles etc..
The NNN case

$$\left(1 + \frac{\sqrt{3}}{2}\right) \approx 1.8660 \sigma < H_d < 2\sigma: \text{ the NNN case. Figures for } H_d = 1.95\sigma \text{ when } \phi_{\text{max}} \approx 0.8074 \text{ and } \phi_K \approx 0.8053.$$
Configurational Entropy for the NNN case

\[ H_d = 1.95 \sigma, \quad \phi_{max} = 0.8074 \]

(from S. S. Ashwin and R. K. Bowles, PRL 102, 235701 (2009)).
The transfer matrix for the NNN problem is complicated.
Is there a feature in the equation of state associated with the “kink” in $S_c$?

There is an “apparent” divergence of $\frac{1}{\beta F \sigma}$ for $\phi = \phi_K \approx 0.8053 < \phi_{\text{max}}$. 
\( \xi_3 = 1 / \ln(\lambda_1/\lambda_3) \), corresponding to “crystalline” order as in the \( S(k) \) of the hard rod gas as \( \phi \to \phi_{\text{max}} \).

\( \xi_c = 1 / \ln(\lambda_1/|\lambda_c|) \), corresponding to the growth of buckled crystalline order.
(a) The “kink” in $S_c$, (b) the apparent divergence in the pressure (force), and (c) the peak in $\xi_3$ are all close to $\phi = \phi_K$.

There is no true singularity at $\phi_K$: the “transition” is avoided.

Question: Does behaviour near $\phi_K$ mimic what is expected for hard spheres at $\phi_{rcp}$?

At $\phi_{rcp}$, the pressure apparently diverges, just as at $\phi_K$, and the jammed states for $\phi > \phi_{rcp}$ have increasing amounts of fcc order.

The correlation length associated with $\phi_d$ in the NNN model is still the length scale associated with the growing zig-zag order i.e.

$$\xi = 1 / \ln(\lambda_1/|\lambda_2|).$$

There are multiple length scales, e.g. $\xi$, $\xi_3$ and $\xi_c$ (and therefore time) scales in the system.