the mean energy $\langle E \rangle_\beta$ at the temperature $T = 1/\beta$ is obtained by calculating the integral.

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where the summation is performed over $N_c$ configurations at equilibrium.
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$C_v$ is given by $k_b \beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$.
Time driven algorithm

\[\langle A \rangle = \frac{1}{t} \sum_{0}^{t} A(t') dt'\] (3)

One assumes an ergodicity time smaller than the simulation time.

Event-driven algorithm

\[\langle A \rangle = \frac{1}{T_{N_{c}}} \sum_{i}^{N_{c}} A_{i} t_{i}\] (4)

where \(t_{i}\) is time interval between the \(i\)th and \((i+1)\)th event (collision).
Molecular Dynamics

Time driven algorithm

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Spatial correlation functions

- Point particle system: \( N \) identical particles
Correlation functions

Spatial correlation functions

- Point particle system: \( N \) identical particles
- Microscopic density

\[
\rho(r) = \sum_{i=1}^{N} \delta(r - r_i)
\]
Spatial correlation functions

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- Microscopic density

\[
\rho(r) = \sum_{i=1}^{N} \delta(r - r_i)
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- Microscopic pair density

\[
\rho(r, r') = \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \delta(r - r_i) \delta(r' - r_j)
\]
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- Take the average over "similar" configurations \( \overline{\rho(r)} = \langle \rho(r) \rangle \)
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$$\overline{\rho(r)} = N \int \cdots \int \exp(-\beta V(r^N)) dr^{N-1} \overline{Z_N(V, T)}$$
Correlation functions

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  \[
  \overline{\rho(r, r')} = N(N - 1) \int \cdots \int \frac{\exp(-\beta V(r^N))}{Z_N(V, T)} dr^{N-2}
  \]
Correlation functions

Spatial correlation functions

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  $$\overline{\rho(r)} = N \int \ldots \int \exp(-\beta V(r^N)) dr^{N-1} \frac{1}{Z_N(V, T)}$$
- For the Microscopic pair density
  $$\overline{\rho(r, r')} = N(N - 1) \int \ldots \int \exp(-\beta V(r^N)) dr^{N-2} \frac{1}{Z_N(V, T)}$$
- Sum rules
  $$\int \overline{\rho(r)} dr = N$$
  $$\int \overline{\rho(r, r')} dr dr' = N(N - 1)$$
Spatial correlation functions

- The pair distribution function is defined as (I remove the overline notation)

\[ g(r, r') = \frac{\rho(r, r')}{\rho(r)\rho(r')} \]
Spatial correlation functions

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For an isotropic and homogeneous system,

\[ g(r, r) = g(|r - r'|) \]
Implementation in a simulation.

- When the distance $|r - r'|$ is large, the radial distribution function goes to $1 - \frac{1}{N}$.
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For an homogeneous system and homogeneous system,

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\rho^2 g(|r - r'|) = \langle \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \delta(r - r_i) \delta(r' - r_j) \rangle
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$$

Using the change of variable $r, r' \rightarrow r, s = r' - r$ and integrating over $r$

$$
\rho g(s) = \frac{1}{N} \langle \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \delta(s - r_i + r_j) \rangle
$$
Implementation in a simulation.

- In a simulation box in 3D, space discretization of \( g(r) \)

\[
\rho g(\Delta r(j + 0.5)) = \frac{1}{N(V_{j+1} - V_j)} 2N_p(r),
\]

where \( N_p(r) \) is the number of distinct pairs whose center to center distances are between \( j\Delta r \) and \( (j + 1)\Delta r \) and where \( V_j = \frac{4\pi}{3}((j + 1)\Delta r)^3 \).
Implementation in a simulation.

- In a simulation box in 3D, space discretization of $g(r)$

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where $N_p(r)$ is the number of distinct pairs whose center to center distances are between $j\Delta r$ and $(j + 1)\Delta r$ and where $V_j = \frac{4\pi}{3} ((j + 1)\Delta r)^3$.

- The maximum distance of $g(r)$ is the half of the linear size of the simulation box.
Structure factor

**Definition**

\[ S(k) = \frac{1}{N} \langle \rho_k \rho_{-k} \rangle \]

where \( \rho_k \) is the Fourier transform of the microscopic density \( \rho(r) \).
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- Due to the periodic boundary conditions, the wavelengths are discretized \( k = \pm n\pi/L \) where \( n \) is an integer.

\[
S(k) = 1 + \frac{1}{N} \left\langle \int \int \exp(-ik(r - r')) \sum_{i=1}^{N} \sum_{j=1,\, i \neq j} \delta(r - r_i)\delta(r - r_j) \, dr \, dr' \right\rangle
\]

which gives

\[
S(k) = 1 + \frac{1}{N} \int \int \exp(-ik(r - r')) \rho(r, r') \, dr \, dr'.
\]
For an isotropic and uniform fluid

\[ S(k) = 1 + \frac{\rho^2}{N} \int \int \exp(-ik(r-r')) g(r,r') dr dr' \]

The radial distribution function only depends on \(|r-r'|\). One then obtains

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The Fourier transform only depends on the modulus \(|k|

\[ S(k) = 1 + 2\pi\rho \int r^2 g(r) \int_0^\pi \exp(-ikr \cos(\theta)) \sin(\theta) d\theta dr \]

\[ S(k) = 1 + 4\pi\rho \int_0^\infty r^2 g(r) \frac{\sin(kr)}{kr} dr. \]
For the Ising model, one defines the spin-spin time correlation function

\[ C(t) = \frac{1}{N} \sum_{i=1}^{N} \langle S_i(0)S_i(t) \rangle \]
For the Ising model, one defines the spin-spin time correlation function

\[ C(t) = \frac{1}{N} \sum_{i=1}^{N} \langle S_i(0)S_i(t) \rangle \]

For a simple liquid made of point particles, the density autocorrelation function is

\[ C(t) = \frac{1}{V} \int dr \langle \delta \rho(r, t)\delta \rho(r, 0) \rangle \] (5)

where \( \delta \rho(r, t) \) denotes the local density fluctuation. This autocorrelation function
Time average of a correlation function (or others quantities) at equilibrium uses a fundamental property of equilibrium systems, namely, time translational invariance. In other words, if one calculates $\langle S_i(t')S_i(t' + t) \rangle$, the result is independent of $t'$. Define a timestep for $C(t)$, define a matrix of $N_c$ columns and $N$ rows ($N$ is the total number of spins), and once equilibrated, one defines a real vector of $N_c$ components for $C(t)$.
Time correlation functions

Implementation

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- In other words, if one calculates $\langle S_i(t')S_i(t' + t) \rangle$, the result is independent of $t'$.

\[
C(t) = \frac{1}{NM} \sum_{j=1}^{M} \sum_{i=1}^{N} S_i(t_j)S_i(t_j + t).
\]

- Define a timestep for $C(t)$.

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$$C(t) = \frac{1}{NM} \sum_{j=1}^{M} \sum_{i=1}^{N} S_i(t_j)S_i(t_j + t).$$

- $\tau_{eq} \ll N_c \Delta t_c \ll T_{sim}$ (6)
Consider a system at equilibrium described by the Hamiltonian $\mathcal{H}_0$. At time $t = 0$, an external force $F(t)$ is applied and the additional Hamiltonian $\mathcal{H}'$ is given by

$$\mathcal{H}' = -A(r^N) F(t)$$

where $A(r^N)$ is the conjugate variable.
Consider a system at equilibrium described by the Hamiltonian $H_0$. At time $t = 0$, an external force $F(t)$ is applied and the additional Hamiltonian $H'$ is given by

$$H' = -A(r^N)F(t)$$

where $A(r^N)$ is the conjugate variable.

$F(t) \to 0$ when $t \to \infty$

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

$$\frac{\partial f^{(N)}(r^N, p^N, t)}{\partial t} = -i\mathcal{L}f^{(N)}(r^N, p^N, t)$$

$$= \{H_0 + H', f^{(N)}(r^N, p^N, t)\}$$

$$= - i\mathcal{L}_0 f^{(N)}(r^N, p^N, t) - \{A, f^{(N)}(r^N, p^N, t)\}F(t)$$
Implementation

Because the system was initially at equilibrium, one has

\[ f^{(N)}(r^N, p^N, 0) = C \exp(-\beta \mathcal{H}_0(r^N, p^N)), \]
Because the system was initially at equilibrium, one has

\[ f^{(N)}(r^N, p^N, 0) = C \exp(-\beta \mathcal{H}_0(r^N, p^N)), \]

Since the external force is weak, one performs a perturbative expansion of \( f^{(N)}(r^N) \) around equilibrium. One writes

\[ f^{(N)}(r^N, p^N, t) = f_0^{(N)}(r^N, p^N) + f_1^{(N)}(r^N, p^N, t) \]

\[ f_1^{(N)}(r^N, p^N, t) = -\int_{-\infty}^{t} \exp(-i(t - s)\mathcal{L}_0)\{A, f_0^{(N)}\} F(s) ds. \]
Therefore, the variable $\langle \Delta B(t) \rangle = \langle B(t) \rangle - \langle B(-\infty) \rangle$ evolves as

$$\langle \Delta B(t) \rangle = \int \int dr^N dp^N \left( f^{(N)}(r^N, p^N, t) - f_0^{(N)}(r^N, p^N) \right) B(r^N) dr^N dp^N.$$
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$$\langle \Delta B(t) \rangle = - \int \int dr^N dp^N \int_{-\infty}^{t} \exp(-i(t - s)\mathcal{L}_0) \{ A, f_0^{(N)} \} B(r^N) F(s) ds$$

$$= - \int \int dr^N dp^N \int_{-\infty}^{t} \{ A, f_0^{(N)} \} \exp(i(t - s)\mathcal{L}_0) B(r^N) F(s) ds$$
Calculating the Poisson bracket, one obtains that

\[
\{ A, f_0^{(N)} \} = \sum_{i=1}^{N} \left( \frac{\partial A}{\partial r_i} \frac{\partial f_0^{(N)}}{dp_i} - \frac{\partial A}{\partial p_i} \frac{\partial f_0^{(N)}}{dr_i} \right)
\]

\[
= -\beta \sum_{i=1}^{N} \left( \frac{\partial A}{\partial r_i} \frac{\partial H_0^{(N)}}{dp_i} - \frac{\partial A}{\partial p_i} \frac{\partial H_0^{(N)}}{dr_i} \right) f_0^{(N)}
\]

\[
= -\beta i L_0 A f_0^{(N)}
\]

\[
= -\beta \frac{dA(0)}{dt} f_0^{(N)}
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\]

\[
= - \beta i \mathcal{L}_0 A f_0^{(N)}
\]

\[
= - \beta \frac{dA(0)}{dt} f_0^{(N)}
\]

Using

\[
B(r^N(t)) = \exp(it\mathcal{L}_0)B(r^N(0))
\]

\[
\langle \Delta B(t) \rangle = \beta \int_{-\infty}^{t} ds \left\langle \frac{dA(0)}{dt} B(t - s) \right\rangle F(s)
\]
\[ \langle \Delta B(t) \rangle = \int_{-\infty}^{\infty} ds \chi(t, s)F(s) + O(F^2) \]

where \( \chi(t, s) \) is the response function.
Linear response theory: results and transport coefficients

\[ \langle \Delta B(t) \rangle = \int_{-\infty}^{\infty} ds \chi(t, s) F(s) + \mathcal{O}(F^2) \]

where \( \chi(t, s) \) is the response function

\[
\chi(t) = \begin{cases} 
-\beta \frac{d}{dt} \langle A(0) B(t) \rangle & t > 0 \\
0 & t < 0
\end{cases}
\]

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

2. \( \chi(t, s) = 0, \quad t - s \leq 0 \)

3. The equilibrium response function is translationally invariant in time

\[ \chi(t, s) = \chi(t - s) \]
When $A = B$, the autocorrelation function is

$$C_A(t) = \langle A(0)A(t) \rangle,$$

and we have

$$\chi(t) = \begin{cases} 
-\beta \frac{dC_A(t)}{dt} & t > 0 \\
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When \( A = B \), the autocorrelation function is

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\chi(t) = \begin{cases} 
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0 & t < 0 
\end{cases}
\]

By defining the linear integrated response as

\[
R(t) = \int_0^t \chi(s)ds
\]

The fluctuation-dissipation theorem is expressed as

\[
R(t) = \begin{cases} 
\beta(C_A(0) - C_A(t)) & t > 0 \\
0 & t < 0 
\end{cases}
\]
Van Hove function

\[ \rho G(r, r'; t) = \langle \rho(r' + r, t) \rho(r', 0) \rangle \]
Space-time correlation functions

Van Hove function

\[ \rho G(r, r'; t) = \langle \rho(r' + r, t)\rho(r', 0) \rangle \]

This function can be expressed from the microscopic densities as

\[ \rho G(r, r'; t) = \left\langle \sum_{i=1}^{N} \sum_{j=1}^{N} \delta(r' + r - r_i(t))\delta(r - r_j(0)) \right\rangle \]
**Van Hove function**

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\]

For a homogeneous system, \( G(r, r'; t) \) only depends on the relative distance. Integrating over volume, one obtains

\[
G(r, t) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sum_{j=1}^{N} \delta(r - r_i(t) + r_j(0)) \right\rangle
\]
Van Hove function

At $t = 0$, the Van Hove function $G(r, t)$ is simplified and one obtains

$$G(r, 0) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sum_{j=1}^{N} \delta(r + r_i(0) - r_j(0)) \right\rangle$$

$$= \delta(r) + \rho g(r)$$
Space-time correlation functions

Van Hove function

Function splitting

\[ G(r, t) = G_s(r, t) + G_d(r, t) \]

with

\[ G_s(r, t) = \frac{1}{N} \langle \sum_{i=1}^{N} \delta((r + r_{i}(0) - r_{i}(t))) \rangle \]

and

\[ G_d(r, t) = \frac{1}{N} \langle \sum_{i \neq j} \delta(r + r_{j}(0) - r_{i}(t)) \rangle \]
**Van Hove function**

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Physical interpretation
Van Hove function

- Normalization rules

\[ \int d\mathbf{r} G_s(\mathbf{r}, t) = 1 \]

In the long time limit, the system loses memory of the initial configuration and the correlation functions becomes independent of the distance \( r \).

\[ \lim_{r \to \infty} G_s(\mathbf{r}, t) = \lim_{t \to \infty} G_s(\mathbf{r}, t) \approx 1 \]

\[ \lim_{r \to \infty} G_d(\mathbf{r}, t) = \lim_{t \to \infty} G_s(\mathbf{r}, t) \approx N - 1 \]
Space-time correlation functions

Van Hove function

- Normalization rules

\[ \int dr G_s(r, t) = 1 \]

\[ \int dr G_d(r, t) = N - 1 \]
Van Hove function

- Normalization rules
  \[ \int dr G_s(r, t) = 1 \]
  \[ \int dr G_d(r, t) = N - 1 \]

- In the long time limit, the system loses memory of the initial configuration and the correlation functions become independent of the distance \( r \).
  \[ \lim_{r \to \infty} G_s(r, t) = \lim_{t \to \infty} G_s(r, t) \simeq \frac{1}{V} \simeq 0 \]
  \[ \lim_{r \to \infty} G_d(r, t) = \lim_{t \to \infty} G_s(r, t) \simeq \frac{N - 1}{V} \simeq \rho \]
Intermediate scattering function

\[ F(k, t) = \int dk G(r, t) e^{-ik \cdot rt} \]
Space-time correlation functions

Intermediate scattering function

\[ F(k, t) = \int d^3k G(r, t) e^{-i k \cdot r} \]

self part of the function

\[ F_s(k, t) = \int d^3k G_s(r, t) e^{-i k \cdot r} \]
Intermediate scattering function

\[ F(k, t) = \int dkG(r, t)e^{-ik.r}t \]

- self part of the function

\[ F_s(k, t) = \int dkG_s(r, t)e^{-ikrt} \]

- distinct part of the function

\[ F_d(k, t) = \int dkG_d(r, t)e^{-ikrt} \]
Space-time correlation functions

Dynamic structure factor

\[ S(k, \omega) = \int dt F(k, t) e^{i\omega t} \]
Space-time correlation functions

Dynamic structure factor

\[ S(k, \omega) = \int dt F(k, t) e^{i \omega t} \]

- Evident sum rule

\[ \int d\omega S(k, \omega) = S(k) \]
Dynamic structure factor

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- To be continued... 4—point correlation function, point-to-set function...