Extended Dynamical Equations of the Period Vectors of Crystals under Constant External Stress to Many-body Interactions

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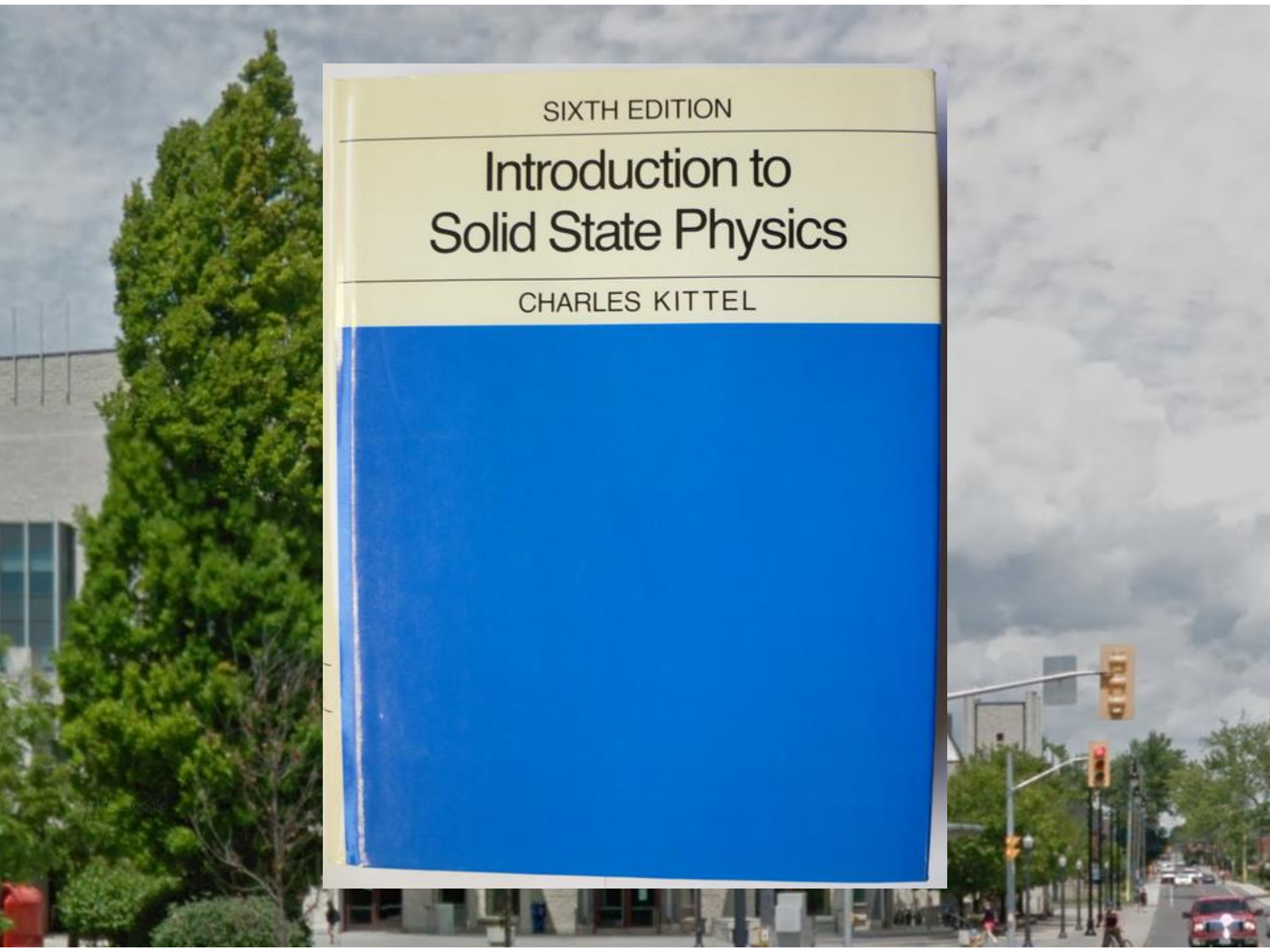
SIXTH EDITION
Introduction to
Solid State Physics
CHARLES KITTEL

As shown in most solid state physics books, crystals are made of periodic structures in space.

Then all position vectors of particles in one cell, and the three period vectors are the full degrees of freedom of the whole system.

The period vectors, I call here, are the cell edge vectors, and also known as the basic vectors or primitive translation vectors.

What about the period vectors?

In classical physics, the dynamics of particles is described by Newton's second law.

The period vectors can be determined by minimizing (Gibbs) free energy or enthalpy for crystals under constant external pressure.

What about the general situation with constant external stress?

As a matter of fact, external stress

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will definitely cause its internal structure to change

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Molecular dynamics (MD) simulations have been widely used with the periodic boundary condition applied, then the whole system becomes a crystal.

Then we face the same basic physics problem to determine the period vectors theoretically in MD.

A great amount of effort has been devoted to derive the dynamics of the period vectors. Since the Lagrangian/Hamiltonian Dynamics is used, dynamical equations of the particles are re-generated as well.

Three typical problems in the effort

The re-generated dynamical equations of particles usually deviated from Newton's second law to some extent.

The generated dynamical equations of the period vectors under external stress are not in a form where the period vectors are driven by the imbalance of the internal and external stresses. Then when the system reaches an equilibrium state, the internal and external stresses may not balance each other.

The generated internal stress may not contain the kinetic-energy term or only contain fractional coordinate velocities.

Without

Parrinello and Rahman theory (constant external pressure)

$$L = \tfrac{1}{2}\sum m_i \dot{\vec{s}}_i' \underline{G} \dot{\vec{s}}_i - \sum_i \sum_{j>i} \varphi(r_{ij}) + \tfrac{1}{2} W \,\mathrm{Tr}(\dot{\underline{h}}' \dot{\underline{h}}) - p_{\mathrm{ext}} \Omega. \qquad (1)$$

$$\ddot{\vec{s}}_i = m_i^{-1} \sum_{j \neq i} \chi(r_{ij})(\vec{s}_i - \vec{s}_j) - \underline{G}^{-1} \dot{\underline{G}} \dot{\vec{s}}_i, \qquad (2)$$

$$\ddot{\underline{h}} = W^{-1}(\underline{\pi} - p_{\mathrm{ext}})\underline{\sigma}. \qquad (3)$$

$$\Omega \vec{\pi} = \sum_i m_i \vec{v}_i \vec{v}_i + \sum_i \sum_{j>i} \chi(r_{ij})(\vec{r}_i - \vec{r}_j)(\vec{r}_i - \vec{r}_j), \qquad (4)$$

with $\underline{h}$ be the matrix formed by $\{\vec{a}, \vec{b}, \vec{c}\}$

$\vec{r}_i = \xi_i \vec{a} + \eta_i \vec{b} + \zeta_i \vec{c} = \underline{h} \vec{s}_i$, $\qquad (\xi_i, \eta_i, \zeta_i)$

$\chi(r)$ to denote $-d\varphi/rdr$, the vector $\vec{v}_i$ being $\underline{h}\dot{\vec{s}}_i$.

Phys. Rev. Lett. **45**, 1196 (1980)

In 1983, Nosé and Klein pointed out

The result is the usual Newton's second law equation with a correction term arising from the change in shape of the MD cell.

$$m_i \ddot{\mathbf{s}}_i = \mathbf{h}^{-1} \mathbf{f}_i - m_i \mathbf{G}^{-1} \dot{\mathbf{G}} \dot{\mathbf{s}}_i. \qquad (2.5)$$

in the paper

MOLECULAR PHYSICS, 1983, VOL. 50, NO. 5, 1055–1076

This implies that the generated dynamical equations for particles in PR theory are not consistent with Newton's second law.

PR theory (constant external stress)

The generated dynamical equation for the periods under constant external stress $\mathbf{S}$

$$W\ddot{\mathbf{h}} = (\boldsymbol{\pi} - p)\boldsymbol{\sigma} - \mathbf{h}\boldsymbol{\Sigma}. \qquad (2.25)$$

$$\boldsymbol{\Sigma} = \mathbf{h}_0^{-1}(\mathbf{S} - p)\mathbf{h}_0'^{-1}\boldsymbol{\Omega}_0. \qquad (2.24)$$

in the paper J. Appl. Phys. **52**, 7182 (1981).

We recently derived

Can. J. Phys. 93: 974–978 (2015), dx.doi.org/10.1139/cjp-2014-0518

NRC Research Press

ARTICLE

Dynamical equations for the period vectors in a periodic system under constant external stress[1]

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Abstract: The purpose of this paper is to derive the dynamical equations for the period vectors of a periodic system under constant external stress. The explicit starting point is Newton's second law applied to halves of the system. Later statistics over indistinguishable translated states and forces associated with transport of momentum are applied to the resulting dynamical equations. In the final expressions, the period vectors are driven by the imbalance between internal and external stresses. The internal stress is shown to have both full interaction and kinetic energy terms.

Key words: dynamical equations, crystal period vectors, periodic boundary conditions, stress, molecular dynamics.

by following Newtonian Dynamics only, where Newton's laws are strictly reserved and used repeatedly.

As a result,

Newton's second law on the particles

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i \quad (i = 1, 2, \cdots, n)$$

is always kept as original (then only work for periods);

our dynamical equations are in the form where the periods are driven by the imbalance between internal and external stresses;

our internal stress has both a full kinetic-energy term and a full interaction term.

Typicals

Since this work deals with pair-potential only

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Key words: dynamical equations, crystal period vectors, periodic boundary conditions, stress, molecular dynamics.

Let us do it again with many-body interactions.

Three major steps

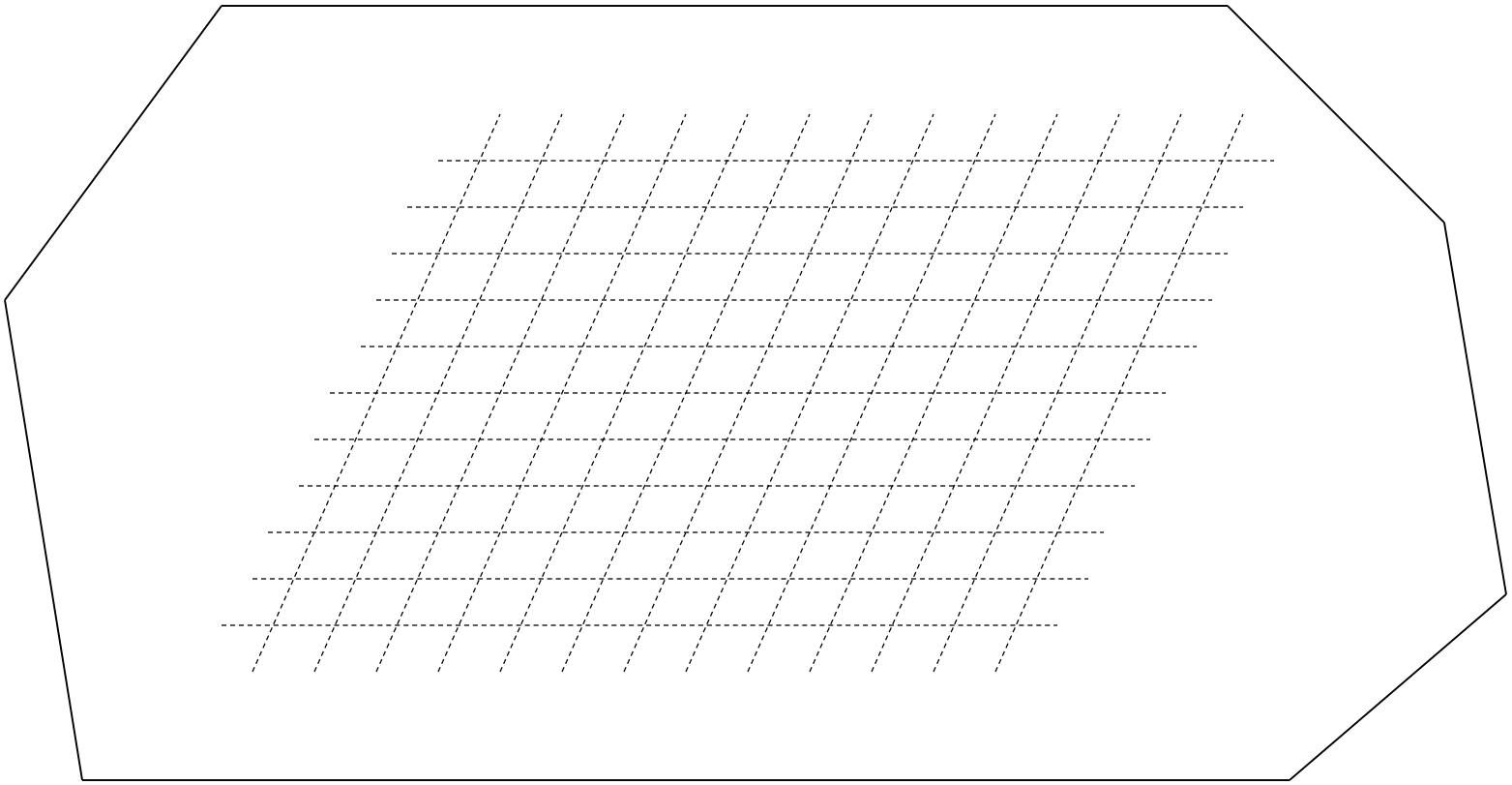
Newton's second law is applied on halves of the crystal to get instantaneous dynamical equations of the period vectors.

Statistics of the above dynamical equations over indistinguishable translated states is carried out.

Forces associated with momentum transportation and statistics over particles' moving directions are further implemented in the dynamical equations.

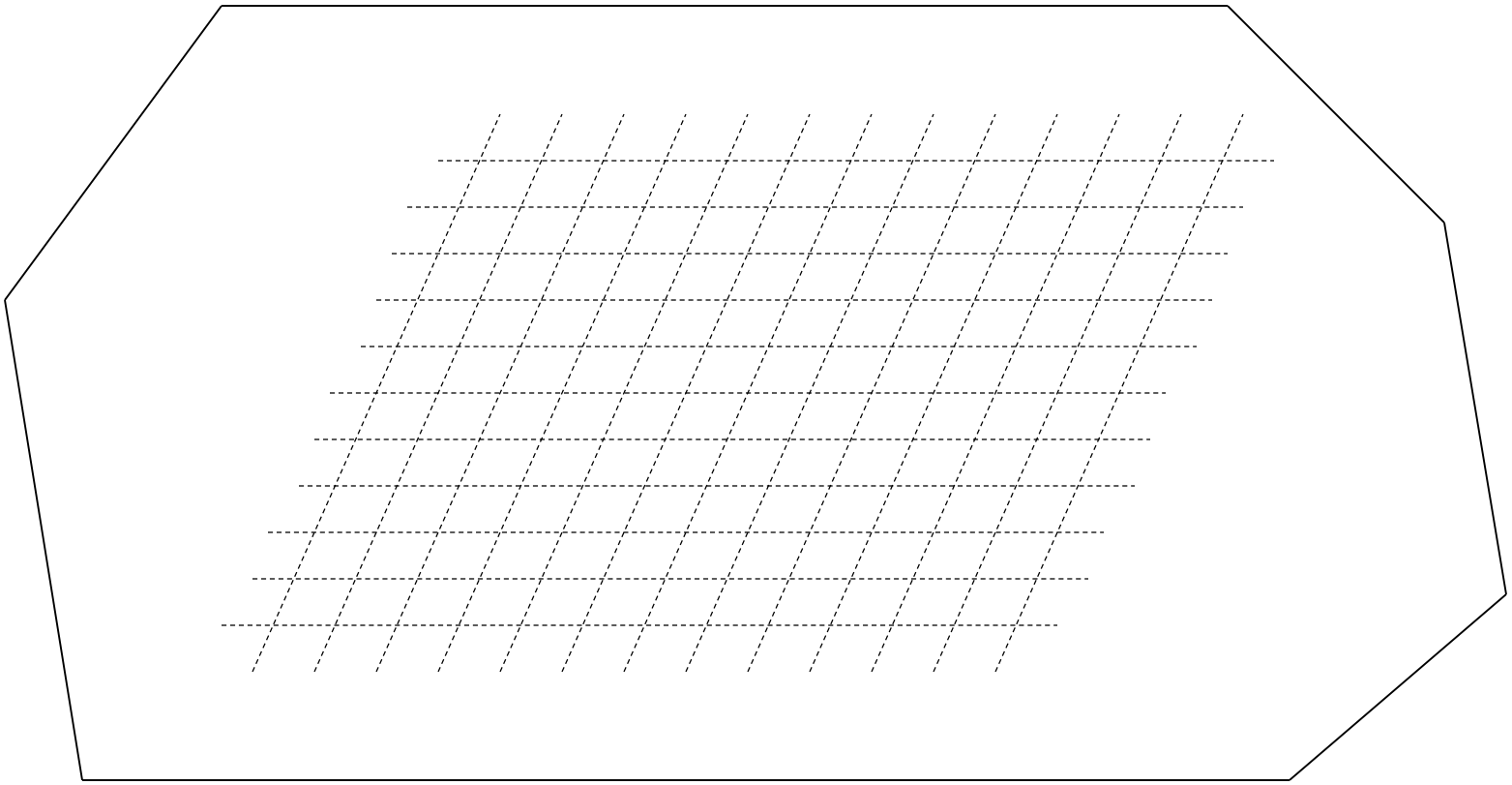
Some preparation first

In this work, the whole system is modeled as a limited macroscopic bulk, composed of an unlimited number of repeated microscopic cells in three dimensions, with surface effect ignored.



As usual, the cell in the center

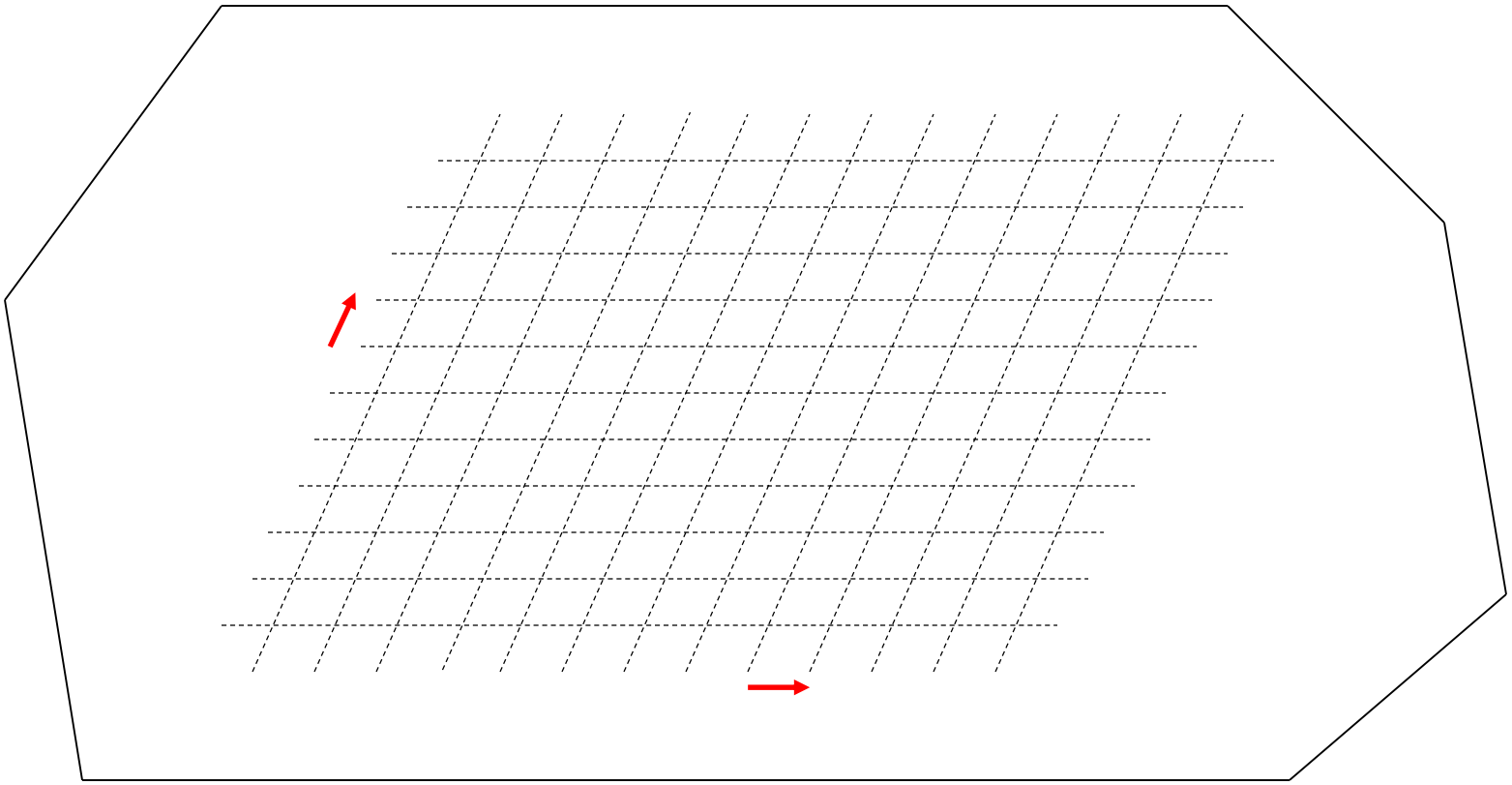
is called MD cell. Particles in it called MD particles with position vectors $\mathbf{r}_i$, $i = 1, 2, \cdots, n$.



For each cell, the three edge vectors

$\mathbf{a}, \mathbf{b}, \mathbf{c}$ (forming a right-handed triad)

are the period vectors of the system.



Some notation

By using the periods $\mathbf{a},\ \mathbf{b},\ \mathbf{c}$, any cell can be represented with $\mathbf{T} = T_{\mathbf{a}}\mathbf{a} + T_{\mathbf{b}}\mathbf{b} + T_{\mathbf{c}}\mathbf{c},$ where $T_{\mathbf{a}},\ T_{\mathbf{b}},\ T_{\mathbf{c}}$ are integers.

For the MD cell $\mathbf{T} = 0$.

Cell volume $\Omega = (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}$

Cell surface vectors:

$$\sigma_{\mathbf{a}} = \mathbf{b} \times \mathbf{c},\ \sigma_{\mathbf{b}} = \mathbf{c} \times \mathbf{a},\ \sigma_{\mathbf{c}} = \mathbf{a} \times \mathbf{b}$$

$$\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \text{or}\ \mathbf{c}$$

More notation

External stress $\overleftrightarrow{\Upsilon}$

with external pressure p as a special case

$$\overleftrightarrow{\Upsilon} = p \, \overleftrightarrow{I}$$

where $\overleftrightarrow{I}$ is a unit matrix.

More notation

For identifying a particle in the many-body interactions across the whole crystal effectively, let us use a simplified form of index I_k for it, so that its position vector can be expressed as

$$\mathbf{r}_{I_k} = I_{k,\mathbf{a}}\mathbf{a} + I_{k,\mathbf{b}}\mathbf{b} + I_{k,\mathbf{c}}\mathbf{c} + \mathbf{r}_{i_k},$$

where $I_{k,\mathbf{a}}$, $I_{k,\mathbf{b}}$, and $I_{k,\mathbf{c}}$ are integers, and i_k is its image particle in the MD cell. Namely, I_k means four integers of

$$(I_{k,\mathbf{a}},\ I_{k,\mathbf{b}},\ I_{k,\mathbf{c}},\ i_k)$$

More notation

For $\text{any pair of indexes } I_k \text{ and } I_{k'}$

$$(I_{k,\mathbf{a}} - I_{k',\mathbf{a}})^2 + (I_{k,\mathbf{b}} - I_{k',\mathbf{b}})^2 + (I_{k,\mathbf{c}} - I_{k',\mathbf{c}})^2 + (i_k - i_{k'})^2 \neq 0$$

is always assumed, as no pair of particles can share the same physical location.

More notation

For $\text{up to } M\text{-body}$ interactions, the $m\text{-body}$ potential is

$$\varphi^{(m)}(\mathbf{r}_{I_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m})$$

then the force on particle I_k is

$$\mathbf{f}_{I_k}^{(m)}(\mathbf{r}_{I_1}, \mathbf{r}_{I_2}, \cdots, \mathbf{r}_{I_m})$$
$$= -\nabla_{\mathbf{r}_{I_k}} \varphi^{(m)}(\mathbf{r}_{I_1}, \mathbf{r}_{I_2}, \cdots, \mathbf{r}_{I_m})$$

Force properties

Based on the essence of Newton's third law,

$$\sum_{k=1}^{m} \mathbf{f}_{I_k}^{(m)}(\mathbf{r}_{I_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m}) = 0$$

Further considering the crystal's periodicity,

$$\sum_{i_1=1}^{n} \mathbf{F}_{i_1}^{(m)} = 0,$$

where

$$\mathbf{F}_{i_1}^{(m)} = \frac{1}{(m-1)!} \sum_{\{I_2, I_3, \cdots, I_m\}} \mathbf{f}_{i_1}^{(m)}(\mathbf{r}_{i_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m})$$

Force Independence

As different body interactions are independent on each other, the total potential or forces should a summation of all of them. For example,

$$\mathbf{F}_i = \sum_{m=2}^{M} \mathbf{F}_i^{(m)}$$

Stationary coordinate system

Since $$\sum_{i=1}^{n} m_i \ddot{\mathbf{r}}_i = \sum_{i=1}^{n} \mathbf{F}_i = 0$$

the center-of-mass coordinate system of MD cell will be employed.

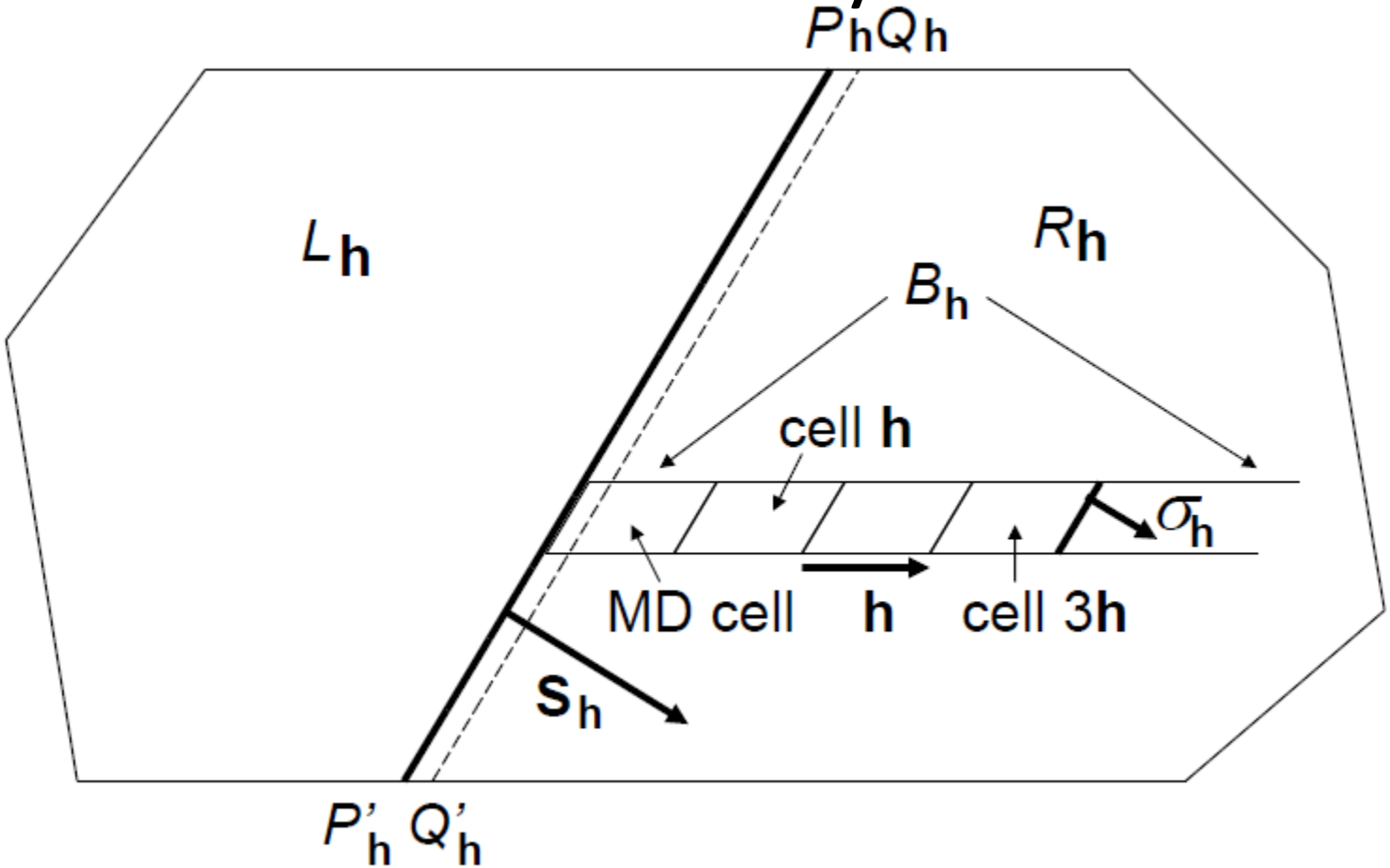
The first major step

Instantaneous dynamical equations of the period vectors.

Statistics of the above dynamical equations over indistinguishable translated states is carried out.

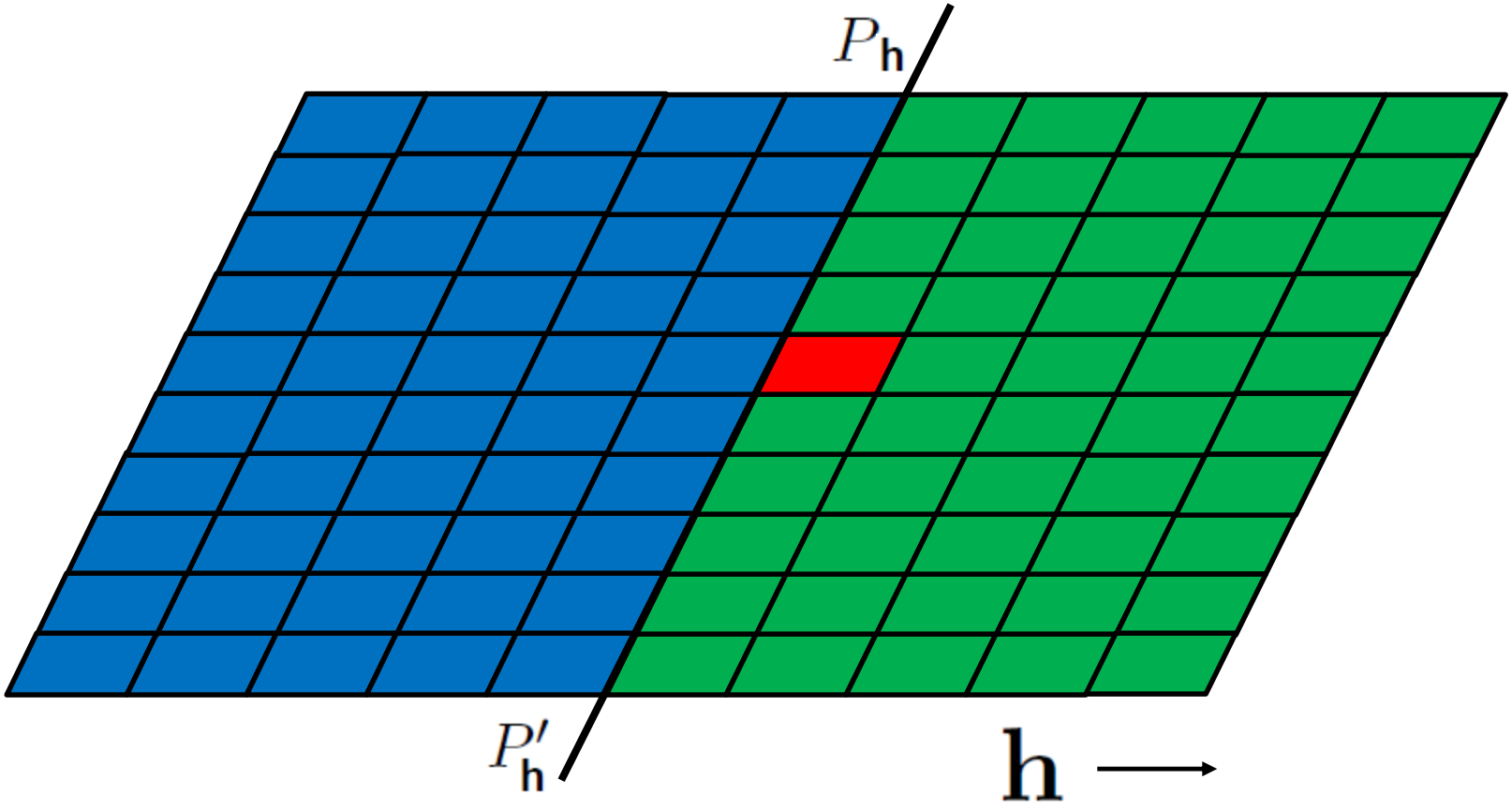
Forces associated with momentum transportation and statistics over particle's moving directions are further implemented in the dynamical equations.

Now let us first cut the system into two parts



with plane $P_{\mathbf{h}}P'_{\mathbf{h}}$, so that for a given period $\mathbf{h}$, the right $(R_{\mathbf{h}})$ part contains $\mathbf{T} = T_{\mathbf{a}}\mathbf{a} + T_{\mathbf{b}}\mathbf{b} + T_{\mathbf{c}}\mathbf{c}$ cells of $T_{\mathbf{h}} \geq 0$, the rest in the left $(L_{\mathbf{h}})$ part.

A detailed illustration

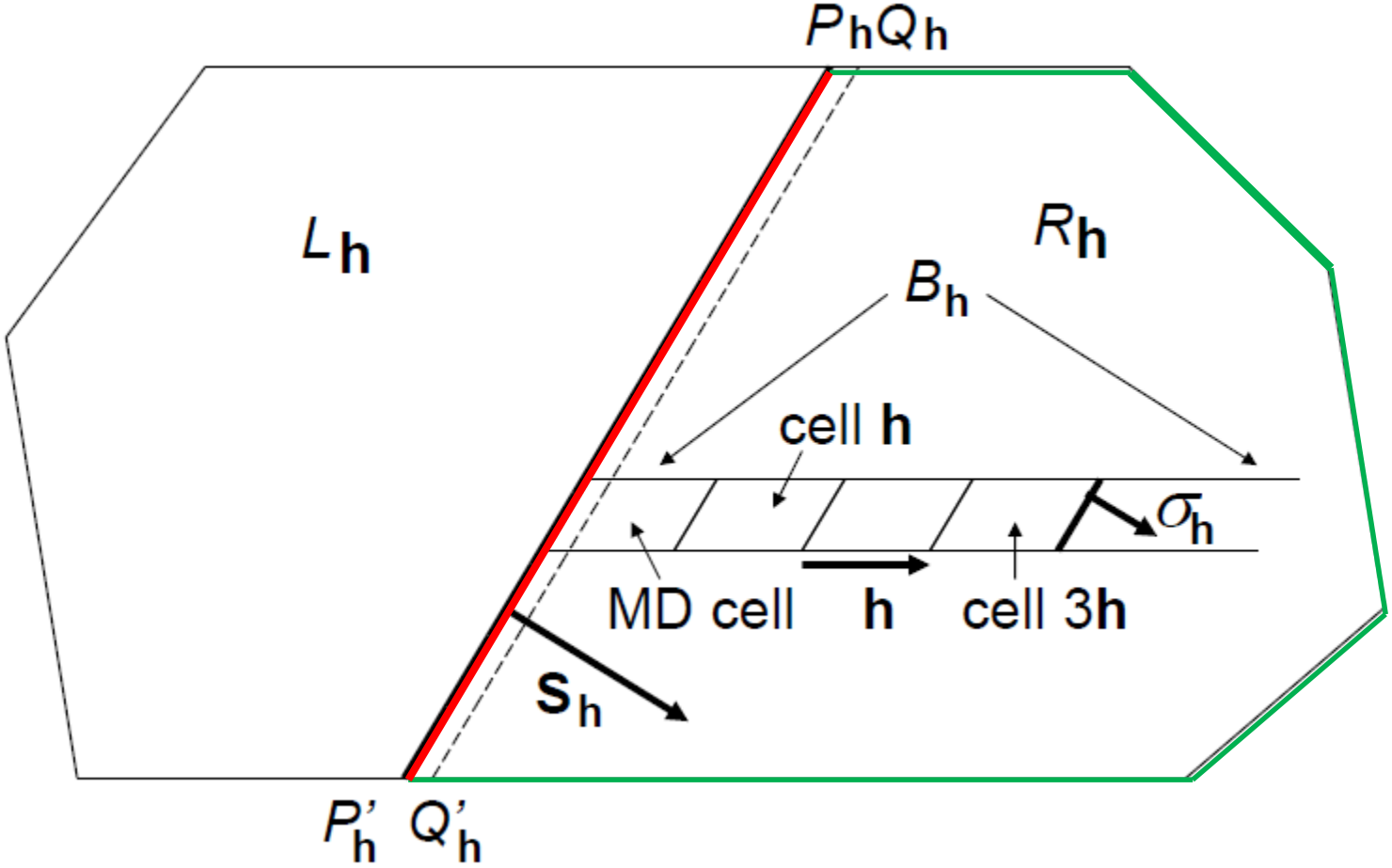


The red is the MD cell.

The net external force on $R_{\mathbf{h}}$

$$\mathbf{F}_{E,R} = \int_{R_{\mathbf{h}},sf} \overrightarrow{\overrightarrow{\Upsilon}} \cdot d\mathbf{s} = \overrightarrow{\overrightarrow{\Upsilon}} \cdot \int_{R_{\mathbf{h}},sf} d\mathbf{s} = \overrightarrow{\overrightarrow{\Upsilon}} \cdot \mathbf{S}_{\mathbf{h}}$$

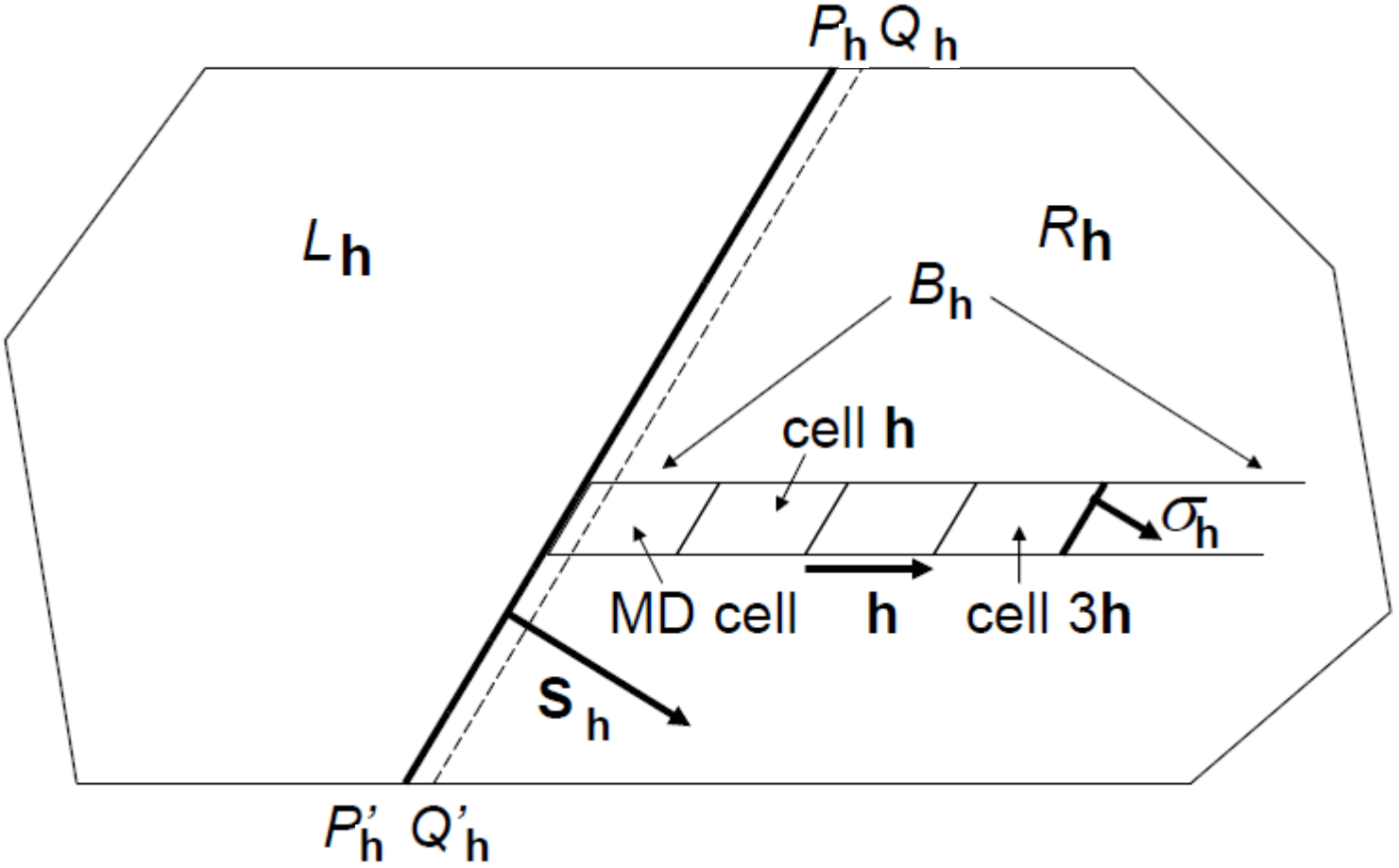
$\mathbf{S}_{\mathbf{h}}$ is the cross section vector in plane $P_{\mathbf{h}}P'_{\mathbf{h}}$



Newton's Second Law on $R_{\mathbf{h}}$

$$M_R \ddot{\mathbf{r}}_{RC} = \mathbf{F}_{L\to R} + \overrightarrow{\overrightarrow{\Upsilon}} \cdot \mathbf{S}_{\mathbf{h}}$$

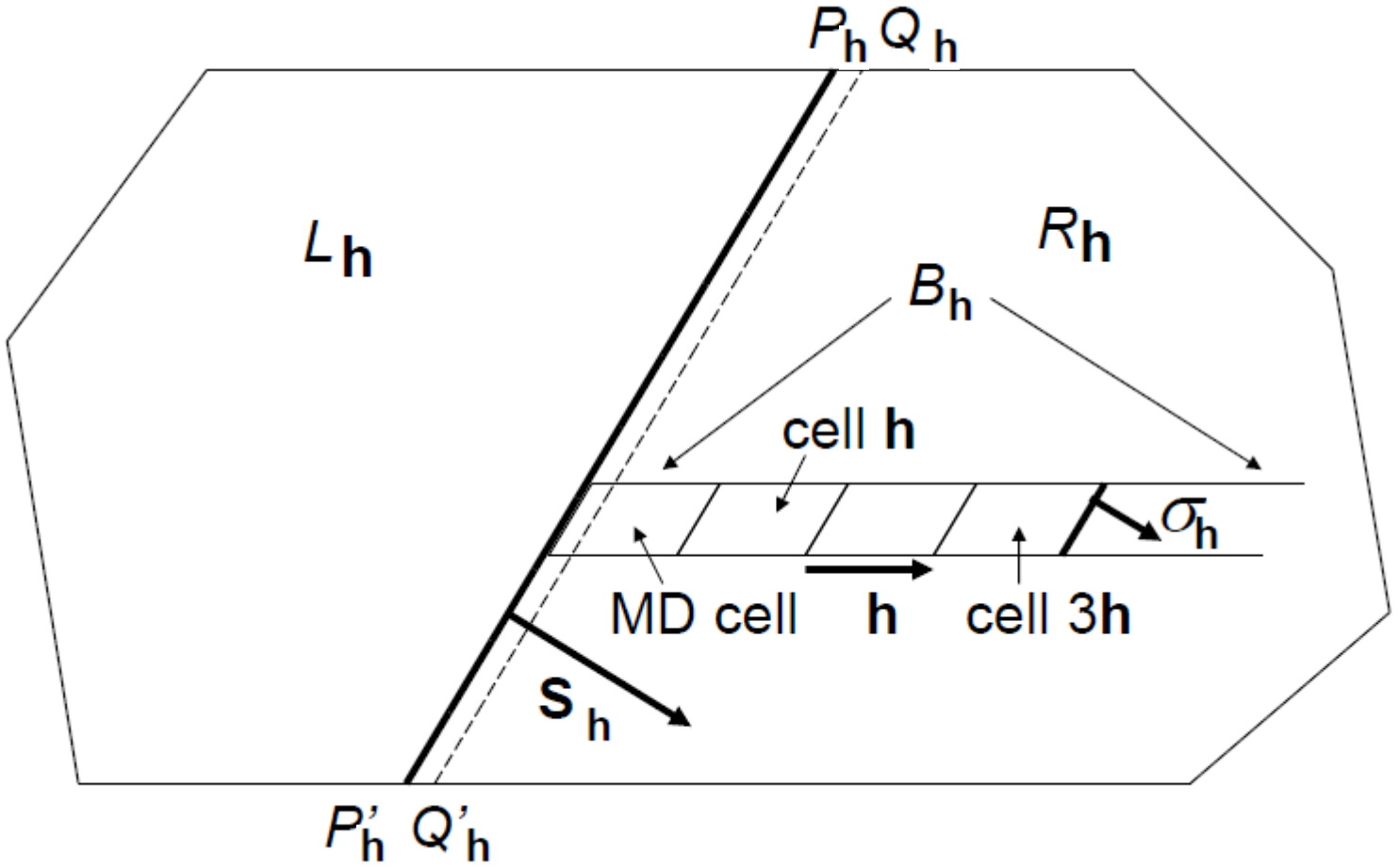
$\mathbf{F}_{L\to R}$ is the net force on $R_{\mathbf{h}}$ by $L_{\mathbf{h}}$



Newton's Second Law on $R_{\mathbf{h}}$

$$M_R \ddot{\mathbf{r}}_{RC} = \mathbf{F}_{L\to R} + \overrightarrow{\overrightarrow{\Upsilon}} \cdot \mathbf{S}_{\mathbf{h}} \qquad N_{\mathbf{h}} = |\mathbf{S}_{\mathbf{h}}| \,/\, |\sigma_{\mathbf{h}}|$$

$$\frac{1}{N_{\mathbf{h}}} M_R \ddot{\mathbf{r}}_{RC} = \mathbf{F}_{\mathbf{h}} + \overrightarrow{\overrightarrow{\Upsilon}} \cdot \sigma_{\mathbf{h}} \qquad \mathbf{F}_{\mathbf{h}} = \frac{1}{N_{\mathbf{h}}} \mathbf{F}_{L\to R}$$



The left side of $\frac{1}{N_{\mathbf{h}}} M_R \ddot{\mathbf{r}}_{RC} = \mathbf{F}_{\mathbf{h}} + \overline{\overline{\Upsilon}} \cdot \sigma_{\mathbf{h}}$

$$\frac{1}{N_{\mathbf{h}}} M_R \ddot{\mathbf{r}}_{RC} = \frac{1}{N_{\mathbf{h}}} \sum_{\mathbf{T} \in R_{\mathbf{h}}} \sum_{i=1}^{n} m_i \left(\ddot{\mathbf{r}}_i + \ddot{\mathbf{T}} \right) = \frac{M_{cell}}{N_{\mathbf{h}}} \sum_{\mathbf{T} \in R_{\mathbf{h}}} \ddot{\mathbf{T}}$$

where $M_{cell} = \sum_{i=1}^{n} m_i$ and $\ddot{\mathbf{T}} = T_{\mathbf{a}} \ddot{\mathbf{a}} + T_{\mathbf{b}} \ddot{\mathbf{b}} + T_{\mathbf{c}} \ddot{\mathbf{c}}$

and $\sum_{i=1}^{n} m_i \ddot{\mathbf{r}}_i = \sum_{i=1}^{n} \mathbf{F}_i = 0.$ is used.

The left side of $\frac{1}{N_{\mathbf{h}}} M_R \ddot{\mathbf{r}}_{RC} = \mathbf{F}_{\mathbf{h}} + \overrightarrow{\Upsilon} \cdot \sigma_{\mathbf{h}}$

$$\frac{1}{N_{\mathbf{h}}} M_R \ddot{\mathbf{r}}_{RC} = \alpha_{\mathbf{h},\mathbf{a}} \ddot{\mathbf{a}} + \alpha_{\mathbf{h},\mathbf{b}} \ddot{\mathbf{b}} + \alpha_{\mathbf{h},\mathbf{c}} \ddot{\mathbf{c}},$$

where $\alpha_{\mathbf{h},\mathbf{h}'} = \frac{M_{cell}}{N_{\mathbf{h}}} \sum_{\mathbf{T} \in R_{\mathbf{h}}} T_{\mathbf{h}'} \quad (\mathbf{h}' = \mathbf{a},\ \mathbf{b},\ \mathbf{c}).$

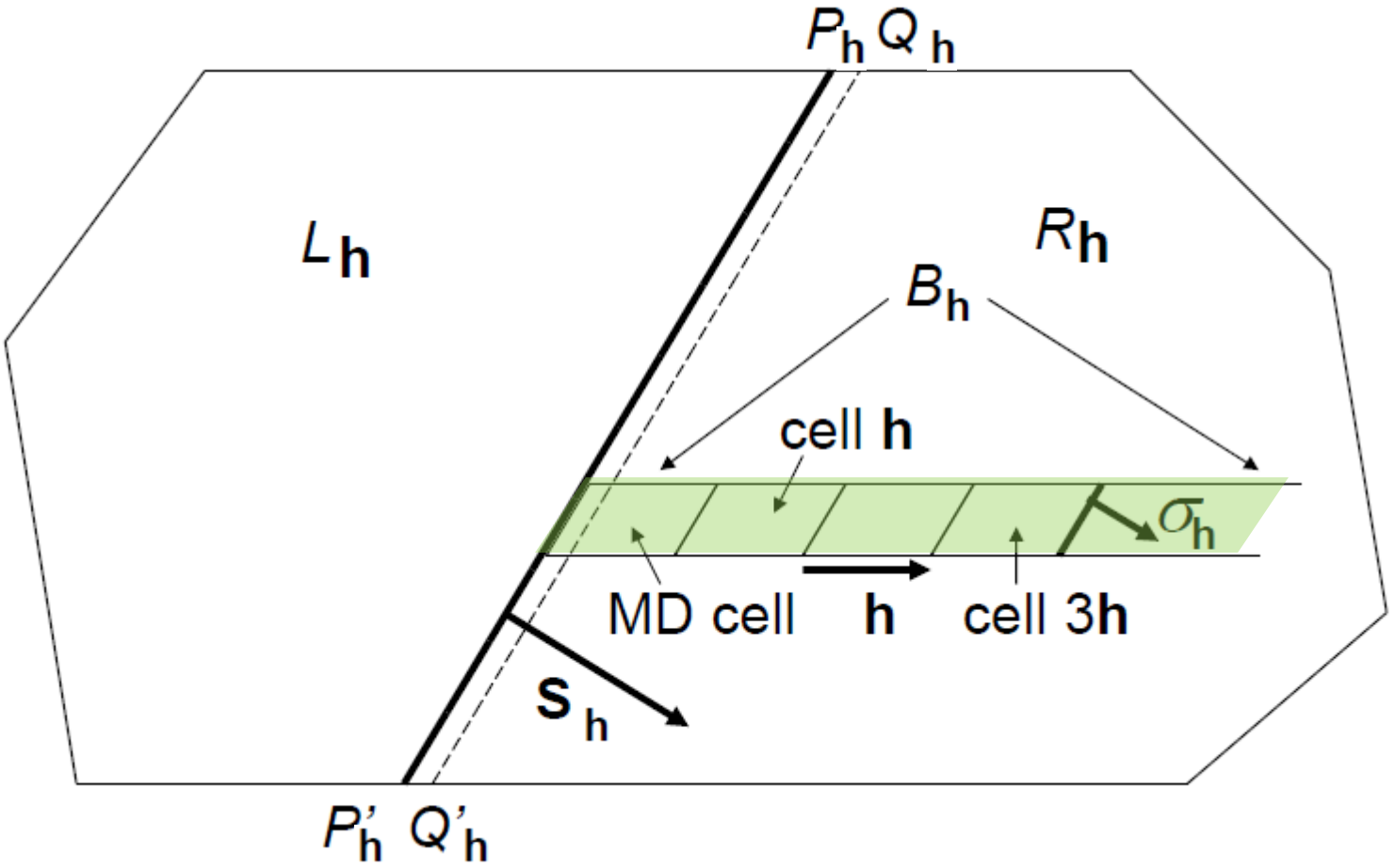
Since in $R_{\mathbf{h}}$, any $T_{\mathbf{h}}$ is non-negative, and for any $T_{\mathbf{h}' \neq \mathbf{h}}$, there exists $-T_{\mathbf{h}'}$ to cancel it, then $\alpha_{\mathbf{h},\mathbf{h}' \neq \mathbf{h}}$ is zero.

$$\frac{1}{N_{\mathbf{h}}} M_R \ddot{\mathbf{r}}_{RC} = \alpha_{\mathbf{h},\mathbf{h}} \ddot{\mathbf{h}}$$

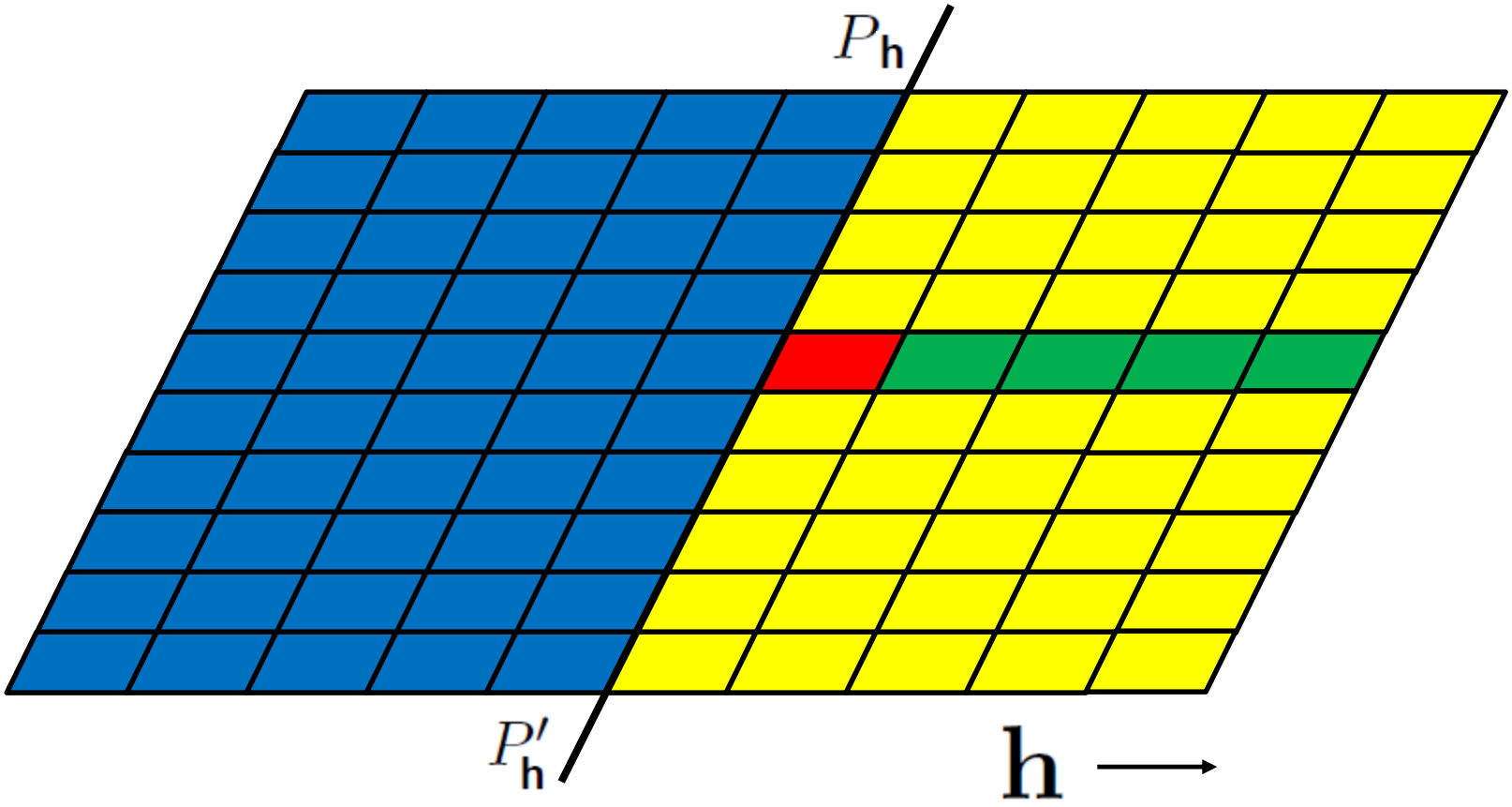
Newton's Second Law on $R_{\mathbf{h}}$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \mathbf{F}_{\mathbf{h}} + \overrightarrow{\Upsilon} \cdot \sigma_{\mathbf{h}}. \qquad \mathbf{F}_{\mathbf{h}} = \frac{1}{N_{\mathbf{h}}}\mathbf{F}_{L\to R}$$

$B_{\mathbf{h}}$ "half cell bar"



$\mathbf{F_h}$ is the net force of blues on red and greens



The red is the MD cell.

Newton's Second Law on $R_{\mathbf{h}}$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \mathbf{F}_{\mathbf{h}} + \overleftrightarrow{\Upsilon} \cdot \sigma_{\mathbf{h}}. \qquad \mathbf{F}_{\mathbf{h}} = \frac{1}{N_{\mathbf{h}}}\mathbf{F}_{L\to R}$$

Considering all m-body interactions with total t particles $(m > t \geq 1)$ in the $R_{\mathbf{h}}$ part

$$\begin{aligned}
\mathbf{F}_{t,\mathbf{h}}^{(m)} &= \frac{1}{N_{\mathbf{h}}}\frac{1}{t!\,(m-t)!}\sum_{\{I_1,I_2,\cdots,I_t\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{t,\mathbf{h}}\geq 0)}\ \sum_{\{I_{t+1},I_{t+2},\cdots,I_m\}}^{(I_{t+1,\mathbf{h}},I_{t+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}<0)}\ \sum_{\mu=1}^{t}\mathbf{f}_{I_\mu}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{N_{\mathbf{h}}}\frac{1}{t!\,(m-t)!}\sum_{\{I_1,I_2,\cdots,I_t\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{t,\mathbf{h}}\geq 0)}\ \sum_{\{I_{t+1},I_{t+2},\cdots,I_m\}}^{(I_{t+1,\mathbf{h}},I_{t+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}<0)} t\mathbf{f}_{I_1}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{N_{\mathbf{h}}}\frac{1}{(t-1)!\,(m-t)!}\sum_{\{I_1,I_2,\cdots,I_t\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{t,\mathbf{h}}\geq 0)}\ \sum_{\{I_{t+1},I_{t+2},\cdots,I_m\}}^{(I_{t+1,\mathbf{h}},I_{t+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}<0)}\mathbf{f}_{I_1}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})
\end{aligned}$$

Newton's Second Law on $R_{\mathbf{h}}$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \mathbf{F}_{\mathbf{h}} + \overline{\overline{\Upsilon}} \cdot \sigma_{\mathbf{h}}. \qquad \mathbf{F}_{\mathbf{h}} = \frac{1}{N_{\mathbf{h}}}\mathbf{F}_{L\to R}$$

By using crystal's periodicity, it can be reduced to

$$\mathbf{F}_{t,\mathbf{h}}^{(m)} = \frac{1}{(t-1)!\,(m-t)!}\sum_{l=0}^{-\infty}\sum_{i_1=1}^{n}\sum_{\{I_2,I_3,\cdots,I_t\}}^{(I_{2,\mathbf{h}},I_{3,\mathbf{h}},\cdots,I_{t,\mathbf{h}}\geq l)}\sum_{\{I_{t+1},I_{t+2},\cdots,I_m\}}^{(I_{t+1,\mathbf{h}},I_{t+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}<l)}\mathbf{f}_{i_1}^{(m)}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})$$

$$\begin{aligned}\mathbf{F}_{\mathbf{h}} &= \sum_{m=2}^{M}\sum_{t=1}^{m-1}\mathbf{F}_{t,\mathbf{h}}^{(m)} \\ &= \sum_{m=2}^{M}\sum_{t=1}^{m-1}\frac{1}{(t-1)!\,(m-t)!}\sum_{l=0}^{-\infty}\sum_{i_1=1}^{n}\sum_{\{I_2,I_3,\cdots,I_t\}}^{(I_{2,\mathbf{h}},I_{3,\mathbf{h}},\cdots,I_{t,\mathbf{h}}\geq l)}\sum_{\{I_{t+1},I_{t+2},\cdots,I_m\}}^{(I_{t+1,\mathbf{h}},I_{t+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}<l)}\mathbf{f}_{i_1}^{(m)}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})\end{aligned}$$

Total cell potential energy

For m-body potential $\varphi^{(m)}(\mathbf{r}_{I_1}, \mathbf{r}_{I_2}, \cdots, \mathbf{r}_{I_m})$, supposing s $(m \geq s \geq 1)$ particles in the cell, then s/m of the potential should belong to the cell

$$E^{(m)}_{p,cell,s} = \frac{s}{m}\frac{1}{s!(m-s)!} \overbrace{\sum_{i_1,i_2,\cdots,i_s}}^{\text{(inside the cell)}} \overbrace{\sum_{\{I_{s+1},I_{s+2},\cdots,I_m\}}}^{\text{(outside the cell)}} \varphi^{(m)}(\mathbf{r}_{i_1}, \mathbf{r}_{i_2}, \cdots, \mathbf{r}_{i_s}, \mathbf{r}_{I_{s+1}}, \mathbf{r}_{I_{s+2}}, \cdots, \mathbf{r}_{I_m})$$

$$E^{(m)}_{p,cell} = \sum_{s=1}^{m} E^{(m)}_{p,cell,s}$$

$$= \frac{1}{m!} \sum_{i_1=1}^{n} \sum_{\{I_2,I_3,\cdots,I_m\}} \varphi^{(m)}(\mathbf{r}_{i_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m})$$

$$E_{p,cell} = \sum_{m=2}^{M} E^{(m)}_{p,cell}$$

Take a derivative

$$
\begin{aligned}
-\frac{\partial}{\partial \mathbf{h}} E^{(m)}_{p,cell} &= \frac{1}{m!} \sum_{i_1=1}^{n} \sum_{\{I_2, I_3, \cdots, I_m\}} \sum_{k=2}^{m} I_{k,\mathbf{h}} \mathbf{f}^{(m)}_{I_k}(\mathbf{r}_{i_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m}) \\
&= \frac{1}{m!} \sum_{i_1=1}^{n} \sum_{\{I_2, I_3, \cdots, I_m\}} (m-1) I_{m,\mathbf{h}} \mathbf{f}^{(m)}_{I_m}(\mathbf{r}_{i_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m}) \\
&= \frac{1}{m\,(m-2)!} \sum_{i_1=1}^{n} \sum_{\{I_2, I_3, \cdots, I_m\}} I_{m,\mathbf{h}} \mathbf{f}^{(m)}_{I_m}(\mathbf{r}_{i_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m})
\end{aligned}
$$

where

$$
\mathbf{f}^{(m)}_{I_k}(\mathbf{r}_{I_1}, \mathbf{r}_{I_2}, \cdots, \mathbf{r}_{I_m}) = -\nabla_{\mathbf{r}_{I_k}} \varphi^{(m)}(\mathbf{r}_{I_1}, \mathbf{r}_{I_2}, \cdots, \mathbf{r}_{I_m})
$$

Split it based on signs

$$-\frac{\partial}{\partial \mathbf{h}} E^{(m)}_{p,cell} = \mathbf{F}^{(m)}_{\mathbf{h},+} + \mathbf{F}^{(m)}_{\mathbf{h},-}$$

where

$$\begin{aligned}
\mathbf{F}^{(m)}_{\mathbf{h},+} &= \frac{1}{m\,(m-2)!} \sum_{i_1=1}^{n} \sum_{\{I_2,I_3,\cdots,I_m\}}^{I_{m,\mathbf{h}}>0} I_{m,\mathbf{h}} \mathbf{f}^{(m)}_{I_m}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{m\,(m-2)!} \sum_{l=0}^{+\infty} \sum_{i_1=1}^{n} \sum_{\{I_2,I_3,\cdots,I_m\}}^{I_{m,\mathbf{h}}>l} \mathbf{f}^{(m)}_{I_m}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}), \\
\mathbf{F}^{(m)}_{\mathbf{h},-} &= \frac{1}{m\,(m-2)!} \sum_{i_1=1}^{n} \sum_{\{I_2,I_3,\cdots,I_m\}}^{I_{m,\mathbf{h}}<0} I_{m,\mathbf{h}} \mathbf{f}^{(m)}_{I_m}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{-1}{m\,(m-2)!} \sum_{l=0}^{-\infty} \sum_{i_1=1}^{n} \sum_{\{I_2,I_3,\cdots,I_m\}}^{I_{m,\mathbf{h}}<l} \mathbf{f}^{(m)}_{I_m}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}).
\end{aligned}$$

Expand it and more effort

$$\mathbf{F}_{\mathbf{h},+}^{(m)} = \frac{1}{m}\sum_{t'=0}^{m-2}\sum_{l=0}^{+\infty}\sum_{i_1=1}^{n}\sum_{I_m}^{I_{m,\mathrm{h}}>l}\sum_{\{I_2,I_3,\cdots,I_{t'+1}\}}^{(I_{2,\mathrm{h}},I_{3,\mathrm{h}},\cdots,I_{t'+1,\mathrm{h}}>0)}\sum_{\{I_{t'+2},I_{t'+3},\cdots,I_{m-1}\}}^{(I_{t'+2,\mathrm{h}},I_{t'+3,\mathrm{h}},\cdots,I_{m-1,\mathrm{h}}\le 0)}\frac{\mathbf{f}_{I_m}^{(m)}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})}{t'!\,(m-2-t')!}$$

$$= \frac{1}{m}\sum_{t'=0}^{m-2}\sum_{l=0}^{-\infty}\sum_{I_1}^{I_{1,\mathrm{h}}<l}\sum_{i_m=1}^{n}\sum_{\{I_2,I_3,\cdots,I_{t'+1}\}}^{(I_{2,\mathrm{h}},I_{3,\mathrm{h}},\cdots,I_{t'+1,\mathrm{h}}\ge l)}\sum_{\{I_{t'+2},I_{t'+3},\cdots,I_{m-1}\}}^{(I_{t'+2,\mathrm{h}},I_{t'+3,\mathrm{h}},\cdots,I_{m-1,\mathrm{h}}<l)}\frac{\mathbf{f}_{i_m}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{i_m})}{t'!\,(m-2-t')!}$$

$$= \frac{1}{m}\sum_{t'=0}^{m-2}\sum_{l=0}^{-\infty}\sum_{I_m}^{I_{m,\mathrm{h}}<l}\sum_{i_1=1}^{n}\sum_{\{I_2,I_3,\cdots,I_{t'+1}\}}^{(I_{2,\mathrm{h}},I_{3,\mathrm{h}},\cdots,I_{t'+1,\mathrm{h}}\ge l)}\sum_{\{I_{t'+2},I_{t'+3},\cdots,I_{m-1}\}}^{(I_{t'+2,\mathrm{h}},I_{t'+3,\mathrm{h}},\cdots,I_{m-1,\mathrm{h}}<l)}\frac{\mathbf{f}_{i_1}^{(m)}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})}{t'!\,(m-2-t')!}$$

$$= \frac{1}{m}\sum_{t'=0}^{m-2}\sum_{l=0}^{-\infty}\sum_{i_1=1}^{n}\sum_{\{I_2,I_3,\cdots,I_{t'+1}\}}^{(I_{2,\mathrm{h}},I_{3,\mathrm{h}},\cdots,I_{t'+1,\mathrm{h}}\ge l)}\sum_{\{I_{t'+2},I_{t'+3},\cdots,I_{m-1}\}}^{(I_{t'+2,\mathrm{h}},I_{t'+3,\mathrm{h}},\cdots,I_{m-1,\mathrm{h}}<l)}\sum_{I_m}^{I_{m,\mathrm{h}}<l}\frac{\mathbf{f}_{i_1}^{(m)}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})}{t'!\,(m-2-t')!}$$

$$= \frac{1}{m}\sum_{t'=0}^{m-2}\sum_{l=0}^{-\infty}\sum_{i_1=1}^{n}\sum_{\{I_2,I_3,\cdots,I_{t'+1}\}}^{(I_{2,\mathrm{h}},I_{3,\mathrm{h}},\cdots,I_{t'+1,\mathrm{h}}\ge l)}\sum_{\{I_{t'+2},I_{t'+3},\cdots,I_{m-1},I_m\}}^{(I_{t'+2,\mathrm{h}},I_{t'+3,\mathrm{h}},\cdots,I_{m-1,\mathrm{h}},I_{m,\mathrm{h}}<l)}\frac{\mathbf{f}_{i_1}^{(m)}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})}{t'!\,(m-2-t')!}$$

We get

$$\mathbf{F}^{(m)}_{\mathbf{h},+} = \sum_{t=1}^{m-1} \frac{m-t}{m} \mathbf{F}^{(m)}_{t,\mathbf{h}}$$

$$\mathbf{F}^{(m)}_{\mathbf{h},-} = \sum_{t=1}^{m-1} \frac{t}{m} \mathbf{F}^{(m)}_{t,\mathbf{h}}$$

Newton's Second Law on $R_{\mathbf{h}}$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \mathbf{F_h} + \overrightarrow{\overrightarrow{\Upsilon}} \cdot \sigma_{\mathbf{h}}. \qquad \mathbf{F_h} = \frac{1}{N_{\mathbf{h}}}\mathbf{F}_{L\to R}$$

$$\mathbf{F_h} = \sum_{m=2}^{M}\sum_{t=1}^{m-1}\mathbf{F}_{t,\mathbf{h}}^{(m)} = \sum_{m=2}^{M}\left(\mathbf{F}_{\mathbf{h},+}^{(m)} + \mathbf{F}_{\mathbf{h},-}^{(m)}\right)$$

$$= \sum_{m=2}^{M} -\frac{\partial}{\partial \mathbf{h}} E_{p,cell}^{(m)} = -\frac{\partial}{\partial \mathbf{h}} E_{p,cell}$$

Introducing main interaction tensor/dyad

$$\overrightarrow{\overrightarrow{\varepsilon}}_{main} = \frac{-1}{\Omega}\left[\left(\frac{\partial E_{p,cell}}{\partial \mathbf{a}}\right)\mathbf{a} + \left(\frac{\partial E_{p,cell}}{\partial \mathbf{b}}\right)\mathbf{b} + \left(\frac{\partial E_{p,cell}}{\partial \mathbf{c}}\right)\mathbf{c}\right]$$

$$= \sum_{m=2}^{M} \overrightarrow{\overrightarrow{\varepsilon}}^{(m)}_{main}$$

$$\overrightarrow{\overrightarrow{\varepsilon}}^{(m)}_{main} = \frac{-1}{\Omega}\left[\left(\frac{\partial E^{(m)}_{p,cell}}{\partial \mathbf{a}}\right)\mathbf{a} + \left(\frac{\partial E^{(m)}_{p,cell}}{\partial \mathbf{b}}\right)\mathbf{b} + \left(\frac{\partial E^{(m)}_{p,cell}}{\partial \mathbf{c}}\right)\mathbf{c}\right]$$

$$\mathbf{F}_{\mathbf{h}} = \overrightarrow{\overrightarrow{\varepsilon}}_{main} \cdot \sigma_{\mathbf{h}}$$

where $\mathbf{h} \cdot \sigma_{\mathbf{h}'} = \Omega \delta_{\mathbf{h},\mathbf{h}'}$

First form of the period dynamics

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}}_{main} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \quad (\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c}).$$

from Newton's second law

$$M_R\ddot{\mathbf{r}}_{RC} = \mathbf{F}_{L\to R} + \overrightarrow{\overrightarrow{\Upsilon}} \cdot \mathbf{S}_{\mathbf{h}} \qquad N_{\mathbf{h}} = |\mathbf{S}_{\mathbf{h}}| \,/\, |\sigma_{\mathbf{h}}|$$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \mathbf{F}_{\mathbf{h}} + \overrightarrow{\overrightarrow{\Upsilon}} \cdot \sigma_{\mathbf{h}}. \qquad \mathbf{F}_{\mathbf{h}} = \overrightarrow{\overrightarrow{\varepsilon}}_{main} \cdot \sigma_{\mathbf{h}}$$

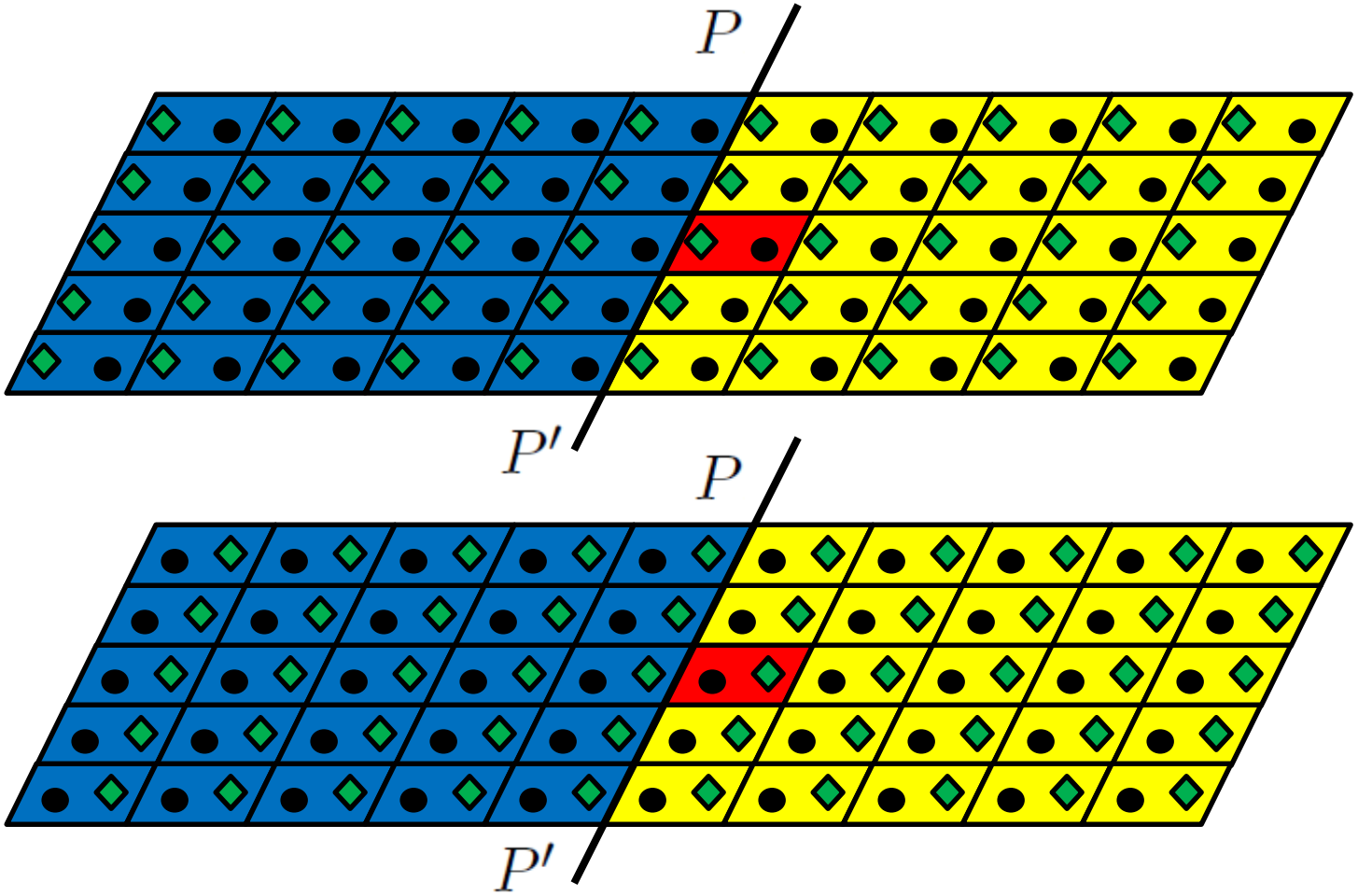
The second major step

Instantaneous dynamical equations of the period vectors.

Statistics of the above dynamical equations over indistinguishable translated states

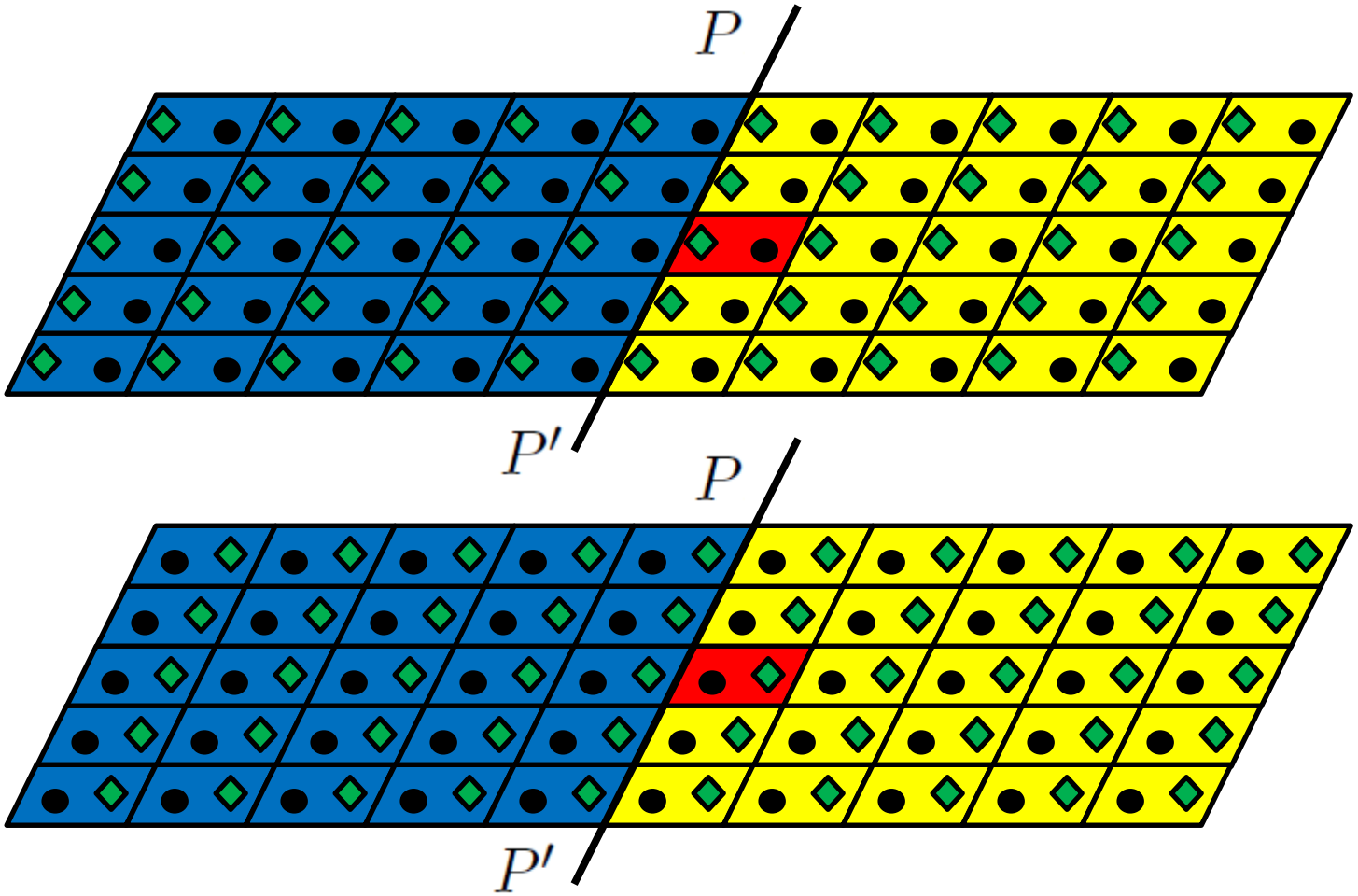
Forces associated with momentum transportation and statistics over particle's moving directions are further implemented in the dynamical equations.

Now let us consider two states



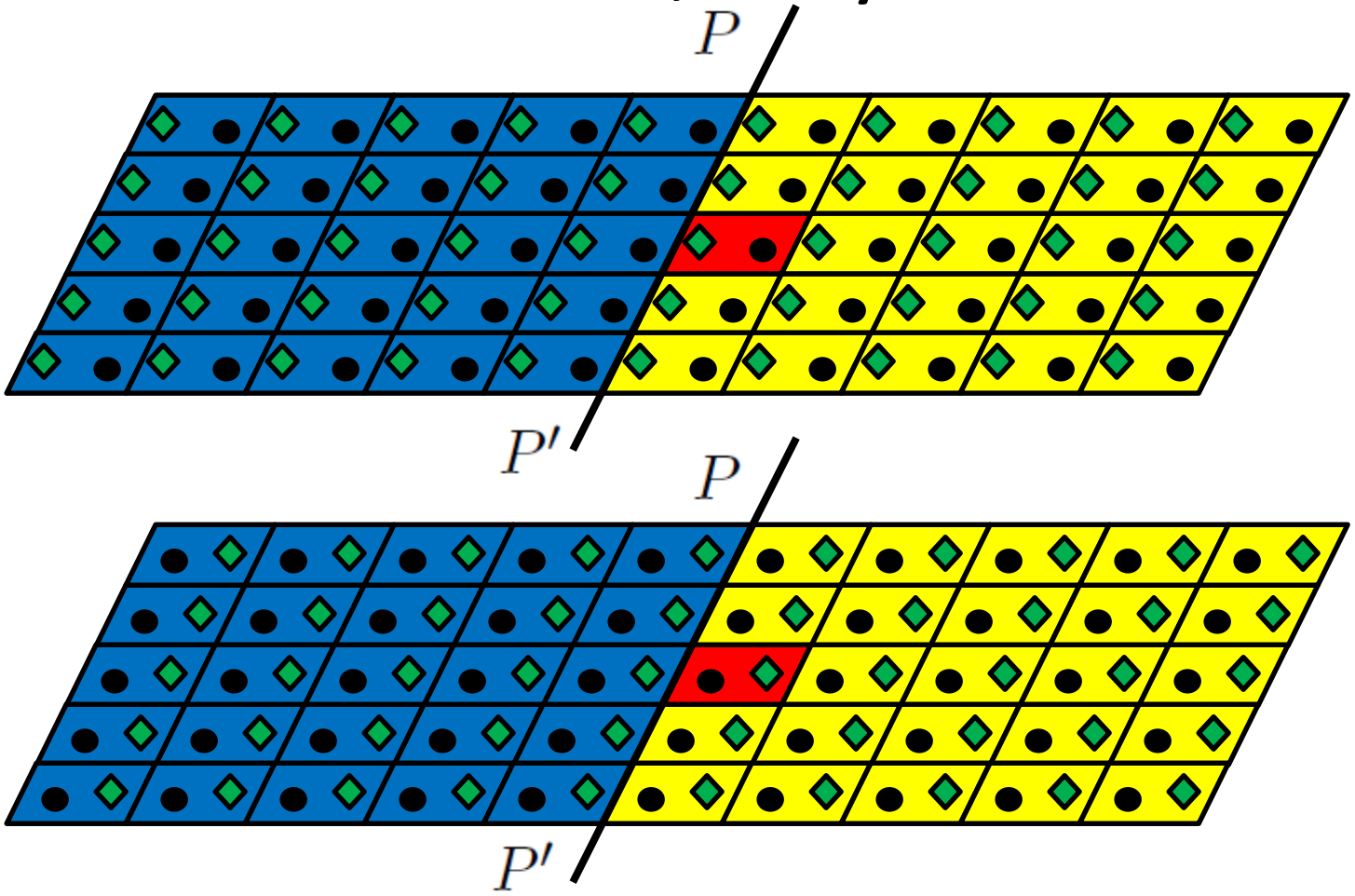
Only difference is translation between them from microscopic point of view.

Since they are indistinguishable from macroscopic



We should take an unweighted average of the dynamical equations over all such states.

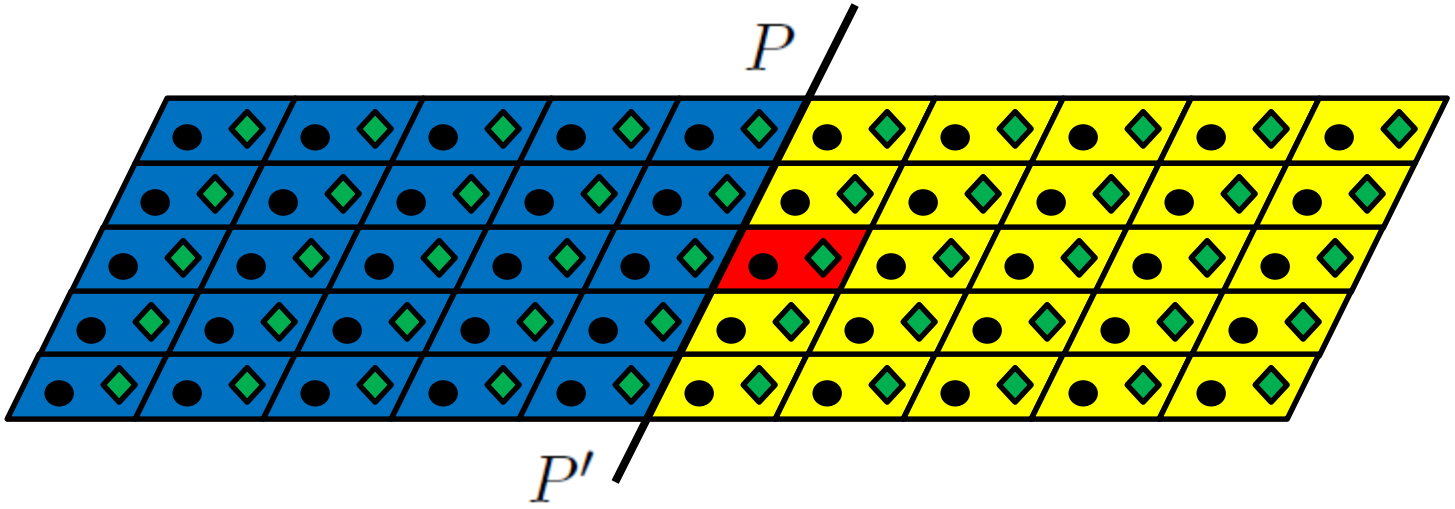
In all such states, only $\overrightarrow{\overrightarrow{\varepsilon}}_{main}$ differs



$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}}_{main} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \quad (\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c}).$$

What we really need is the unweighted average of

$\overrightarrow{\overrightarrow{\varepsilon}}_{main}$ or $\mathbf{F_h}$



What we really need is the unweighted average of

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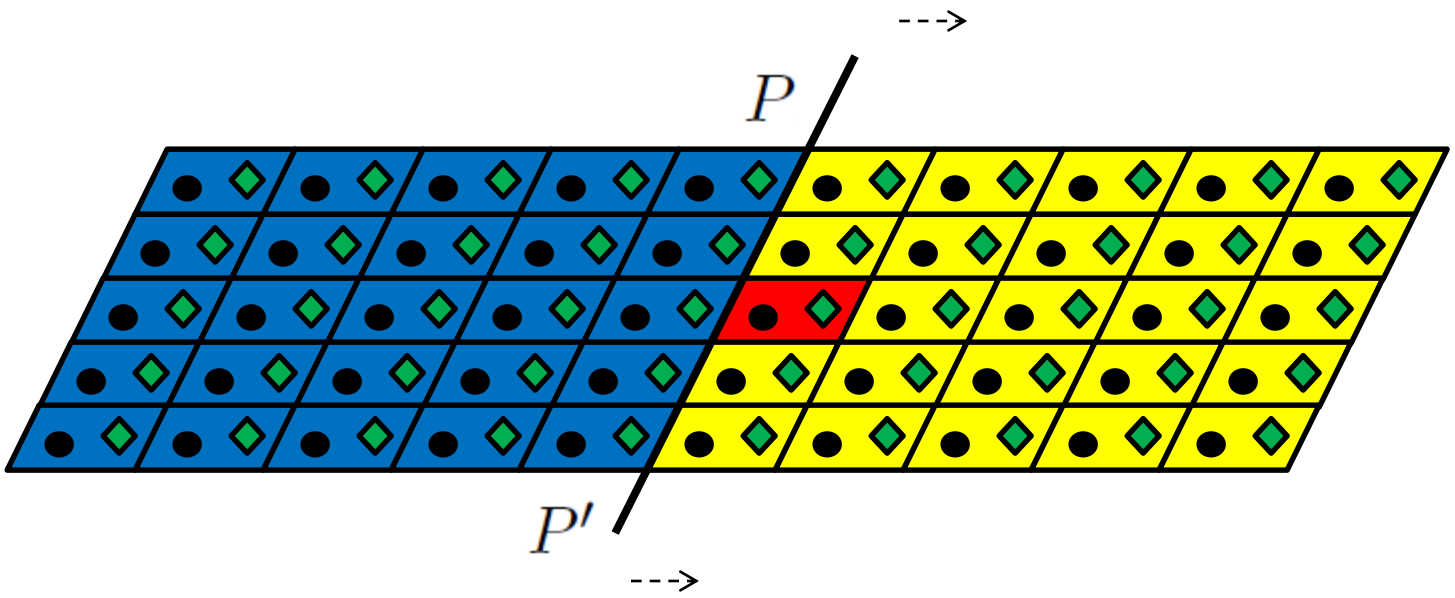
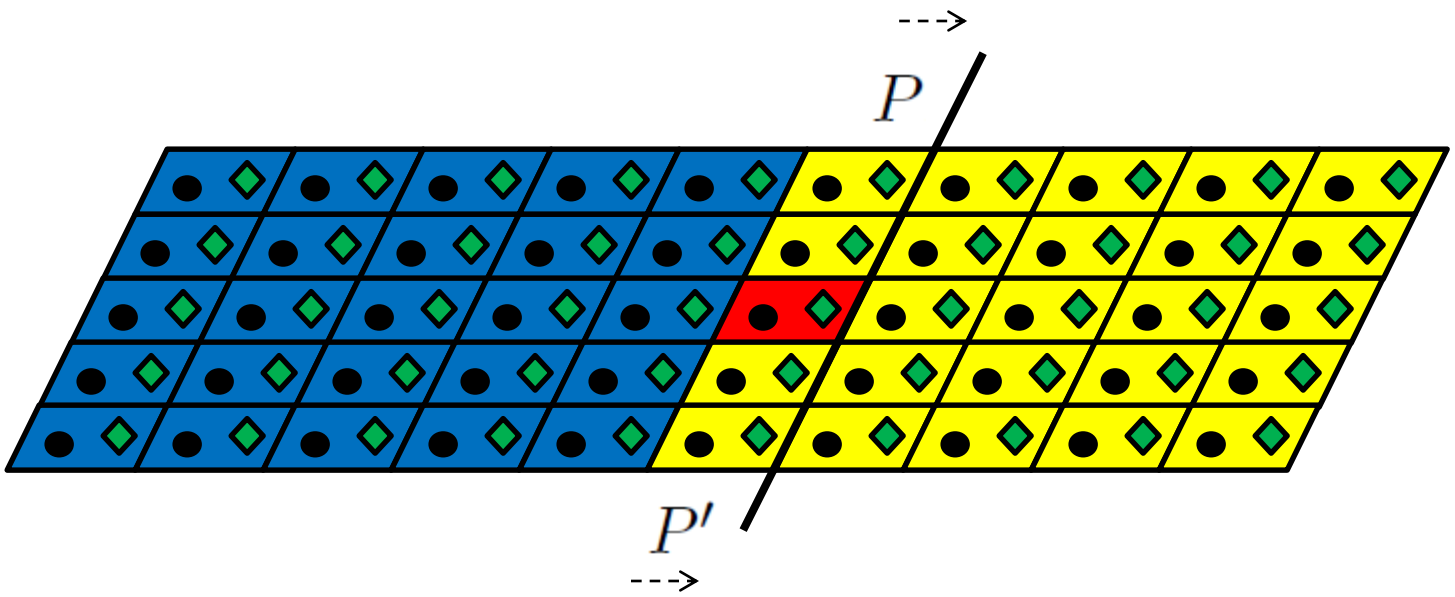


The total amount of such states can be represented by the volume of the MD cell Ω .

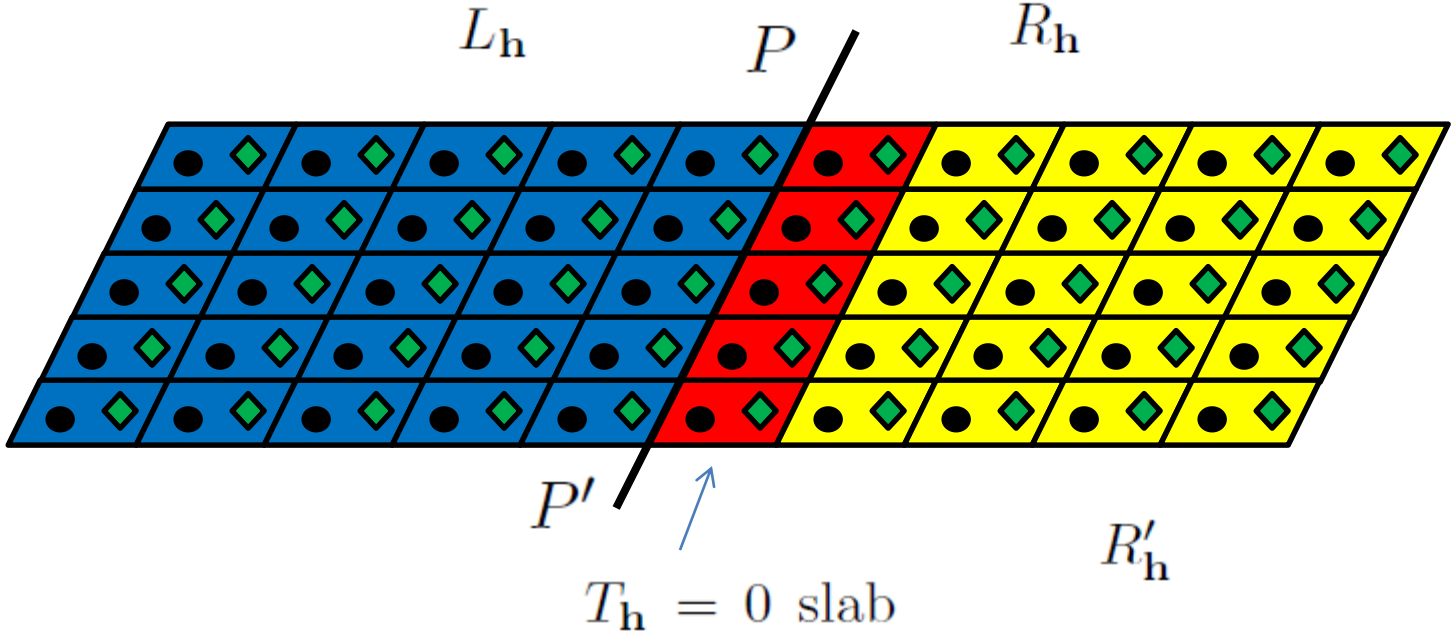
What we really need is the unweighted average of

$\overrightarrow{\overrightarrow{\varepsilon}}_{main}$ or $\mathbf{F_h}$



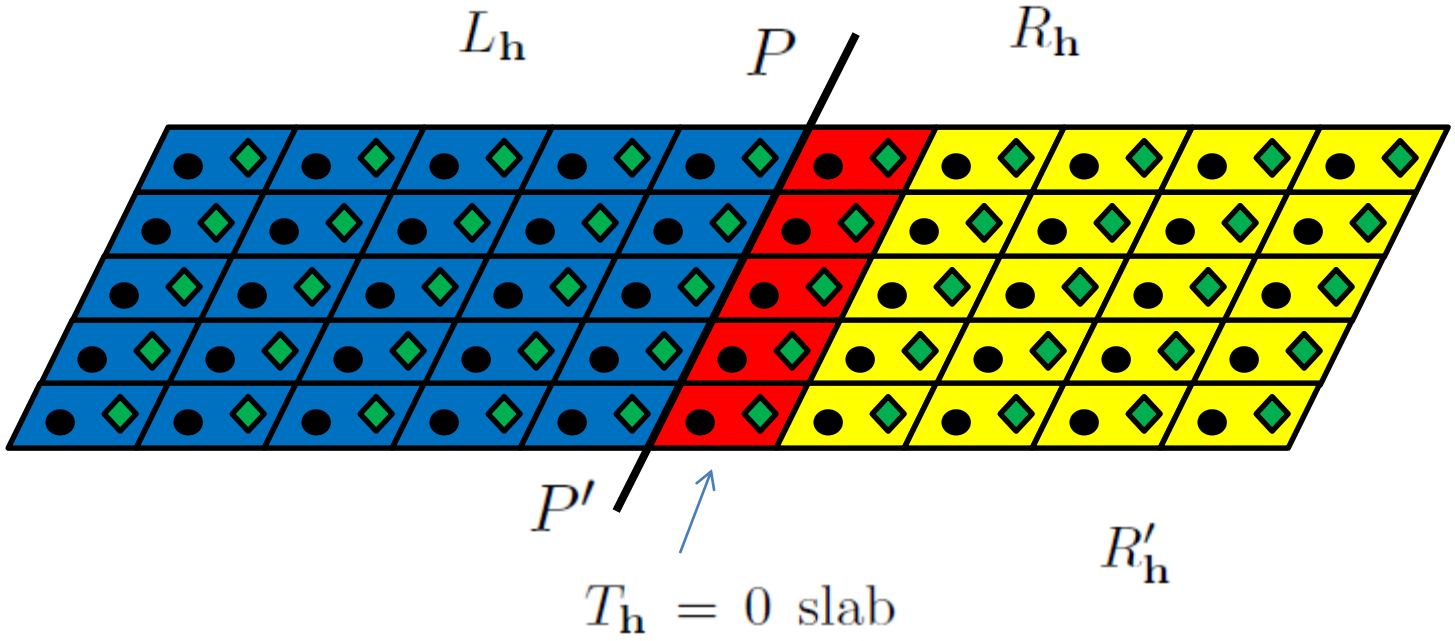
The total amount of such states can be represented by the volume of the MD cell Ω .

For easy description, let us divide the $R_{\mathbf{h}}$ part of the crystal into $T_{\mathbf{h}} = 0$ slab (red area) and $R'_{\mathbf{h}}$ part (yellow area).



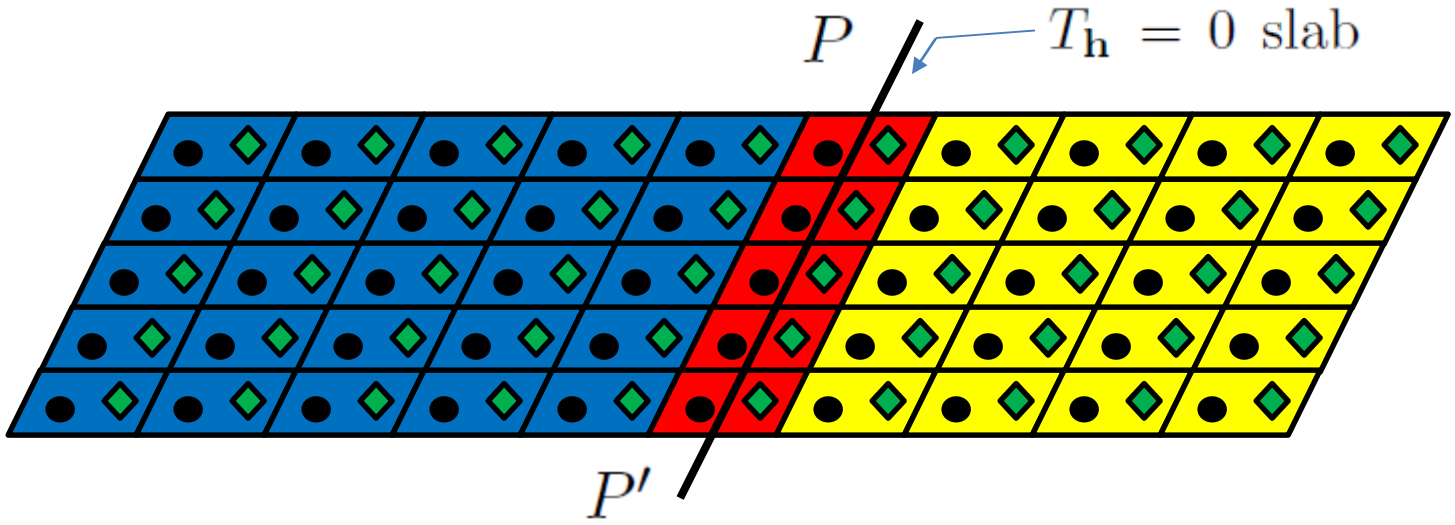
$$\mathbf{T} = T_{\mathbf{a}}\mathbf{a} + T_{\mathbf{b}}\mathbf{b} + T_{\mathbf{c}}\mathbf{c},$$

We will only consider anything new in the averaged $\mathbf{F_h}$, compared with $\mathbf{F_h}$ itself. This means there must be $s \geq 1$ particle(s) in $T_\mathbf{h} = 0$ slab in all-body interactions.



$$\mathbf{T} = T_\mathbf{a}\mathbf{a} + T_\mathbf{b}\mathbf{b} + T_\mathbf{c}\mathbf{c},$$

Supposing all possible locations for PP' plane is Ω , the probability for $\mathrm{MD\ particle}\ i_k$ appearing on the left side of it is

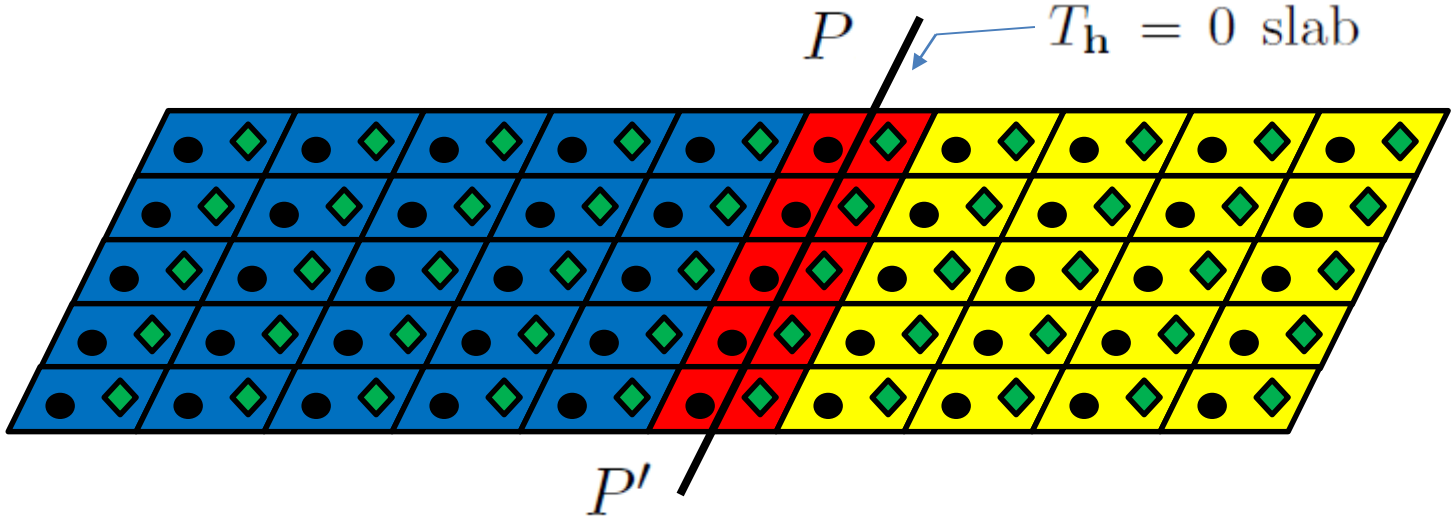


$$\frac{(\mathbf{h} - (\mathbf{r}_{i_k} - \mathbf{r}_0)) \cdot \sigma_{\mathbf{h}}}{\Omega} = \frac{(\mathbf{h}_0 - \mathbf{r}_{i_k}) \cdot \sigma_{\mathbf{h}}}{\Omega}$$

$\mathbf{r}_0$ is the position of the left-bottom and far-away vertex of the MD cell and $\mathbf{h}_0 = \mathbf{h} + \mathbf{r}_0$

A total of three cases

Case 1, additional $t \geq 1$ particle(s) in m-body interactions in the $L_{\mathbf{h}}$ part.



averaged net force acting on the s particles by the rest m particles

$$\mathbf{F}^{(m)}_{c1,s,t,\mathbf{h}} = \frac{1}{N_{\mathbf{h}}} \frac{1}{s!t!\,(m-t-s)!} \sum_{\{I_1,I_2,\cdots,I_s\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{s,\mathbf{h}}=0)} \sum_{\{I_{s+1},I_{s+2},\cdots,I_{s+t}\}}^{(I_{s+1,\mathbf{h}},I_{s+2,\mathbf{h}},\cdots,I_{s+t,\mathbf{h}}<0)} \sum_{\{I_{s+t+1},I_{s+t+2},\cdots,I_m\}}^{(I_{s+t+1,\mathbf{h}},I_{s+t+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}>0)} \times$$
$$\sum_{\mu=1}^{s} \frac{\left(\mathbf{h}_0 - \mathbf{r}_{i_\mu}\right)\cdot\sigma_{\mathbf{h}}}{\Omega} \mathbf{f}^{(m)}_{I_\mu}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m})$$

should be excluded from $\mathbf{F}_{\mathbf{h}}$, as it was unconditionally included in the $\mathbf{F}_{\mathbf{h}}$ previously.

Considering all possible

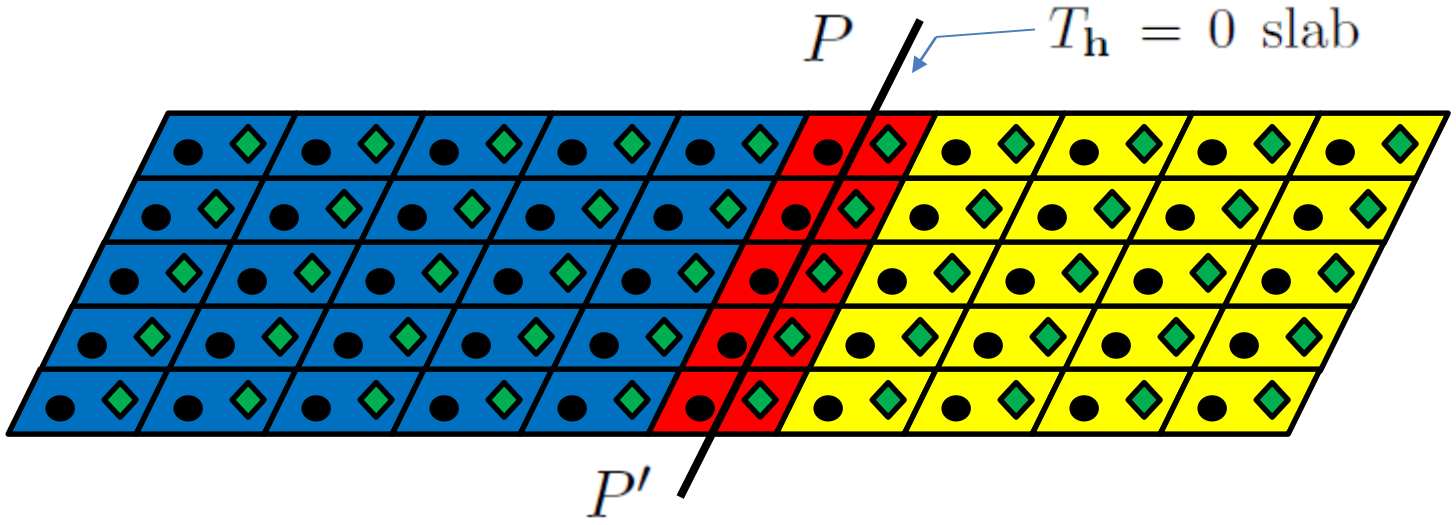
$$s' = s - 1 = 0, 1, 2, \cdots, m - t - 1$$

it can be reduced to

$$\mathbf{F}^{(m)}_{\boldsymbol{c1},t,\mathbf{h}} = \sum_{s'=0}^{m-t-1} \mathbf{F}^{(m)}_{\boldsymbol{c1},s,t,\mathbf{h}} =$$

$$= \sum_{i_1=1}^{n} \frac{(\mathbf{h}_0 - \mathbf{r}_{i_1}) \cdot \sigma_{\mathbf{h}}}{\Omega t! \, (m-t-1)!} \sum_{\{I_2, I_3, \cdots, I_{t+1}\}}^{(I_{2,\mathbf{h}}, I_{3,\mathbf{h}}, \cdots, I_{t+1,\mathbf{h}} < 0)} \sum_{\{I_{t+2}, I_{t+3}, \cdots, I_m\}}^{(I_{t+2,\mathbf{h}}, I_{t+3,\mathbf{h}}, \cdots, I_{m,\mathbf{h}} \geq 0)} \mathbf{f}^{(m)}_{i_1}(\mathbf{r}_{i_1}, \mathbf{r}_{I_2}, \mathbf{r}_{I_3}, \cdots, \mathbf{r}_{I_m}).$$

Case 2, no particles in $L_{\mathbf{h}}$ but at least one in the $R'_{\mathbf{h}}$ part of m-body interactions



Employing Newton's third law

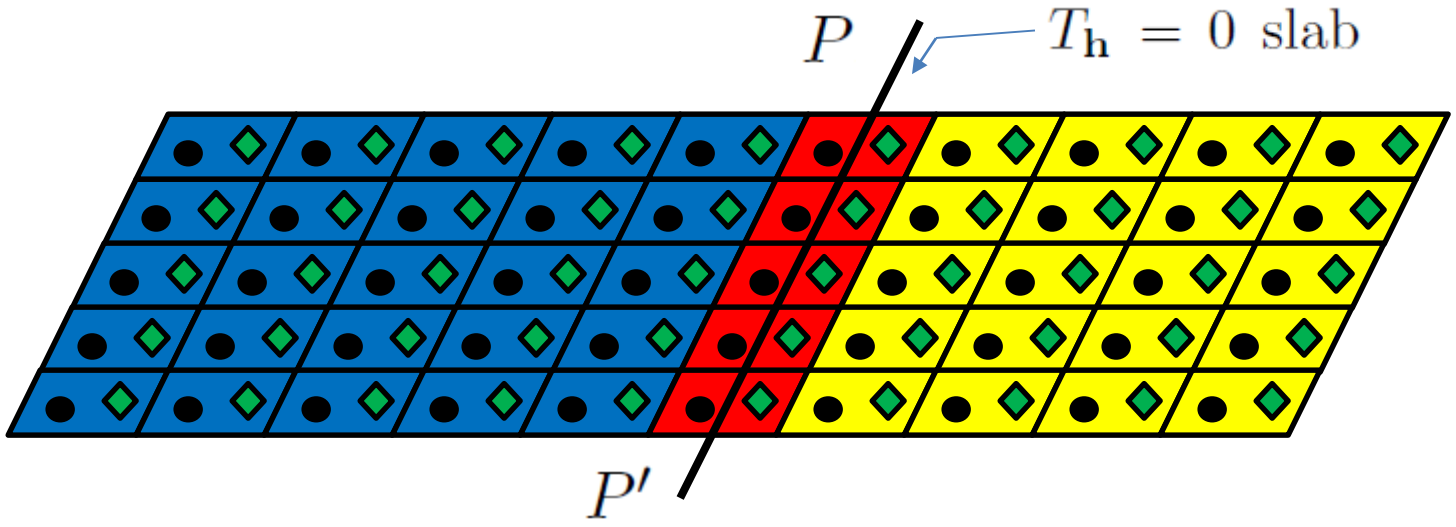
the following averaged force

$$\begin{aligned}
\mathbf{F}^{(m)}_{c2,s,\mathbf{h}} &= \frac{1}{N_{\mathbf{h}}}\frac{1}{s!\,(m-s)!}\sum_{\{I_1,I_2,\cdots,I_s\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{s,\mathbf{h}}=0)}\sum_{\{I_{s+1},I_{s+2},\cdots,I_m\}}^{(I_{s+1,\mathbf{h}},I_{s+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}>0)}\sum_{\mu=1}^{s}\frac{(\mathbf{h}_0-\mathbf{r}_{i_\mu})\cdot\sigma_{\mathbf{h}}}{\Omega}\mathbf{f}^{(m)}_{I_\mu}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{N_{\mathbf{h}}}\frac{1}{s!\,(m-s)!}\sum_{\{I_1,I_2,\cdots,I_s\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{s,\mathbf{h}}=0)}\sum_{\{I_{s+1},I_{s+2},\cdots,I_m\}}^{(I_{s+1,\mathbf{h}},I_{s+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}>0)}s\frac{(\mathbf{h}_0-\mathbf{r}_{i_1})\cdot\sigma_{\mathbf{h}}}{\Omega}\mathbf{f}^{(m)}_{I_1}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{(s-1)!\,(m-s)!}\sum_{i_1=1}^{n}\sum_{\{I_2,I_3,\cdots,I_s\}}^{(I_{2,\mathbf{h}},I_{3,\mathbf{h}},\cdots,I_{s,\mathbf{h}}=0)}\sum_{\{I_{s+1},I_{s+2},\cdots,I_m\}}^{(I_{s+1,\mathbf{h}},I_{s+2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}>0)}\frac{(\mathbf{h}_0-\mathbf{r}_{i_1})\cdot\sigma_{\mathbf{h}}}{\Omega}\mathbf{f}^{(m)}_{i_1}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}).
\end{aligned}$$

should be substracted from $\mathbf{F}_{\mathbf{h}}$.

Case 3, all particles in the m-body interactions are in the $T_{\mathbf{h}} = 0$ slab. Supposing particle I_m is the nearest to the right, the probability for PP' is between particle I_k and particle I_m is

$$\left(\mathbf{r}_{i_m} - \mathbf{r}_{i_k}\right) \cdot \sigma_{\mathbf{h}} / \Omega$$



Also using Newton's third law

the following averaged force

$$
\begin{aligned}
\mathbf{F}_{c3,\mathbf{h}}^{(m)} &= \frac{1}{N_{\mathbf{h}}}\frac{1}{m!}\sum_{\{I_1,I_2,\cdots,I_m\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}=0)}\sum_{\mu=1}^{m}\frac{\left(\mathbf{r}_{i_m}-\mathbf{r}_{i_\mu}\right)\cdot\sigma_{\mathbf{h}}}{\Omega}\mathbf{f}_{I_\mu}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{N_{\mathbf{h}}}\frac{1}{m!}\sum_{\{I_1,I_2,\cdots,I_m\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}=0)}\sum_{\mu=1}^{m}\frac{\left(\mathbf{h}_0-\mathbf{r}_{i_\mu}\right)\cdot\sigma_{\mathbf{h}}}{\Omega}\mathbf{f}_{I_\mu}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{N_{\mathbf{h}}}\frac{1}{m!}\sum_{\{I_1,I_2,\cdots,I_m\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}=0)}m\frac{\left(\mathbf{h}_0-\mathbf{r}_{i_1}\right)\cdot\sigma_{\mathbf{h}}}{\Omega}\mathbf{f}_{I_1}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{N_{\mathbf{h}}\Omega\,(m-1)!}\sum_{\{I_1,I_2,\cdots,I_m\}}^{(I_{1,\mathbf{h}},I_{2,\mathbf{h}},\cdots,I_{m,\mathbf{h}}=0)}\left(\mathbf{h}_0-\mathbf{r}_{i_1}\right)\cdot\sigma_{\mathbf{h}}\mathbf{f}_{I_1}^{(m)}(\mathbf{r}_{I_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}) \\
&= \frac{1}{\Omega\,(m-1)!}\sum_{i_1=1}^{n}\sum_{\{I_2,I_3,\cdots,I_m\}}^{(I_{2,\mathbf{h}},I_{3,\mathbf{h}},\cdots,I_{m,\mathbf{h}}=0)}\left(\mathbf{h}_0-\mathbf{r}_{i_1}\right)\cdot\sigma_{\mathbf{h}}\mathbf{f}_{i_1}^{(m)}(\mathbf{r}_{i_1},\mathbf{r}_{I_2},\mathbf{r}_{I_3},\cdots,\mathbf{r}_{I_m}).
\end{aligned}
$$

should be substracted from $\mathbf{F}_{\mathbf{h}}$.

Then $\mathbf{F_h}$ should be updated to the averaged

$$\overline{\mathbf{F}}'_{\mathbf{h}} = \mathbf{F_h} - \mathbf{F}^{(m)}_{c3,\mathbf{h}} - \sum_{s'=0}^{m-2} \mathbf{F}^{(m)}_{c2,s,\mathbf{h}} - \sum_{t=1}^{m-1} \mathbf{F}^{(m)}_{c1,t,\mathbf{h}}$$

$$= \mathbf{F_h} + \frac{1}{\Omega} \sum_{i_1=1}^{n} \mathbf{F}_{i_1} \mathbf{r}_{i_1} \cdot \sigma_{\mathbf{h}},$$

where

$$\mathbf{F}_{i_1} = \sum_{m=2}^{M} \mathbf{F}^{(m)}_{i_1}.$$

Then $\mathbf{F_h}$ should be updated to the averaged

$$\overline{\mathbf{F}}'_{\mathbf{h}} = \mathbf{F_h} + \frac{1}{\Omega}\sum_{i_1=1}^{n} \mathbf{F}_{i_1}\mathbf{r}_{i_1} \cdot \sigma_{\mathbf{h}} = \mathbf{F_h} + \overline{\overline{\varepsilon}}_p \cdot \sigma_{\mathbf{h}}$$

$$= \left(\overline{\overline{\varepsilon}}_{main} + \overline{\overline{\varepsilon}}_p\right) \cdot \sigma_{\mathbf{h}} = \overline{\overline{\varepsilon}} \cdot \sigma_{\mathbf{h}}$$

where

$$\overline{\overline{\varepsilon}} = \overline{\overline{\varepsilon}}_{main} + \overline{\overline{\varepsilon}}_p$$

$$\overline{\overline{\varepsilon}}_p = \frac{1}{\Omega}\sum_{i_1=1}^{n} \mathbf{F}_{i_1}\mathbf{r}_{i_1}$$

Then $\mathbf{F_h}$ should be updated to the averaged

$$\overline{\mathbf{F}}'_{\mathbf{h}} = \mathbf{F_h} + \vec{\vec{\varepsilon}}_p \cdot \sigma_{\mathbf{h}} = \vec{\vec{\varepsilon}} \cdot \sigma_{\mathbf{h}}$$

where $\vec{\vec{\varepsilon}} = \vec{\vec{\varepsilon}}_{main} + \vec{\vec{\varepsilon}}_p$, $\vec{\vec{\varepsilon}}_p = \frac{1}{\Omega} \sum_{i_1=1}^{n} \mathbf{F}_{i_1} \mathbf{r}_{i_1}$

Since

$$\vec{\vec{\varepsilon}}_{main} = \frac{-1}{\Omega} \left[\left(\frac{\partial E_{p,cell}}{\partial \mathbf{a}} \right) \mathbf{a} + \left(\frac{\partial E_{p,cell}}{\partial \mathbf{b}} \right) \mathbf{b} + \left(\frac{\partial E_{p,cell}}{\partial \mathbf{c}} \right) \mathbf{c} \right], \quad \mathbf{F}_i = -\frac{\partial E_{p,cell}}{\partial \mathbf{r}_i}$$

$$\vec{\vec{\varepsilon}} = -\frac{1}{\Omega} \sum_{\mathbf{z} \in \mathrm{DOF}} \left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}} \right) \mathbf{z}$$

DOF means all degrees of freedom, which are the period vectors and MD particle position vectors:

$$\mathbf{a},\ \mathbf{b},\ \mathbf{c},\quad \mathbf{r}_1, \mathbf{r}_2, \cdots, \text{and } \mathbf{r}_n.$$

Period Dynamics $(\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c})$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}}_{main} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \qquad \text{(first form)}$$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \qquad \text{(improved)}$$

where the full interaction tensor

$$\overrightarrow{\overrightarrow{\varepsilon}} = -\frac{1}{\Omega} \sum_{\mathbf{z} \in \mathrm{DOF}} \left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right) \mathbf{z}$$

The last major step

Instantaneous dynamical equations of the period vectors.

Statistics of the above dynamical equations over indistinguishable translated states

Forces associated with momentum transportation and statistics over particles' moving directions

Now let us consider

forces associated with transportation of momentum across geometric planes,

even without collision or any other interactions

Forces only due to momentum transportation

But what is such a force?

This seemingly controversial topic has been debated extensively.

Considering a single particle $m \neq 0$

without being acted by any regular force,
but running with a constant velocity $\mathbf{v} \neq 0$

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Since it passes through many planes, is there any additional force acting on it?

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As a matter of fact,

systems can be defined in two ways.

The first way,

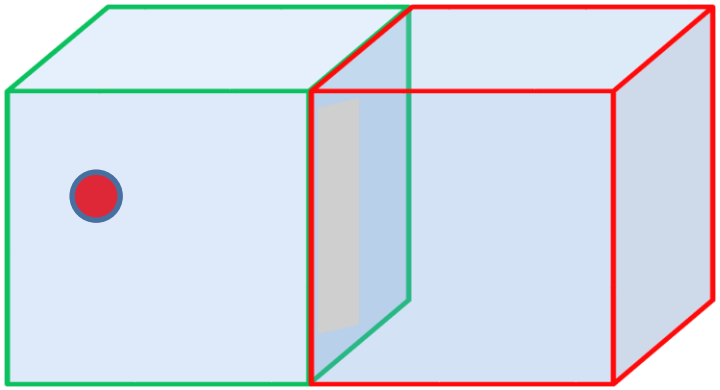
systems are defined based on materials or particles, as we do normally.

For example, the above single particle can be employed to define such a system, then no additional forces need to be considered, in order to satisfy Newton's Laws.

The other way,

systems are defined based on space.

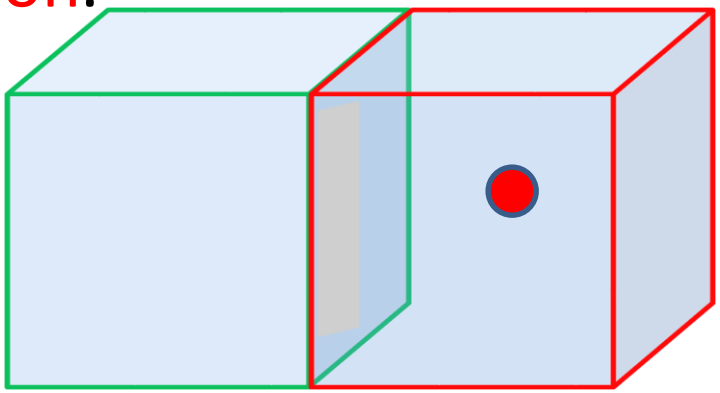
For example, for the same single particle running process, we can define systems like red and green boxes, only based on space.



Anything inside such a closed space belongs to the system. Otherwise, it is not.

When the particle passes through

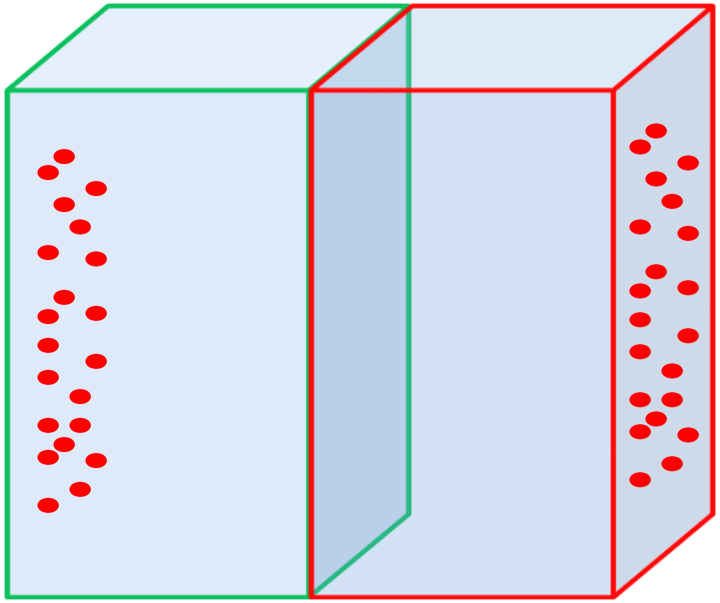
the plane between the red and green systems in $\triangle t$ the momentum of each system changes. In order to satisfy Newton's laws, we can say there are forces between the two systems: $m\mathbf{v}/\triangle t$ and $-m\mathbf{v}/\triangle t$ This is the force purely associated with momentum transportation.



These action and reaction forces between the two space-based systems satisfy Newton's third law.

An ideal gas

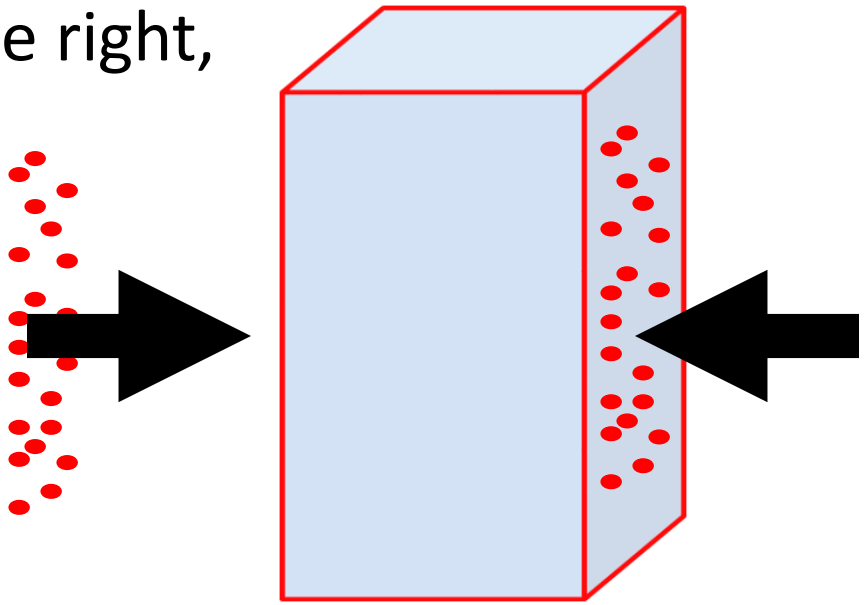
in a macroscopic equilibrium state in a closed container is cut into two halves:



Sorry for extremely simplified gas particles!

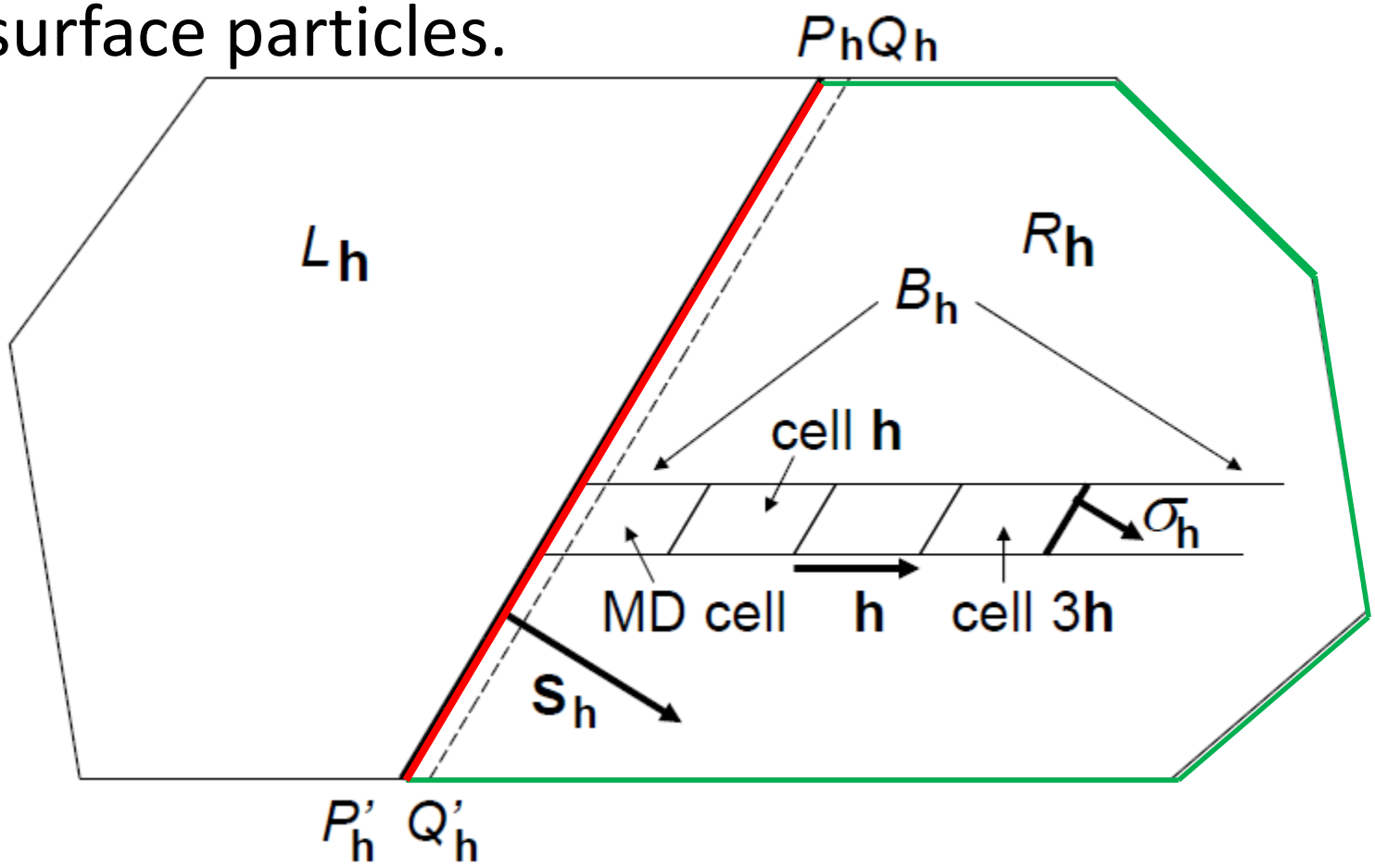
On the right half system

the force associated with momentum transportation on the left should be balanced by the regular force acted by the container during collisions with the gas particles on the right,



so that the right half gas can be in a macroscopic equilibrium state.

Our previous half systems are indeed defined based on space. Otherwise particles should be traced down when crossing the $P_{\mathrm{h}}P'_{\mathrm{h}}$ plane. Then such forces should be considered, while the external stress includes the forces in collisions between the external walls and the surface particles.

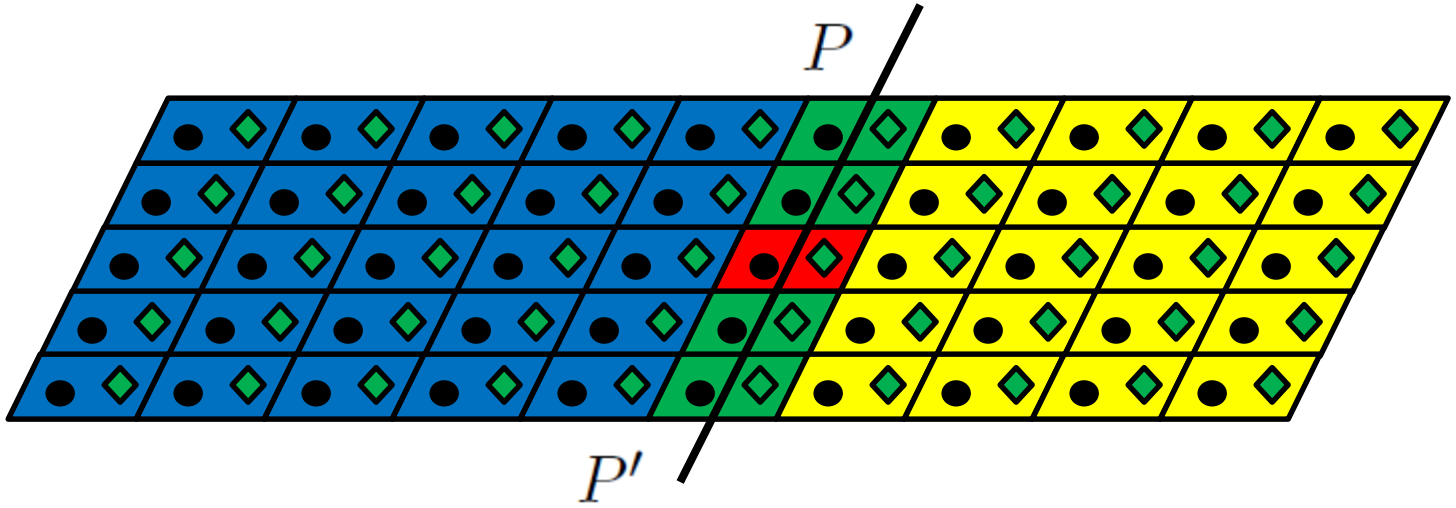


In all the previous translated-only states

During a unit time, particles pass $|\dot{\mathbf{r}}_i \cdot \sigma_{\mathbf{h}}|$ amount of states. Then the total

$$\frac{1}{\Omega}\sum_{i=1}^{n} m_i \dot{\mathbf{r}}_i \dot{\mathbf{r}}_i \cdot \sigma_{\mathbf{h}}$$

should be added into the dynamical equation.



Period Dynamics $(\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c})$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}}_{main} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \qquad \text{(first form)}$$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \qquad \text{(improved)}$$

$$\overrightarrow{\overrightarrow{\varepsilon}} = -\frac{1}{\Omega} \sum_{\mathbf{z} \in \mathrm{DOF}} \left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right) \mathbf{z}$$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\pi}}' + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \qquad \text{(further improved)}$$

where the instantaneous internal stress

$$\overrightarrow{\overrightarrow{\pi}}' = \overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\tau}}' \qquad \overrightarrow{\overrightarrow{\tau}}' = \frac{1}{\Omega} \sum_{i=1}^{n} m_i \dot{\mathbf{r}}_i \dot{\mathbf{r}}_i$$

The last consideration

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overline{\overline{\pi}}' + \overline{\overline{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}}$$ (further improved)

where the instantaneous internal stress

$$\overline{\overline{\pi}}' = \overline{\overline{\varepsilon}} + \overline{\overline{\tau}}'$$

$$\overline{\overline{\varepsilon}} = -\frac{1}{\Omega}\sum_{\mathbf{z}\in \mathrm{DOF}}\left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right)\mathbf{z} \quad , \quad \overline{\overline{\tau}}' = \frac{1}{\Omega}\sum_{i=1}^{n} m_i \dot{\mathbf{r}}_i \dot{\mathbf{r}}_i$$

The periods should not depend on the instantaneous directions of particles' microscopic motion, as they can be measured macroscopically under constant external pressure and temperature.

The last unweighted average of the

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overline{\overline{\pi}}' + \overline{\overline{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}}$$

(further improved)

where the instantaneous internal stress

$$\overline{\overline{\pi}}' = \overline{\overline{\varepsilon}} + \overline{\overline{\tau}}'$$

$$\overline{\overline{\varepsilon}} = -\frac{1}{\Omega}\sum_{\mathbf{z}\in \mathrm{DOF}}\left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right)\mathbf{z} \quad , \quad \overline{\overline{\tau}}' = \frac{1}{\Omega}\sum_{i=1}^{n} m_i \dot{\mathbf{r}}_i \dot{\mathbf{r}}_i$$

over all particles' moving directions.

Period Dynamics $(\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c})$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\pi}}' + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}}$$

(further improved)

$$\overrightarrow{\overrightarrow{\pi}}' = \overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\tau}}' \qquad \overrightarrow{\overrightarrow{\tau}}' = \frac{1}{\Omega}\sum_{i=1}^{n} m_i \dot{\mathbf{r}}_i \dot{\mathbf{r}}_i$$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\pi}} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}}$$

(last)

where the internal stress $\overrightarrow{\overrightarrow{\pi}} = \overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\tau}}$

$$\overrightarrow{\overrightarrow{\varepsilon}} = -\frac{1}{\Omega}\sum_{\mathbf{z}\in \mathrm{DOF}} \left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right)\mathbf{z}$$

$$\overrightarrow{\overrightarrow{\tau}} = \frac{1}{3\Omega}\sum_{i=1}^{n} m_i \left|\dot{\mathbf{r}}_i\right|^2 \overrightarrow{\overrightarrow{I}} = \frac{2}{3\Omega} E_{k,MD} \overrightarrow{\overrightarrow{I}}$$

Period Dynamics $(\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c})$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}}_{main} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}}$$ (first form)

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}}$$ (improved)

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$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\pi}} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}}$$

$$\overrightarrow{\overrightarrow{\tau}} = \frac{2}{3\Omega} E_{k,MD}\ \overrightarrow{\overrightarrow{I}}$$ (last)

$$\overrightarrow{\overrightarrow{\pi}} = \overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\tau}}$$

Summary

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i \quad (i = 1, 2, \cdots, n),$$

$$\alpha_{\mathbf{h},\mathbf{h}} \ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\pi}} + \overrightarrow{\overrightarrow{\Upsilon}} \right) \cdot \sigma_{\mathbf{h}} \qquad (\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c})$$

$$\overrightarrow{\overrightarrow{\pi}} = \overrightarrow{\overrightarrow{\varepsilon}} + \overrightarrow{\overrightarrow{\tau}}$$

$$\overrightarrow{\overrightarrow{\tau}} = \frac{2}{3\Omega} E_{k,MD} \overrightarrow{\overrightarrow{I}}$$

$$\overrightarrow{\overrightarrow{\varepsilon}} = -\frac{1}{\Omega} \sum_{\mathbf{z} \in \mathrm{DOF}} \left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}} \right) \mathbf{z}$$

Further extension

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\pi}} + \overrightarrow{\overrightarrow{\Upsilon}}\right) \cdot \sigma_{\mathbf{h}} \qquad (\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c})$$

$$\overrightarrow{\overrightarrow{\pi}} = -\frac{1}{\Omega} \sum_{\mathbf{z} \in \mathrm{DOF}} \left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right) \mathbf{z} + \frac{2}{3\Omega} E_{k,MD}\ \overrightarrow{\overrightarrow{I}}$$

by combining with forces based on Quantum mechanics, then applied, especially in piezoelectric and piezomagnetic simulations.

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Questions?

Thank you much very for your attention!

More details:
https://arxiv.org/abs/cond-mat/0209372
https://arxiv.org/abs/cond-mat/0505251
and some reprints available for picking up.

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Appendixes

GROMACS

Groningen Machine for Chemical Simulations

USER MANUAL

Version 5.0.7

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If you allow full anisotropic deformations and use constraints you might have to scale more slowly or decrease your timestep to avoid errors from the constraint algorithms. It is important to note that although the Berendsen pressure control algorithm yields a simulation with the correct average pressure, it does not yield the exact NPT ensemble, and it is not yet clear exactly what errors this approximation may yield.

Parrinello-Rahman pressure coupling

In cases where the fluctuations in pressure or volume are important *per se* (*e.g.* to calculate thermodynamic properties), especially for small systems, it may be a problem that the exact ensemble is not well defined for the weak-coupling scheme, and that it does not simulate the true NPT ensemble.

GROMACS also supports constant-pressure simulations using the Parrinello-Rahman approach [39, 40], which is similar to the Nosé-Hoover temperature coupling, and in theory gives the true NPT ensemble. With the Parrinello-Rahman barostat, the box vectors as represented by the matrix $\boldsymbol{b}$ obey the matrix equation of motion[2]

$$\frac{\mathrm{d}\boldsymbol{b}^2}{\mathrm{d}t^2} = V\boldsymbol{W}^{-1}\boldsymbol{b}'^{-1}\left(\boldsymbol{P}-\boldsymbol{P}_{ref}\right). \tag{3.62}$$

The volume of the box is denoted V, and $\boldsymbol{W}$ is a matrix parameter that determines the strength of the coupling. The matrices $\boldsymbol{P}$ and $\boldsymbol{P}_{ref}$ are the current and reference pressures, respectively.

The equations of motion for the particles are also changed, just as for the Nosé-Hoover coupling. In most cases you would combine the Parrinello-Rahman barostat with the Nosé-Hoover thermostat, but to keep it simple we only show the Parrinello-Rahman modification here:

$$\frac{\mathrm{d}^2\boldsymbol{r}_i}{\mathrm{d}t^2} = \frac{\boldsymbol{F}_i}{m_i} - \boldsymbol{M}\frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t}, \tag{3.63}$$

$$\boldsymbol{M} = \boldsymbol{b}^{-1}\left[\boldsymbol{b}\frac{\mathrm{d}\boldsymbol{b}'}{\mathrm{d}t} + \frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}t}\boldsymbol{b}'\right]\boldsymbol{b}'^{-1}. \tag{3.64}$$

Comparison

$$\frac{\mathrm{d}\boldsymbol{b}^2}{\mathrm{d}t^2} = V\boldsymbol{W}^{-1}\boldsymbol{b}'^{-1}\left(\boldsymbol{P} - \boldsymbol{P}_{ref}\right)$$

$$\alpha_{\mathbf{h},\mathbf{h}}\ddot{\mathbf{h}} = \left(\overrightarrow{\overrightarrow{\pi}} + \overrightarrow{\overrightarrow{\Upsilon}}\right)\cdot\sigma_{\mathbf{h}} \qquad (\mathbf{h} = \mathbf{a},\ \mathbf{b},\ \mathbf{c})$$

$$\overrightarrow{\overrightarrow{\pi}} = -\frac{1}{\Omega}\sum_{\mathbf{z}\in\mathrm{DOF}}\left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right)\mathbf{z} + \frac{2}{3\Omega}E_{k,MD}\ \overrightarrow{\overrightarrow{I}}$$

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LAMMPS Users Manual

4 May 2017 version

http://lammps.sandia.gov - Sandia National Laboratories

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where U is the system potential energy, P_t is the desired hydrostatic pressure, V and V_0 are the system and reference volumes, respectively. *E_strain* is the strain energy expression proposed by Parrinello and Rahman (Parrinello1981). Taking derivatives of E w.r.t. the box dimensions, and setting these to zero, we find that at the minimum of the objective function, the global system stress tensor **P** will satisfy the relation:

750

LAMMPS Users Manual

$$\mathbf{P} = P_t\mathbf{I} + \mathbf{S}_t \left(\mathbf{h}_0^{-1}\right)^t \mathbf{h}_{0d}$$

where **I** is the identity matrix, **h**_0 is the box dimension tensor of the reference cell, and **h**_0*d* is the diagonal part of **h**_0. **S**_*t* is a symmetric stress tensor that is chosen by LAMMPS so that the upper-triangular components of **P** equal the stress tensor specified by the user.

This equation only applies when the box dimensions are equal to those of the reference dimensions. If this is not the case, then the converged stress tensor will not equal that specified by the user. We can resolve this problem by periodically resetting the reference dimensions. The keyword *nreset_ref* controls how often this is done. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. A value of *nstep* means that every *nstep* minimization steps, the reference dimensions are set to those of the current simulation domain. Note that resetting the reference dimensions changes the objective function and gradients, which sometimes causes the minimization to fail. This can be resolved by changing the value of *nreset*, or simply continuing the minimization from a restart file.

Comparison

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$$\overrightarrow{\overrightarrow{\pi}} = -\frac{1}{\Omega} \sum_{\mathbf{z} \in \mathrm{DOF}} \left(\frac{\partial E_{p,cell}}{\partial \mathbf{z}}\right) \mathbf{z} + \frac{2}{3\Omega} E_{k,MD}\ \overrightarrow{\overrightarrow{I}}$$

Formula