

Appendix **A**

Reference models

After a century of considerable progress in Statistical Physics, several Hamiltonian have become reference models, because they describe many phenomena using basic assumptions. The purpose of this appendix is to give a non exhaustive list of these models as well as a brief description of their significant properties.

A.1 Lattice models

A.1.1 XY model

The *XY* model is a lattice model where variables are two dimensional vectors. The dimension of the lattice can be one, two or higher. The corresponding Hamiltonian reads

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (\text{A.1})$$

The bracket $\langle i, j \rangle$ denote a double summation where i is an index running over all sites and j over nearest neighbor sites of i (each link of the lattice must be account for once). $\mathbf{S}_i \cdot \mathbf{S}_j$ is a scalar product between vectors \mathbf{S}_i and \mathbf{S}_j . The upper critical dimension of this system is 4 and the Mermin-Wagner theorem [23] prevents finite temperature transition in two dimensions 2 when the order parameter is the magnetization. Indeed, it appears a phase transition at finite temperature associated to the topological defects which undergo a phase transition between a phase where defects are bounded at low temperature as pairs and dissociated at high temperature. (About topological defects in condensed matter physics, see the review rather exhaustive by Mermin[22]). This transition was described by Kosterlitz et Thouless[19].

In two dimensions, this transition is rather smooth, because, the derivatives of the thermodynamic potential are continuous. Signature of the transition can be observed by monitoring the quantity called helicity.

In three dimensions, this transition is continuous as expected. Note that α is negative.

A.1.2 Heisenberg model

The Heisenberg model is a lattice model, where variables are three-dimensional vectors. Formally, the Hamiltonian is given by the equation

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (\text{A.2})$$

with \mathbf{S}_i is a three-dimensional vector, the other parameters are already defined in the XY model. The lower critical dimension is two, where the critical temperature is equal to zero. When temperature is non zero, the magnetization goes to zero. Conversely to the XY model, this system does not exhibit topological defects, because the vectors can rotate in the third dimension[22]. In three dimension, the system has a continuous transition between a paramagnetic phase and a ferromagnetic phase at a finite temperature.

A.1.3 $O(n)$ model

The generalization of these models is simple, because one considers spins described by a n -component vector. There is physical examples described interacting spins where spins are four-dimensional vectors. By considering the general case n , there is theoretical interest: when n goes to infinity, the limit is the spherical model which is solvable in many cases and provides a non trivial phase diagram. Moreover, one has perturbative methods which are able to give quantitative results when n is large ($1/n$ expansion) useful when these results are applied for a given n .

A.2 Off-lattice models

A.2.1 Introduction

In these lecture notes, two simple liquid models have been largely used, namely the hard sphere model and the Lennard-Jones model. The first one accounts for the exclusion effects and has a phase diagram exhibiting a liquid-solid transition (for a dimension greater than two) and the Lennard-Jones

model which has a attractive part of the potential at long distance (which corresponds to Van der Waals forces) has a more complex diagram, which includes a liquid-gas coexistence curve finishing in a critical point. In the dense region, and at low temperature, one finds a line of liquid-solid transition (of first order in three dimensions) finishing in a triple point at low temperature.

A.2.2 StockMayer model

The Lennard-Jones model is suitable for describing neutral atoms or apolar molecules. This situation is obviously too restrictive for describing ubiquitous liquids like polar liquids. For instance, water which is basically composed of H_2O molecules (neglecting at first order the ionic dissociation) has a huge dipole moment. A basic description can be obtained with the Stockmayer Hamiltonian consisting of a Lennard-Jones Hamiltonian with an additional dipole interaction between particles.

$$\mathcal{H} = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + \frac{\epsilon}{2} \sum_{i \neq j}^N \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] + \frac{1}{r_{ij}^3} (\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j - 3\boldsymbol{\mu}_i \cdot \hat{\mathbf{r}}_i \boldsymbol{\mu}_j \cdot \hat{\mathbf{r}}_j) \quad (\text{A.3})$$

A.2.3 Kob-Andersen model

Glassforming liquids show a spectacular increase of the relaxation time when the temperature decreases. This relaxation time increases of 15 orders of magnitude until the system, generally unable to crystallize, becomes in an amorphous state for temperatures below the glass transition and the system remains in non equilibrium state. This transition temperature is not unique, but depends on the tempering rate. No apparent diverging length occurs at the transition, and more generally the structure of amorphous states is similar to that observed in liquids. Because this phenomenon is present for many liquids, one can imagine that simple liquid models can display this transition. But, in three dimensions, simple liquids (hard spheres, Lennard-Jones liquid) easily crystallize and it is difficult to supercool these systems, even if the tempering rate is slow (in simulation, this rate is always quite large compared to experiments). A well-known model which avoids crystallization and can be supercooled is the Kob-Andersen model[16, 18, 17] It corresponds to a mixture of two species of spherical particles interacting with a Lennard-Jones potential

$$v_{\alpha\beta} = 4\epsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r} \right)^6 \right] \quad (\text{A.4})$$

Reference models

The two species are denoted A and B and the species ratio is equal to 80% of A particles and 20% of B particles. Interaction parameters are $\epsilon_{AA} = 1$, $\epsilon_{AB} = 1.5$, and $\epsilon_{BB} = 0.5$, and particle sizes are given by $\sigma_{AA} = 1$, $\sigma_{AB} = 0.8$ and $\sigma_{BB} = 0.88$.

Appendix B

Linear response theory

Consider a system at equilibrium described by the Hamiltonian \mathcal{H}_0 . At time $t = 0$, this system is submitted to an external force and the Hamiltonian \mathcal{H}' is given by

$$\mathcal{H}' = -A(\mathbf{r}^N)F(t) \quad (\text{B.1})$$

where $F(t)$ is an external time-dependent force and $A(\mathbf{r}^N)$ is the variable conjugate to the force F . One assumes that this force goes to zero when $t \rightarrow \infty$ such that the system goes to equilibrium. It is possible to consider a space-dependent force, but for sake of simplicity, we restrict here the analysis to a uniform force.

The time evolution of the system is described by the Liouville equation

$$\frac{\partial f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t)}{\partial t} = -i\mathcal{L}f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t) \quad (\text{B.2})$$

$$= \{\mathcal{H}_0 + \mathcal{H}', f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t)\} \quad (\text{B.3})$$

$$= -i\mathcal{L}_0 f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t) - \{A, f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t)\}F(t) \quad (\text{B.4})$$

where \mathcal{L}_0 denotes the Liouville operator associated with \mathcal{H}_0

$$\mathcal{L}_0 = i\{\mathcal{H}_0, \} \quad (\text{B.5})$$

Because the system was initially at equilibrium, one has

$$f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, 0) = C \exp(-\beta\mathcal{H}_0(\mathbf{r}^N, \mathbf{p}^N)), \quad (\text{B.6})$$

where C is a normalization constant. Since the external force is weak, one performs a perturbative expansion of equation (B.4) to first order. One writes

$$f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t) = f_0^{(N)}(\mathbf{r}^N, \mathbf{p}^N) + f_1^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t) \quad (\text{B.7})$$

To the lowest order, one has

$$\frac{\partial f_1^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t)}{\partial t} = -i\mathcal{L}_0 f_1^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t) - \{A(\mathbf{r}^N), f_0^{(N)}(\mathbf{r}^N, \mathbf{p}^N)\} F(t). \quad (\text{B.8})$$

Equation (B.8) is solved formally with the initial condition given by equation (B.6). This gives

$$f_1^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t) = - \int_{-\infty}^t \exp(-i(t-s)\mathcal{L}_0) \{A, f_0^{(N)}\} F(s) ds. \quad (\text{B.9})$$

Therefore, the variable $\langle \Delta B(t) \rangle = \langle B(t) \rangle - \langle B(-\infty) \rangle$ evolves as

$$\langle \Delta B(t) \rangle = \int \int d\mathbf{r}^N d\mathbf{p}^N \left(f^{(N)}(\mathbf{r}^N, \mathbf{p}^N, t) - f_0^{(N)}(\mathbf{r}^N, \mathbf{p}^N) \right) B(\mathbf{r}^N) d\mathbf{r}^N d\mathbf{p}^N. \quad (\text{B.10})$$

To lowest order, the difference of Liouville distributions is given by equation (B.9) and equation (B.10) becomes

$$\langle \Delta B(t) \rangle = - \int \int d\mathbf{r}^N d\mathbf{p}^N \int_{-\infty}^t \exp(-i(t-s)\mathcal{L}_0) \{A, f_0^{(N)}\} B(\mathbf{r}^N) F(s) ds \quad (\text{B.11})$$

$$= - \int \int d\mathbf{r}^N d\mathbf{p}^N \int_{-\infty}^t \{A, f_0^{(N)}\} \exp(i(t-s)\mathcal{L}_0) B(\mathbf{r}^N) F(s) ds \quad (\text{B.12})$$

by using the fact that the Liouville operator is Hermitian.

Calculating the Poisson bracket, one obtains that

$$\{A, f_0^{(N)}\} = \sum_{i=1}^N \left(\frac{\partial A}{\partial \mathbf{r}_i} \frac{\partial f_0^{(N)}}{\partial \mathbf{p}_i} - \frac{\partial A}{\partial \mathbf{p}_i} \frac{\partial f_0^{(N)}}{\partial \mathbf{r}_i} \right) \quad (\text{B.13})$$

$$= -\beta \sum_{i=1}^N \left(\frac{\partial A}{\partial \mathbf{r}_i} \frac{\partial \mathcal{H}_0^{(N)}}{\partial \mathbf{p}_i} - \frac{\partial A}{\partial \mathbf{p}_i} \frac{\partial \mathcal{H}_0^{(N)}}{\partial \mathbf{r}_i} \right) f_0^{(N)} \quad (\text{B.14})$$

$$= -\beta i \mathcal{L}_0 A f_0^{(N)} \quad (\text{B.15})$$

$$= -\beta \frac{dA(0)}{dt} f_0^{(N)} \quad (\text{B.16})$$

By inserting equation (B.16) in Eq. (B.12), one has

$$\langle \Delta B(t) \rangle = \beta \int \int d\mathbf{r}^N d\mathbf{p}^N f_0^{(N)} \int_{-\infty}^t \frac{dA(0)}{dt} \exp(-i(t-s)\mathcal{L}_0) B(\mathbf{r}^N) F(s) ds \quad (\text{B.17})$$

By using the fact that

$$B(\mathbf{r}^N(t)) = \exp(it\mathcal{L}_0)B(\mathbf{r}^N(0)) \quad (\text{B.18})$$

Eq. (B.17) becomes

$$\langle \Delta B(t) \rangle = \beta \int_{-\infty}^t ds \left\langle \frac{dA(0)}{dt} B(t-s) \right\rangle F(s) \quad (\text{B.19})$$

One defines the linear response function of B with respect to F as

$$\langle \Delta B(t) \rangle = \int_{-\infty}^{\infty} ds \chi(t,s) F(s) + \mathcal{O}(F^2) \quad (\text{B.20})$$

With Eq. (B.19), one finds the following properties

1. By equating Eqs. (B.19) and (B.20), one obtains the fluctuation-dissipation theorem

$$\chi(t) = \begin{cases} -\beta \frac{d}{dt} \langle A(0)B(t) \rangle & t > 0 \\ 0 & t < 0 \end{cases} \quad (\text{B.21})$$

2. A system cannot respond to a perturbation before it is applied. This property is a consequence of the causality.

$$\chi(t,s) = 0, \quad t - s \leq 0 \quad (\text{B.22})$$

3. The equilibrium response function is translationally invariant in time

$$\chi(t,s) = \chi(t-s) \quad (\text{B.23})$$

When $A = B$, one denotes the autocorrelation function as

$$C_A(t) = \langle A(0)A(t) \rangle, \quad (\text{B.24})$$

and we have

$$\chi(t) = \begin{cases} -\beta \frac{dC_A(t)}{dt} & t > 0 \\ 0 & t < 0 \end{cases} \quad (\text{B.25})$$

By defining the linear response as

$$R(t) = \int_0^t \chi(s) ds \quad (\text{B.26})$$

The fluctuation-dissipation theorem is expressed as

$$R(t) = \begin{cases} \beta(C_A(0) - C_A(t)) & t > 0 \\ 0 & t < 0 \end{cases} \quad (\text{B.27})$$

Appendix C

Ewald sum for the Coulomb potential

Ewald sum

Let us consider N charged particles. The system has a total charge equal to 0, $\sum_i q_i = 0$, in a simulation cell with periodic boundary conditions. A particle i at the position \mathbf{r}_i in the reference box corresponds to an infinity of images located in the replica of this original box and labeled with the coordinates $\mathbf{r}_i + \mathbf{n}L$, where \mathbf{n} is a vector whose components (n_x, n_y, n_z) are integer. The total energy of the system reads

$$U_{coul} = \frac{1}{2} \sum_{i=1}^N q_i \phi(\mathbf{r}_i), \quad (\text{C.1})$$

where $\phi(\mathbf{r}_i)$ is the electrostatic potential at site i ,

$$\phi(\mathbf{r}_i) = \sum_{j, \mathbf{n}}^* \frac{q_j}{|\mathbf{r}_{ij} + \mathbf{n}L|}. \quad (\text{C.2})$$

L'étoile indique que la somme est faite sur toutes les boîtes et sur toutes les particules, hormis $j = i$ quand $\mathbf{n} = 0$.

Pour des potentiels à courte portée (décroissance plus rapide que $1/r^3$), l'interaction entre deux particules i et j est en très bonne approximation calculée comme l'interaction entre la particule i et l'image de j la plus proche de i (convention d'image minimale). Cela signifie que cette image n'est pas nécessairement dans la boîte initiale. Dans le cas de potentiels à longue portée, cette approximation n'est pas suffisante car l'énergie d'interaction entre deux particules décroît trop lentement pour qu'on puisse se limiter à la première image. Dans le cas des potentiels coulombiens, il est même

nécessaire de tenir compte de l'ensemble des boîtes, ainsi que de la nature des conditions aux limites à l'infini.

Pour remédier à cette difficulté, la méthode des sommes d'Ewald consiste à séparer (C.1) en plusieurs parties: une partie à courte portée, obtenue en écrantant chaque particule avec une distribution de charge (que l'on prend souvent gaussienne) de même intensité mais de signe opposé à celle de la particule (sa contribution pourra alors être calculée avec la convention d'image minimale) et une autre à longue portée, due à l'introduction d'une distribution de charge symétrique à la précédente et dont la contribution sera calculée dans l'espace réciproque du réseau cubique. De la forme plus ou moins diffuse de la distribution de charge dépendra la convergence de la somme dans l'espace réciproque.

Si on introduit comme distribution de charge une distribution gaussienne,

$$\rho(\mathbf{r}) = \sum_{j=1}^N \sum_{\mathbf{n}} q_j \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \exp[-\alpha|\mathbf{r} - (\mathbf{r}_j + \mathbf{nL})|^2], \quad (\text{C.3})$$

la partie à courte portée est donnée par

$$U_1 = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \sum_{\mathbf{n}} q_i q_j \frac{\text{erfc}(\alpha|\mathbf{r}_{ij} + \mathbf{nL}|)}{|\mathbf{r}_{ij} + \mathbf{nL}|}, \quad (\text{C.4})$$

où la somme sur \mathbf{n} est tronquée à la première image et où erfc est la fonction erreur complémentaire, et la partie à longue portée par

$$U_2 = \frac{1}{2\pi L^3} \sum_{i=1}^N \sum_{j=1}^N \sum_{\mathbf{k} \neq 0} q_i q_j \left(\frac{4\pi^2}{k^2}\right) \exp\left(\frac{-k^2}{4\alpha}\right) \cos(\mathbf{k}\mathbf{r}_{ij}). \quad (\text{C.5})$$

A cette dernière expression, on doit retirer un terme dit d'auto-interaction dû à l'interaction de chaque distribution de charge q_j avec la charge ponctuelle située au centre de la gaussienne. Le terme à retirer est égal à

$$\frac{\alpha}{\pi^{1/2}} \sum_{i=1}^N q_i^2 = -U_3. \quad (\text{C.6})$$

L'énergie d'interaction coulombienne devient donc:

$$U_{coul} = U_1 + U_2 + U_3. \quad (\text{C.7})$$

Pour des charges (ou spins, ou particules) placées sur les sites d'un réseau, il est possible d'effectuer les sommes dans l'espace réciproque une fois pour

toutes, au début de chaque simulation. Il est donc possible de prendre en compte un très grand nombre de vecteurs d'ondes, ce qui assure une très bonne précision pour le calcul de l'énergie coulombienne.

Dans le cas de systèmes continus, on doit effectuer le calcul dans l'espace à chaque fois que les particules sont déplacées, ce qui fait que l'algorithme est pénalisant pour les grands systèmes. Il existe alors des algorithmes plus performants comme ceux basés sur un développement multipolaire.

Remarks

La somme dans l'expression (C.5) n'est effectuée que pour $\mathbf{k} \neq 0$. Ceci résulte de la convergence conditionnelle des sommes d'Ewald et a des conséquences physiques importantes. Dans un système coulombien périodique, la forme de l'énergie dépend en effet de la nature des conditions aux limites à l'infini et le fait de négliger la contribution à l'énergie correspondant à $\mathbf{k} = 0$ revient à considérer que le système est plongé dans un milieu de constante diélectrique infinie (c'est à dire un bon conducteur). C'est la convention qui est utilisée dans les simulations de systèmes ioniques. Dans le cas inverse, c'est à dire si le système se trouve dans un milieu diélectrique, les fluctuations du moment dipolaire du système créent des charges de surface qui sont responsables de l'existence d'un champ dépolarisant. Celui-ci rajoute un terme à l'énergie qui n'est autre que la contribution correspondant à $\mathbf{k} \neq 0$.

Appendix **D**

Hard rod model

D.1 Equilibrium properties

Let us consider a system with N hard core segments of identical length, σ , moving onto a straight line. The Hamiltonian of this system reads

$$\mathcal{H} = \sum_i^N \left(\frac{1}{2} m \left(\frac{dx_i}{dt} \right)^2 + v(x_i - x_j) \right) \quad (\text{D.1})$$

where

$$v(x_i - x_j) = \begin{cases} +\infty & |x_i - x_j| > \sigma \\ 0 & |x_i - x_j| \leq \sigma. \end{cases} \quad (\text{D.2})$$

The partition function can be factorized (like all classical systems) into two parts: the first one corresponds to the kinetic contribution and can be easily calculated (Gaussian integrals), the second one is the configuration integral which, in one dimension, can be also calculated exactly. One has

$$Q_N(L, N) = \int \dots \int \prod_{dx_i} \exp(-\beta/2 \sum_{i \neq j} v(x_i - x_j)). \quad (\text{D.3})$$

As the potential is equal to zero or infinity, the configuration integral is independent of the temperature. Because two particles cannot overlap, one can write the integral Q_N by labeling the particles:

$$Q_N(L, N) = \int_0^{L-N\sigma} dx_1 \int_{x_1+\sigma}^{L-(N-1)\sigma} \dots \int_{x_{N-1}+\sigma}^{L-\sigma} dx_N. \quad (\text{D.4})$$

When all integrations are performed equation (D.4) gives

$$Q_N(L, N) = (L - N\sigma)^N. \quad (\text{D.5})$$

The canonical partition function of the system is thus determined and the equation of state is given by the relation

$$\beta P = \frac{\ln Q_N(L, N)}{L} \quad (\text{D.6})$$

which gives

$$\frac{\beta P}{\rho} = \frac{1}{1 - \sigma\rho} \quad (\text{D.7})$$

where $\rho = N/L$.

The excess chemical potential is given by the relation

$$\exp(-\beta\mu_{ex}) = (1 - \rho) \exp\left(-\frac{\rho}{1 - \rho}\right). \quad (\text{D.8})$$

The correlation functions can be calculated analytically.

D.2 Parking model

The Random sequential addition is a stochastic process where hard particles are added sequentially to a space of dimension D with random positions with the restriction that a new particle can be inserted only if no overlap with previously adsorbed particles exists. Once inserted, the new particle cannot move on the surface.

The one-dimensional version of the model is known as the parking model and was introduced by a Hungarian mathematician, A. Rényi, in 1963[25].

Hard rods of length σ are dropped randomly and sequentially onto a line following the rules given above. If $\rho(t)$ denotes the particle density onto the line at time t , kinetics is described by the following master equation:

$$\frac{\partial\rho(t)}{\partial t} = k_a\Phi(t), \quad (\text{D.9})$$

where k_a is a constant particle flux (which can be set as a time unit) and $\Phi(t)$, which is the insertion probability at time t , is also the available line fraction for inserting a new particle at time t . Particle diameter is chosen as a unit length.

It is useful to introduce the distribution function of intervals $G(h, t)$, which is defined as follows: $G(h, t)dh$ denotes the void density of length comprised between h and $h + dh$ at time t . For an interval of length h , the available space for inserting a new particle is equal to $h - 1$, and consequently,

the available line fraction $\Phi(t)$ is simply the sum of $(h - \sigma)$ over all available intervals, i.e. $G(h, t)$:

$$\Phi(t) = \int_{\sigma}^{\infty} dh(h - 1)G(h, t). \quad (\text{D.10})$$

Since each interval corresponds to a particle, the particle density $\rho(t)$ reads

$$\rho(t) = \int_0^{\infty} dhG(h, t), \quad (\text{D.11})$$

whereas the complementary fraction of the coverage is related to the distribution function of intervals $G(h, t)$ by the relation

$$1 - \rho(t) = \int_0^{\infty} dhG(h, t). \quad (\text{D.12})$$

The above two equations are sum rules of the interval distribution function. During the process, the function $G(h, t)$ evolves as

$$\frac{\partial G(h, t)}{\partial t} = -H(h - 1)(h - 1)G(h, t) + 2 \int_{h+1}^{\infty} dh'G(h', t), \quad (\text{D.13})$$

where $H(x)$ is the Heaviside function. The first term of the right-hand side of equation (D.13) (loss term) corresponds to a particle insertion within a interval of length h (for $h \geq 1$), whereas the second term of the right-hand side of equation (D.13) (creation term) corresponds to the insertion in a interval of length $h' > h + 1$. The factor 2 comes from the two possibilities of creating an interval of length h from an larger interval of length h' . Note that the interval distribution function $G(h, t)$ is conditioned by the existence of intervals larger than h .

We now have a closed set of equations, resulting from the screening property, namely that a particle insertion in a given interval has no effect on other intervals. The partial differential equations can be solved by using the following ansatz, for $h > 1$,

$$G(h, t) = F(t) \exp(-(h - 1)t), \quad (\text{D.14})$$

which leads

$$F(t) = t^2 \exp\left(-2 \int_0^t du \frac{1 - e^{-u}}{u}\right). \quad (\text{D.15})$$

Integrating equation (D.13) by using the solution of $G(h, t)$ for $h > 1$, one gets $G(h, t)$ for $0 < h < 1$,

$$G(h, t) = 2 \int_0^t du \exp(-uh) \frac{F(u)}{u}. \quad (\text{D.16})$$

The three equations (D.10), (D.11) and (D.12) obviously lead to the same result for the density $\rho(t)$,

$$\rho(t) = \int_0^t du \exp\left(-2 \int_0^u dv \frac{1 - e^{-v}}{v}\right). \quad (\text{D.17})$$

This result was first obtained by Rényi.

A non trivial property of this model is the existence of a jamming limit (when $t \rightarrow \infty$) with a density $\rho_\infty \sigma = 0.7476\dots$; this density is significantly smaller than the maximum saturation density ($\rho_\infty = 1$) obtained when particles can move on the line. Moreover, it is easy to see that the jamming limit depends on the initial conditions. Here, the line was empty. Conversely, at equilibrium, the final state of the system is only determined by the chemical potential and has no memory of the initial configuration.

The long time kinetics can be obtained from equation (D.17):

$$\rho_\infty - \rho(t) \simeq \frac{e^{-2\gamma}}{t} \quad (\text{D.18})$$

where γ is the Euler constant, which shows that the long time kinetics has an algebraic scaling law.

Configurations obtained by this irreversible process have non trivial properties. At saturation, the interval distribution function has a (integrable) logarithmic divergence at contact $h \rightarrow 0$,

$$G(h, \infty) \simeq -e^{-2\gamma} \ln(h). \quad (\text{D.19})$$

In addition, pair correlations are extremely short ranged

$$g(r) - 1 \propto \frac{1}{\Gamma(r)} \left(\frac{2}{\ln r}\right)^r \quad (\text{D.20})$$

where $\Gamma(x)$ is the Gamma function : $g(r)$ decays super-exponentially and then is different from equilibrium where $g(r)$ decays exponentially.

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