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Structure of Yukawa (Dusty Plasma) Mixtures

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Parameters characterizing the structure of confined Yukawa system are estimated for 'dusty plasmas', clouds of charged macroscopic particles formed near the boundary between plasma and the sheath and levitated by negatively biased electrode. When we have dust particles with different ratios of charge to mass, they form a two-dimensional Yukawa mixture or separate two-dimensional one-component Yukawa systems, depending on the charge density in the sheath and number density of dust particles. In order to provide a basis for numerical simulations on Yukawa mixtures including Coulombic case, we summarize mathematical expressions necessary for molecular dynamics.

Part I Characteristic Parameters for Mixtures

1 Introduction

Physics of dusty plasmas, assemblies of macroscopic particles immersed in plasmas, have attracted keen interest of researchers as an important practical problem in plasma processes of semiconductor manufacturing and also as a subject of basic statistical physics.[1] Observation of crystal-like structures in dusty plasmas[2, 3, 4, 5] have added a new example to the classical Coulomb lattice which was predicted more than sixty years ago.[6]

In our recent works,[7, 8, 9, 10, 11, 12, 13] we have regarded dust particles as interacting via the isotropic repulsive Yukawa potential

$$\frac{q^2}{r}\exp(-\kappa r), \tag{1.1}$$

where $-q$ is the (negative) charge on a dust particle, and trapped in a one-dimensional potential well of the form

$$v_{ext}(z) = \frac{1}{2}kz^2. \tag{1.2}$$

We have analyzed the phase diagram for the structure of this confined Yukawa system by molecular dynamics simulations and theoretical approaches.

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As for the interaction between dust particles, it has been pointed out that there exists an anisotropic interaction coming from the ion flow in the sheath.[14, 15, 16, 17] The most important result of this anisotropic potential may be the phenomenon of alignment of dust particles along the z-direction often observed in experiments. There also exist, however, experiments where such alignment is not apparent[3] and we may have the cases where the isotropic part of interaction potential plays the central role to determine the overall structure in z-direction, even if the configurations in the xy-plane relative to adjacent layers are affected by the anisotropic part.

Defining the mean distance between dust particles a by

$$a = \frac{1}{(\pi N_S)^{1/2}} \tag{1.3}$$

from the surface number density of dust particles N_S, we express the strength of screening by surrounding plasma by a parameter

$$\xi = \kappa a. \tag{1.4}$$

We have also introduced a parameter η defined by

$$\eta = \frac{\pi^{1/2}}{2} \frac{(1/2)ka^2}{q^2/a} \tag{1.5}$$

to describe the relative strength of mutual repulsions and the confining potential. Structures at low temperatures are determined by a competition between these two forces and are expressed as a phase diagram in the (ξ, η)-plane.[9]

It has been found in experiments that the radius of dust particles of the same kind appearing in plasma processes has rather small dispersion. There may be the cases where different kinds of macroscopic particles coexist in plasmas and their separation is necessary. In this part, we clarify the origin of the one-dimensional confining potential and discuss various possibilities of structures for mixtures of Yukawa particles.

2 Parameters Characterizing Confining Potential

We consider the case where our dusty plasma is formed above a horizontal plane electrode which is wide enough to regard the system under consideration as one-dimensional. A typical example of environment of our dusty plasma is shown in Fig.1. Dust particles are under the vertical gravitational field and are levitated by the electric field between the negatively biased electrode and the bulk part of plasma.

Let us assume that the density of charges in the sheath (except for those of dust particles) is given by en_{sheath}, e being the elementary charge, and is nearly constant in the domain where dust crystals are formed. When we take the z-axis in the opposite direction to the gravitation, the gravitational and the electrostatic potentials for a dust particle of mass m and charge $-q$ is written as mgz and as $2\pi qen_{sheath}z^2$, respectively. Thus dust particles are in the potential well $(z < 0)$

$$\phi_{ext}(z) = 2\pi qen_{sheath}z^2 + mgz = 2\pi qen_{sheath}(z - z_0)^2 + const, \tag{2.1}$$

where

$$z_0 = -\frac{mg}{4\pi qen_{sheath}} = -\frac{g}{4\pi en_{sheath}}\frac{m}{q} < 0. \tag{2.2}$$

In this case, $k = 4\pi q e n_{sheath}$ and η is calculated as

$$\eta = \left(\frac{e}{q}\right)\left(\frac{n_{sheath}}{N_S^{3/2}}\right). \tag{2.3}$$

When we have only one species of dust particles, the structure at low temperatures is completely determined by parameters ξ and η. In the case where there are two or more species of dusts, we have to also take the dependence of z_0 on species into account. We thus define a parameter δ by

$$\delta = -\frac{z_0}{a} = \frac{1}{2}\frac{mga}{2\pi q e n_{sheath} a^2} = \frac{g}{4\pi e n_{sheath} a}\frac{m}{q} \tag{2.4}$$

to represent the separation in z-direction: The equilibrium position which is proportional to the charge to mass ratio q/m is compared with the mean distance a.

For a typical case of dust particle with the charge $q = 10^4 e$ and $m_0 = 10^{-13}\text{kg} = 10^{-10}\text{g}$, parameters η and δ are given by

$$\eta = 10^2 \times \left(\frac{10^4 e}{q}\right)\left(\frac{n_{sheath}}{10^9\text{cm}^{-3}}\right)\left(\frac{1\text{mm}^{-2}}{N_S}\right)^{3/2}, \tag{2.5}$$

$$\delta = 6.1 \cdot 10^{-2} \times \left(\frac{10^4 e}{q}\right)\left(\frac{m}{m_0}\right)\left(\frac{N_S}{1\text{mm}^{-2}}\right)^{1/2}\left(\frac{10^9\text{cm}^{-3}}{n_{sheath}}\right). \tag{2.6}$$

Values of these parameters are shown in Fig.2.

According to the values of η and δ, we have four cases. When $\eta \gg 1$ and $\delta \ll 1$, the Yukawa mixture forms a two-dimensional system or the two-dimensional Yukawa mixture. When $\eta \gg 1$ and $\delta \gg 1$, we have separated two-dimensional Yukawa systems, each being composed of one species. When $\eta \ll 1$ and $\delta \ll 1$, we have a mixture of Yukawa particles with finite thickness. When $\eta \ll 1$ and $\delta \gg 1$, we have two separate one-component Yukawa systems with finite thicknesses. These cases are illustrated in Fig.3.

As shown above, mixtures of Yukawa particles are expected to have a rich class of structures at low temperatures. When the axis of temperature is taken into account, their behavior may be even more interesting. One of powerful methods for the analysis of these classical systems is the large scale molecular dynamics simulation. In the next part, we give mathematical basis of such a simulation which is now in progress.

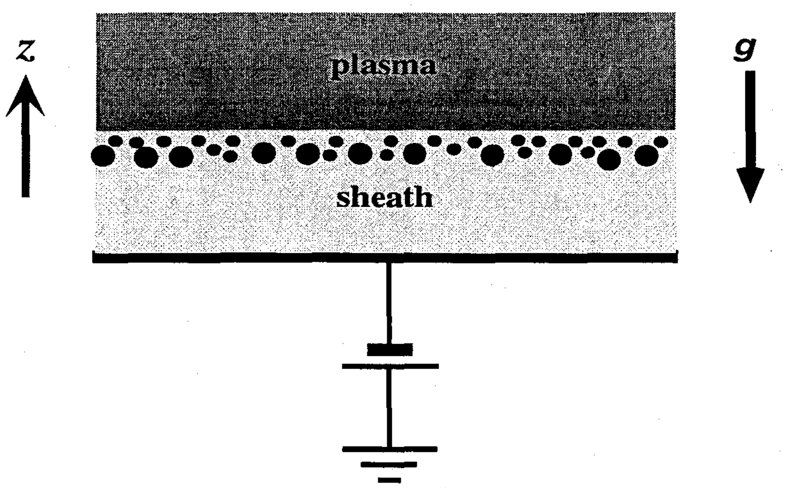

Fig.1. Dusty plasma confined near the boundary of sheath and plasma bulk.

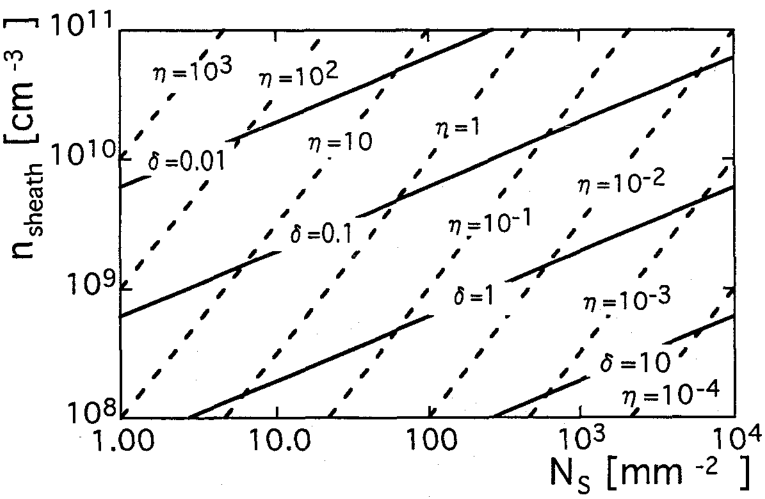

Fig.2. Values of characteristic parameters η and δ.

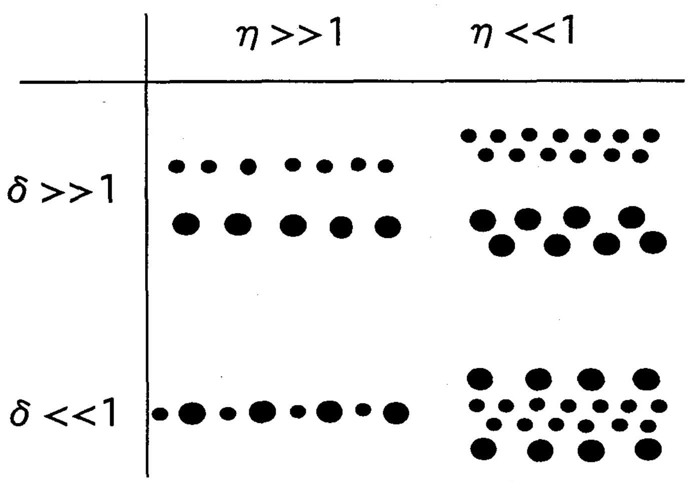

Fig.3. Structures of confined Yukawa mixture.

Part II Molecular Dynamics

3 Formulation for Yukawa Mixtures

In this part, we summarize some mathematical expressions for molecular dynamics of mixtures of Yukawa particles. Our system is composed of particles $i = 1, 2, ..., N$ with mass m_i and charge q_i interacting via the Yukawa interaction

$$q_i q_j v(r) \tag{3.1}$$

where

$$v(r) = \frac{1}{r}\exp(-\kappa r). \tag{3.2}$$

As external conditions, we consider two cases: (1) Three-dimensional system with constant volume or under constant pressure, and (2) The system confined in one direction with constant volume or under constant pressure in remaining two directions. In the first case, we impose periodic boundary conditions in three directions and in the second, in two directions. In order to reduce the effect of boundary conditions on dynamics of the system, we include the deformation of fundamental vectors of periodicity in our formulation.[18, 19]

4 Dynamics for Microcanonical Ensemble

We here summarize molecular dynamics for the microcanonical ensemble. In what follows, the dot denotes the time derivative as

$$\dot{f}(t) = \frac{df(t)}{dt}. \tag{4.1}$$

In order to impose the periodic boundary conditions, we express the coordinates of a particle as

$$\mathbf{r} = \mathsf{h} \cdot \mathbf{x} \tag{4.2}$$

in the case of periodic boundary conditions in three dimensions. Here h is a 3×3 tensor composed of fundamental (column) vectors $\mathbf{a}, \mathbf{b}$, and $\mathbf{c}$ as

$$\mathsf{h} = (\mathbf{a}, \mathbf{b}, \mathbf{c}), \tag{4.3}$$

and the volume of our unit cell is given by

$$V_0 = \det \mathsf{h}. \tag{4.4}$$

For Yukawa system with two-dimensional periodicity $\{\mathbf{P}\}$ in the xy plane, we define h as a 2×2 tensor and express the coordinate

$$\mathbf{r} = (\mathbf{R}, z) \tag{4.5}$$

or

$$\mathbf{r} = \mathbf{R} + z\hat{z} \tag{4.6}$$

as

$$\mathbf{R} = \mathsf{h} \cdot \mathbf{X}, \tag{4.7}$$

$\hat{z}$ being the unit vector in the z-direction. The area of the cross section of the unit cell in xy-plane is given by

$$S_0 = \det \mathsf{h}. \tag{4.8}$$

4.1 Dynamics with fixed periodic boundaries

We first consider the simplest case where the vectors representing the periodicity are fixed. The Lagrangian is given by the standard form as

$$\mathcal{L}(\{\mathbf{r}_i, \dot{\mathbf{r}}_i\}) = \sum_{i=1}^{N} \frac{m_i}{2} \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i - U(\{\mathbf{r}_i\}), \tag{4.9}$$

where $U(\{\mathbf{r}_i\})$ is the potential energy

$$U(\{\mathbf{r}_i\}) = \frac{1}{2} \sum_{i,j(i\neq j)}^{N} q_i q_j v(|\mathbf{r}_i - \mathbf{r}_j|), \tag{4.10}$$

and we have naturally

$$\dot{\mathbf{r}}_i = \mathsf{h} \cdot \dot{\mathbf{x}}_i. \tag{4.11}$$

Equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \mathbf{r}_i} = 0, \tag{4.12}$$

or

$$m_i \frac{d^2}{dt^2} \mathbf{r}_i = -\frac{\partial}{\partial \mathbf{r}_i} U. \tag{4.13}$$

The momentum is defined by

$$\mathbf{p}_i = m_i \dot{\mathbf{r}}_i \tag{4.14}$$

and the Hamiltonian is given by

$$\mathcal{H} = \sum_i \frac{1}{2m_i} \mathbf{p}_i \cdot \mathbf{p}_i + U(\{\mathbf{r}_i\}). \tag{4.15}$$

We have the conservation of total energy in the form

$$\frac{d}{dt}\mathcal{H} = 0. \tag{4.16}$$

4.2 Dynamics with deformable periodic boundaries

4.2.1 Periodicity in three dimensions

A method to take the deformation of fundamental vectors of periodicity is to rewrite the Lagrangian into the form[18]

$$\mathcal{L}(\{\mathbf{x}_i, \dot{\mathbf{x}}_i\}, \mathsf{h}, \dot{\mathsf{h}}) = \sum_i \frac{m_i}{2} \dot{\mathbf{x}}_i \cdot \mathsf{G} \cdot \dot{\mathbf{x}}_i - U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{W}{2} \mathrm{Tr}\left[\dot{\mathsf{h}}^t \cdot \dot{\mathsf{h}}\right], \tag{4.17}$$

where

$$\mathsf{G} = \mathsf{h}^t \cdot \mathsf{h}. \tag{4.18}$$

The positive parameter W corresponds to the mass of the frame of coordinates. The value of W is arbitrary in principle but to be optimized in practice. In this case, velocities are *defined* by

$$\mathbf{v}_i \equiv \mathsf{h} \cdot \dot{\mathbf{x}}_i. \tag{4.19}$$

The equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \mathbf{x}_i} = 0 \tag{4.20}$$

and

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{h}_{\alpha\beta}}\right) - \frac{\partial \mathcal{L}}{\partial h_{\alpha\beta}} = 0, \tag{4.21}$$

or

$$m_i \frac{d}{dt}\mathsf{G} \cdot \frac{d}{dt}\mathbf{x}_i = -\frac{\partial}{\partial \mathbf{x}_i} U \tag{4.22}$$

and

$$W \frac{d^2}{dt^2}\mathsf{h} = \Pi \cdot \sigma. \tag{4.23}$$

Tensors Π and σ are given respectively by

$$\Pi = \frac{1}{V_0}\left\{\sum_i m_i \left(\mathsf{h} \cdot \dot{\mathbf{x}}_i\right)\left(\mathsf{h} \cdot \dot{\mathbf{x}}_i\right) - \frac{1}{2}\sum_{i,j(i\neq j)} q_i q_j \sum_{\mathbf{p}} \frac{\left(\mathbf{r}_{ij} - \mathbf{p}\right)\left(\mathbf{r}_{ij} - \mathbf{p}\right)}{|\mathbf{r}_{ij} - \mathbf{p}|} \frac{\partial v\left(|\mathbf{r}_{ij} - \mathbf{p}|\right)}{\partial |\mathbf{r}_{ij} - \mathbf{p}|}\right\} + \Pi_0, \tag{4.24}$$

$$\Pi_0 = -\frac{1}{2V_0}\left(\sum_i q_i^2\right)\sum_{\mathbf{p}\neq 0} \frac{\mathbf{p}\mathbf{p}}{p}\frac{\partial v\left(p\right)}{\partial p}, \tag{4.25}$$

and

$$\sigma = V_0 \left(\mathsf{h}^t\right)^{-1}. \tag{4.26}$$

The momenta are defined by

$$\mathbf{p}_i = m_i \mathsf{G} \cdot \dot{\mathbf{x}}_i \tag{4.27}$$

and

$$\mu = W\dot{\mathsf{h}}, \tag{4.28}$$

and the Hamiltonian is given by

$$\mathcal{H} = \sum_i \frac{1}{2m_i}(\mathsf{G}^{-1} \cdot \mathbf{p}_i) \cdot \mathbf{p}_i + U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{1}{2W}\mathrm{Tr}(\mu^t \cdot \mu). \tag{4.29}$$

The conservation of Hamiltonian is written as

$$\frac{d}{dt}\mathcal{H} = 0. \tag{4.30}$$

4.2.2 Periodicity in two dimensions

In this case, h, G, and σ are 2×2 tensors defined similarly to the case of three-dimensional periodicity. The Lagrangian is given by

$$\mathcal{L}(\{\mathbf{X}_i, z_i, \dot{\mathbf{X}}_i, \dot{z}_i\}, \mathsf{h}, \dot{\mathsf{h}}) = \sum_i \frac{m_i}{2}\dot{\mathbf{X}}_i \cdot \mathsf{G} \cdot \dot{\mathbf{X}}_i + \sum_i \frac{m_i}{2}\dot{z}_i\dot{z}_i - U(\mathsf{h}, \{\mathbf{X}_i, z_i\}) + \frac{W}{2}\mathrm{Tr}\left[\dot{\mathsf{h}}^t \cdot \dot{\mathsf{h}}\right]. \quad (4.31)$$

Velocities in two dimensions are *defined* by

$$\dot{\mathbf{R}}_i \equiv \mathsf{h} \cdot \dot{\mathbf{X}}_i. \quad (4.32)$$

Equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{X}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \mathbf{X}_i} = 0, \quad (4.33)$$

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{z}_i}\right) - \frac{\partial \mathcal{L}}{\partial z_i} = 0, \quad (4.34)$$

and

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{h}_{\alpha\beta}}\right) - \frac{\partial \mathcal{L}}{\partial h_{\alpha\beta}} = 0, \quad (4.35)$$

or

$$m_i \frac{d}{dt}\mathsf{G} \cdot \frac{d}{dt}\mathbf{X}_i = -\frac{\partial}{\partial \mathbf{X}_i}U, \quad (4.36)$$

$$m_i \frac{d^2}{dt^2}z_i = -\frac{\partial}{\partial z_i}U, \quad (4.37)$$

and

$$W\frac{d^2}{dt^2}\mathsf{h} = \Pi \cdot \sigma. \quad (4.38)$$

Here Π and σ are defined by

$$\Pi = \frac{1}{S_0}\left\{\sum_i m_i \left(\mathsf{h} \cdot \dot{\mathbf{X}}_i\right)\left(\mathsf{h} \cdot \dot{\mathbf{X}}_i\right) - \frac{1}{2}\sum_{i,j(i \neq j)} q_i q_j \sum_{\mathbf{P}} \frac{(\mathbf{R}_{ij} - \mathbf{P})(\mathbf{R}_{ij} - \mathbf{P})}{|\mathbf{r}_{ij} - \mathbf{P}|}\frac{\partial v(|\mathbf{r}_{ij} - \mathbf{P}|)}{\partial |\mathbf{r}_{ij} - \mathbf{P}|}\right\} + \Pi_0, \quad (4.39)$$

$$\Pi_0 = -\frac{1}{2S_0}\left(\sum_i q_i^2\right)\sum_{\mathbf{P} \neq 0}\frac{\mathbf{PP}}{P}\frac{\partial}{\partial P}v(P), \quad (4.40)$$

and

$$\sigma = S_0\left(\mathsf{h}^t\right)^{-1}. \quad (4.41)$$

5 Dynamics with Deformable Periodic Boundaries under External Pressure

The external pressure $p_{ext}(t)$ is taken into account by adding

$$-p_{ext}(t)\det \mathsf{h} = -p_{ext}(t)V_0 \quad (5.1)$$

to the Lagrangian. The Lagrangian is then written as

$$\mathcal{L}(\{\mathbf{x}_i, \dot{\mathbf{x}}_i\}, \mathsf{h}, \dot{\mathsf{h}}, t) = \sum_i \frac{m_i}{2} \dot{\mathbf{x}}_i \cdot \mathsf{G} \cdot \dot{\mathbf{x}}_i - U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{W}{2} \mathrm{Tr}\left[\dot{\mathsf{h}}^t \cdot \dot{\mathsf{h}}\right] - p_{ext}(t) \det \mathsf{h}. \tag{5.2}$$

Equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \mathbf{x}_i} = 0 \tag{5.3}$$

and

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{h}_{\alpha\beta}}\right) - \frac{\partial \mathcal{L}}{\partial h_{\alpha\beta}} = 0, \tag{5.4}$$

or

$$m_i \frac{d}{dt} \mathsf{G} \cdot \frac{d}{dt} \mathbf{x}_i = -\frac{\partial}{\partial \mathbf{x}_i} U \tag{5.5}$$

and

$$W \frac{d^2}{dt^2} \mathsf{h} = [\Pi - p_{ext}(t) \mathsf{I}] \cdot \sigma. \tag{5.6}$$

The momenta are defined by

$$\mathbf{p}_i = m_i \mathsf{G} \cdot \dot{\mathbf{x}}_i \tag{5.7}$$

and

$$\mu = W \dot{\mathsf{h}}, \tag{5.8}$$

and the Hamiltonian is given by

$$\mathcal{H} = \sum_i \frac{1}{2m_i} (\mathsf{G}^{-1} \cdot \mathbf{p}_i) \cdot \mathbf{p}_i + U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{1}{2W} \mathrm{Tr}(\mu^t \cdot \mu) + p_{ext}(t) \det \mathsf{h}. \tag{5.9}$$

In this case, the conservation of Hamiltonian is written as

$$\frac{d}{dt} \mathcal{H} = \det \mathsf{h} \; \frac{d}{dt} p_{ext}(t). \tag{5.10}$$

5.1 Dynamics with Constant volume

The condition of constant volume is realized by adjusting the external pressure so as to keep the volume constant. When the Yukawa system reduces to the Coulomb system without the charge neutrality, the existence of inert rigid background is assumed and this condition is of essential importance.[19]

In the case of three dimensional periodicity, the external pressure is given by

$$p_{ext}(t) = \frac{\mathrm{Tr}(\sigma^t \cdot \Pi \cdot \sigma) - (W/V_0) \mathrm{Tr}(\sigma^t \cdot \dot{\mathsf{h}} \cdot \sigma^t \cdot \dot{\mathsf{h}})}{\mathrm{Tr}(\sigma^t \cdot \sigma)}. \tag{5.11}$$

In the case of two-dimensional periodicity, V_0 is replaced by S_0.

6 Dynamics at Constant Temperature with Deformable Periodic Boundaries under External Pressure

In order to simulate the canonical ensemble, we introduce a variable s and consider the dynamics of a virtual system and then map virtual variables to real ones.[20, 21] The Lagrangian of the virtual system $\mathcal{L}_v$ is given by

$$\mathcal{L}_v(\{\mathbf{x}_i, \dot{\mathbf{x}}_i\}, \mathsf{h}, \dot{\mathsf{h}}, s, \dot{s}, t) = \sum_i \frac{m_i}{2} s^2 \dot{\mathbf{x}}_i \cdot \mathsf{G} \cdot \dot{\mathbf{x}}_i + \frac{W}{2} s^2 \mathrm{Tr}\left[\dot{\mathsf{h}}^t \cdot \dot{\mathsf{h}}\right] + \frac{Q}{2}\dot{s}^2 - U(\mathsf{h}, \{\mathbf{x}_i\}) - p_{ext}(t) \det \mathsf{h} - g k_B T \ln s. \tag{6.1}$$

Here Q is the mass related to the heat reservoir. Though the value of Q does not affect the results so far as one follows the dynamics for a sufficiently long time, it needs to be optimized for practical purposes.

Equations of motion are given by

$$s^2 m_i \frac{d}{dt}\mathsf{G} \cdot \frac{d}{dt}\mathbf{x}_i = -\frac{\partial}{\partial \mathbf{x}_i} U - 2 s \dot{s} m_i \mathsf{G} \cdot \frac{d}{dt}\mathbf{x}_i, \tag{6.2}$$

$$s^2 W \frac{d^2}{dt^2}\mathsf{h} = [\Pi - p_{ext}(t)\mathsf{I}] \cdot \sigma - 2 s \dot{s} W \frac{d}{dt}\mathsf{h}, \tag{6.3}$$

$$Q \frac{d^2}{dt^2} s = \frac{2}{s}\left\{\sum_i \frac{m_i}{2} s^2 \dot{\mathbf{x}}_i \cdot \mathsf{G} \cdot \dot{\mathbf{x}}_i + \frac{W}{2} s^2 \mathrm{Tr}\left[\dot{\mathsf{h}}^t \cdot \dot{\mathsf{h}}\right] - \frac{g}{2} k_B T\right\}. \tag{6.4}$$

The momenta are defined by

$$\mathbf{p}_i = s^2 m_i \mathsf{G} \cdot \dot{\mathbf{x}}_i, \tag{6.5}$$

$$\mu = s^2 W \dot{\mathsf{h}}, \tag{6.6}$$

and

$$p_s = Q \dot{s}, \tag{6.7}$$

and the Hamiltonian is given by

$$\mathcal{H} = \sum_i \frac{1}{2 s^2 m_i} (\mathsf{G}^{-1} \cdot \mathbf{p}_i) \cdot \mathbf{p}_i + U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{1}{2 s^2 W} \mathrm{Tr}(\mu^t \cdot \mu) + \frac{p_s^2}{2Q} + g k_B T \ln s + p_{ext}(t) \det \mathsf{h}. \tag{6.8}$$

The conservation of Hamiltonian is written as

$$\frac{d}{dt}\mathcal{H} = \det \mathsf{h} \, \frac{d}{dt} p_{ext}(t). \tag{6.9}$$

The dynamics of our virtual system is completely determined by these equations.

We now map variables in the virtual system to *real* variables by the relations

$$dt' = \frac{dt}{s(t)} \quad \text{or} \quad t' = \int^t \frac{dt}{s(t)}, \tag{6.10}$$

$$\mathbf{x}'_i = \mathbf{x}_i, \tag{6.11}$$

$$\dot{\mathbf{x}}'_i = \frac{\dot{\mathbf{x}}_i}{s}, \tag{6.12}$$

$$\mathsf{h}' = \mathsf{h}, \tag{6.13}$$

and

$$\dot{\mathsf{h}}' = \frac{\dot{\mathsf{h}}}{s}. \tag{6.14}$$

When $g = 3N + 9 + 1 - 1$, N being the number of particles in the unit cell, the average of real variables taken over uniform intervals of the virtual time follows the canonical distribution. When $g = 3N + 9 - 1$, the average of real variables taken over uniform intervals of the real time follows the canonical distribution. The subtraction of unity comes from the conservation of the volume $\det \mathsf{h}$.

In the case of periodicity in two dimensions, the degrees of freedom accompanying particles are $2N$ and those related to deformation of fundamental vectors are 4. We set $g = 2N + 4 + 1 - 1$ or $g = 2N + 4 - 1$, according to the method of time average.

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Appendix

A Ewald-Type Formulae for Yukawa Lattice Sum

We here describe some Ewald-type expressions for lattice sums[22] in the Yukawa system with three- or two-dimensional periodicity. In order to take the deformation of fundamental vectors, we calculate the pressure tensor in addition to interaction energy and force.[7]

A.1 Interaction energy

A.1.1 Periodicity in three dimensions

We rewrite the Yukawa potential into

$$v(r) = \frac{1}{r}\exp(-\kappa r) = \frac{2}{\sqrt{\pi}}\left(\int_0^G + \int_G^\infty\right) d\rho \exp\left(-r^2\rho^2 - \frac{\kappa^2}{4\rho^2}\right), \tag{A.1}$$

and Fourier-transform the long-range part of the lattice sum:

$$\begin{aligned}
&\sum_{\mathbf{p}} v(|\mathbf{p}-\mathbf{r}|) \\
&= \sum_{\mathbf{p}} \frac{2}{\sqrt{\pi}}\left(\int_0^G + \int_G^\infty\right) d\rho \exp\left(-|\mathbf{p}-\mathbf{r}|^2\rho^2 - \frac{\kappa^2}{4\rho^2}\right) \\
&= \sum_{\mathbf{p}} \frac{1}{2|\mathbf{p}-\mathbf{r}|}\left\{\exp\left(\kappa|\mathbf{p}-\mathbf{r}|\right)\operatorname{erfc}\left(G|\mathbf{p}-\mathbf{r}| + \frac{\kappa}{2G}\right)\right.
\end{aligned}$$

$$+ \quad \exp\left(-\kappa|\mathbf{p}-\mathbf{r}|\right)\mathrm{erfc}\left(G|\mathbf{p}-\mathbf{r}|-\frac{\kappa}{2G}\right)\Bigg\} + \frac{1}{V_0}\sum_{\mathbf{g}}\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \quad (A.2)$$

Here $\{\mathbf{g}\}$ is the reciprocal lattice. The interaction energy between the particle i and its own images or the Madelung energy of lattice $\{\mathbf{p}\}$ is given by $q_i^2\phi_0$ where

$$\begin{aligned}\phi_0 &= \lim_{r\to 0}\left[\sum_{\mathbf{p}} v(|\mathbf{p}-\mathbf{r}|) - v(r)\right] \\ &= \sum_{\mathbf{p}\neq 0}\frac{1}{2p}\left\{\exp(\kappa p)\,\mathrm{erfc}\left(Gp+\frac{\kappa}{2G}\right)+\exp(-\kappa p)\,\mathrm{erfc}\left(Gp-\frac{\kappa}{2G}\right)\right\} \\ &\quad +\frac{1}{V_0}\sum_{\mathbf{g}}\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)+\kappa\,\mathrm{erfc}\left(\frac{\kappa}{2G}\right)-\frac{2}{\sqrt{\pi}}G\exp\left(-\frac{\kappa^2}{4G^2}\right). \qquad (A.3)\end{aligned}$$

The interaction energy U is thus given by

$$\begin{aligned}U &= \frac{1}{2}\sum_{i\neq j} q_i q_j \sum_{\mathbf{p}} v(|\mathbf{r}_{ij}-\mathbf{p}|)+\frac{1}{2}\phi_0\sum_{i=1}^{N} q_i^2 \\ &= \frac{1}{2}\sum_{i\neq j} q_i q_j \sum_{\mathbf{p}}\frac{1}{2|\mathbf{r}_{ij}-\mathbf{p}|}\left\{\exp(\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|+\frac{\kappa}{2G}\right)\right. \\ &\quad \left.+\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|-\frac{\kappa}{2G}\right)\right\} \\ &\quad +\frac{2\pi}{V_0}\sum_{\mathbf{g}}\frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\sum_{i,j}^{N} q_i q_j \exp(i\mathbf{g}\cdot\mathbf{r}_{ij}) \\ &\quad +\frac{1}{2}\left(\sum_{i=1}^{N} q_i^2\right)\sum_{\mathbf{p}\neq 0}\frac{1}{2p}\left\{\exp(\kappa p)\,\mathrm{erfc}\left(Gp+\frac{\kappa}{2G}\right)+\exp(-\kappa p)\,\mathrm{erfc}\left(Gp-\frac{\kappa}{2G}\right)\right\} \\ &\quad +\frac{1}{2}\left(\sum_{i=1}^{N} q_i^2\right)\left[\kappa\,\mathrm{erfc}\left(\frac{\kappa}{2G}\right)-\frac{2}{\sqrt{\pi}}G\exp\left(-\frac{\kappa^2}{4G^2}\right)\right]. \qquad (A.4)\end{aligned}$$

A.1.2 Periodicity in two dimensions

For Yukawa system with two-dimensional periodicity $\{\mathbf{P}\}$, we have

$$\begin{aligned}&\sum_{\mathbf{P}} v(|\mathbf{P}-\mathbf{r}|) \\ &= \sum_{\mathbf{P}}\frac{1}{2|\mathbf{P}-\mathbf{r}|}\left\{\exp(\kappa|\mathbf{P}-\mathbf{r}|)\,\mathrm{erfc}\left(G|\mathbf{P}-\mathbf{r}|+\frac{\kappa}{2G}\right)\right. \\ &\quad \left.+\exp(-\kappa|\mathbf{P}-\mathbf{r}|)\,\mathrm{erfc}\left(G|\mathbf{P}-\mathbf{r}|-\frac{\kappa}{2G}\right)\right\} \\ &\quad +\frac{1}{S_0}\sum_{\mathbf{K}}\frac{\pi}{\sqrt{K^2+\kappa^2}}\exp(i\mathbf{K}\cdot\mathbf{R}) \\ &\quad \times\left(\exp(\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz)\right. \\ &\quad \left.+\exp(-\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz)\right). \qquad (A.5)\end{aligned}$$

Here $\{\mathbf{K}\}$ is the two-dimensional reciprocal lattice and S_0 is the area of the unit cell in two dimensions. The interaction energy between the particle i and its own images or the Madelung energy of two-dimensional lattice $\{\mathbf{P}\}$ is given by $q_i^2\phi_0$ where

$$\begin{aligned}\phi_0 &= \lim_{r\to 0}\{\sum_{\mathbf{P}} v(|\mathbf{P}-\mathbf{r}|) - v(r)\}\\ &= \sum_{\mathbf{P}\neq 0}\frac{1}{2P}\left\{\exp(\kappa P)\mathrm{erfc}\left(GP+\frac{\kappa}{2G}\right)+\exp(-\kappa P)\mathrm{erfc}\left(GP-\frac{\kappa}{2G}\right)\right\}\\ &+ \frac{1}{S_0}\sum_{\mathbf{K}}\frac{2\pi}{\sqrt{K^2+\kappa^2}}\mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G}\right)+\kappa\,\mathrm{erfc}\left(\frac{\kappa}{2G}\right)-\frac{2}{\sqrt{\pi}}G\exp\left(-\frac{\kappa^2}{4G^2}\right).\end{aligned} \tag{A.6}$$

The interaction energy U is given by

$$\begin{aligned}U &= \frac{1}{2}\sum_{i\neq j}q_iq_j\sum_{\mathbf{P}}v(|\mathbf{r}_{ij}-\mathbf{P}|)+\frac{1}{2}\phi_0\left(\sum_i q_i^2\right)\\ &= \frac{1}{2}\sum_{i\neq j}q_iq_j\sum_{\mathbf{P}}\frac{1}{2|\mathbf{P}-\mathbf{r}_{ij}|}\left\{\exp\left(\kappa|\mathbf{P}-\mathbf{r}_{ij}|\right)\mathrm{erfc}\left(G|\mathbf{P}-\mathbf{r}_{ij}|+\frac{\kappa}{2G}\right)\right.\\ &\left.+\exp\left(-\kappa|\mathbf{P}-\mathbf{r}_{ij}|\right)\mathrm{erfc}\left(G|\mathbf{P}-\mathbf{r}_{ij}|-\frac{\kappa}{2G}\right)\right\}\\ &+\frac{\pi}{2S_0}\sum_{i,j}q_iq_j\sum_{\mathbf{K}}\frac{1}{\sqrt{K^2+\kappa^2}}\exp(i\mathbf{K}\cdot\mathbf{R}_{ij})\\ &\times\left(\exp(\sqrt{K^2+\kappa^2}z_{ij})\mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz_{ij}\right)\right.\\ &\left.+\exp(-\sqrt{K^2+\kappa^2}z_{ij})\mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz_{ij}\right)\right)\\ &+\frac{1}{2}\left(\sum_i q_i^2\right)\sum_{\mathbf{P}}{}'\frac{1}{2P}\left\{\exp(\kappa P)\mathrm{erfc}\left(GP+\frac{\kappa}{2G}\right)+\exp(-\kappa P)\mathrm{erfc}\left(GP-\frac{\kappa}{2G}\right)\right\}\\ &+\frac{1}{2}\left(\sum_i q_i^2\right)\left[\kappa\,\mathrm{erfc}\left(\frac{\kappa}{2G}\right)-\frac{2}{\sqrt{\pi}}G\exp\left(-\frac{\kappa^2}{4G^2}\right)\right].\end{aligned} \tag{A.7}$$

A.2 Force

A.2.1 Periodicity in three dimensions

We first note that

$$\frac{\partial}{\partial \mathbf{x}_i}U = \mathsf{h}^t\cdot\frac{\partial}{\partial \mathbf{r}_i}U. \tag{A.8}$$

The second factor is calculated as

$$\begin{aligned}-\frac{\partial}{\partial \mathbf{r}_i}U &= q_i\sum_{j(\neq i)}q_j\sum_{\mathbf{p}}\frac{(\mathbf{r}_i-\mathbf{r}_j-\mathbf{p})}{|\mathbf{r}_{ij}-\mathbf{p}|^3}\\ &\times\left[\frac{1}{2}(1-\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\exp\left(\kappa|\mathbf{r}_{ij}-\mathbf{p}|\right)\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|+\frac{\kappa}{2G}\right)\right.\\ &+\frac{1}{2}(1+\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\exp\left(-\kappa|\mathbf{r}_{ij}-\mathbf{p}|\right)\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|-\frac{\kappa}{2G}\right)\end{aligned}$$

$$+\frac{2}{\sqrt{\pi}}G|\mathbf{r}_{ij}-\mathbf{p}|\exp\left(-G^2|\mathbf{r}_{ij}-\mathbf{p}|^2-\frac{\kappa^2}{4G^2}\right)\Bigg]$$
$$-i\frac{4\pi}{V_0}q_i\sum_{\mathbf{g}}\frac{\mathbf{g}}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\left[\sum_j^N q_j\exp(i\mathbf{g}\cdot\mathbf{r}_{ij})\right]. \tag{A.9}$$

A.2.2 Periodicity in two dimensions

For Yukawa system with two-dimensional periodicity $\{\mathbf{P}=\mathsf{h}\cdot\mathbf{N}\}$, we have

$$\frac{\partial}{\partial\mathbf{X}_i}U=\mathsf{h}^t\cdot\frac{\partial}{\partial\mathbf{R}_i}U, \tag{A.10}$$

$$\begin{aligned}-\frac{\partial}{\partial\mathbf{R}_i}U &= q_i\sum_{j(\neq i)}q_j\sum_{\mathbf{P}}\frac{(\mathbf{R}_i-\mathbf{R}_j-\mathbf{P})}{|\mathbf{r}_{ij}-\mathbf{P}|^3}\\
&\times\left[\frac{1}{2}(1-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|+\frac{\kappa}{2G}\right)\right.\\
&+\frac{1}{2}(1+\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|-\frac{\kappa}{2G}\right)\\
&\left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}_{ij}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}_{ij}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right)\right]\\
&-i\frac{\pi}{S_0}q_i\sum_{\mathbf{K}}\frac{\mathbf{K}}{\sqrt{K^2+\kappa^2}}\sum_j q_j\exp(i\mathbf{K}\cdot\mathbf{R}_{ij})\\
&\times\left(\exp(\sqrt{K^2+\kappa^2}z_{ij})\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz_{ij})\right.\\
&\left.+\exp(-\sqrt{K^2+\kappa^2}z_{ij})\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz_{ij})\right),\end{aligned} \tag{A.11}$$

and

$$\begin{aligned}-\frac{\partial}{\partial z_i}U &= q_i\sum_{j(\neq i)}q_j\sum_{\mathbf{P}}\frac{z_{ij}}{|\mathbf{r}_{ij}-\mathbf{P}|^3}\\
&\times\left[\frac{1}{2}(1-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|+\frac{\kappa}{2G}\right)\right.\\
&+\frac{1}{2}(1+\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|-\frac{\kappa}{2G}\right)\\
&\left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}_{ij}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}_{ij}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right)\right]\\
&-\frac{\pi}{S_0}q_i\sum_{\mathbf{K}}\sum_j q_j\exp(i\mathbf{K}\cdot\mathbf{R}_{ij})\\
&\times\left(\exp(\sqrt{K^2+\kappa^2}z_{ij})\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz_{ij})\right.\\
&\left.-\exp(-\sqrt{K^2+\kappa^2}z_{ij})\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz_{ij})\right).\end{aligned} \tag{A.12}$$

A.3 Pressure tensors

A.3.1 Periodicity in three dimensions

We here give Ewald-type expressions for tensors related to the deformation of unit cell:

$$\begin{aligned}
&\sum_{\mathbf{p}} \frac{(\mathbf{r}-\mathbf{p})(\mathbf{r}-\mathbf{p})}{|\mathbf{r}-\mathbf{p}|} \frac{\partial v(|\mathbf{r}-\mathbf{p}|)}{\partial |\mathbf{r}-\mathbf{p}|} \\
&= -\sum_{\mathbf{p}} \frac{(\mathbf{r}-\mathbf{p})(\mathbf{r}-\mathbf{p})}{|\mathbf{r}-\mathbf{p}|^3} \left\{ \frac{1}{2}(1-\kappa|\mathbf{r}-\mathbf{p}|)\exp(\kappa|\mathbf{r}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{p}|+\frac{\kappa}{2G}\right) \right. \\
&\quad +\frac{1}{2}(1+\kappa|\mathbf{r}-\mathbf{p}|)\exp(-\kappa|\mathbf{r}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{p}|-\frac{\kappa}{2G}\right) \\
&\quad \left. +\frac{2}{\sqrt{\pi}} G|\mathbf{r}-\mathbf{p}|\exp\left(-G^2|\mathbf{r}-\mathbf{p}|^2-\frac{\kappa^2}{4G^2}\right)\right\} \\
&\quad +\frac{8\pi}{V_0}\sum_{\mathbf{g}} \mathbf{g}\mathbf{g}\frac{1}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
&\quad -\mathsf{I}\frac{4\pi}{V_0}\sum_{\mathbf{g}} \frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right), \qquad \text{(A.13)}
\end{aligned}$$

$$\begin{aligned}
&\sum_{\mathbf{p}\neq 0} \frac{\mathbf{p}\mathbf{p}}{p}\frac{\partial v(p)}{\partial p} \\
&= -\sum_{\mathbf{p}\neq 0} \frac{\mathbf{p}\mathbf{p}}{p^3}\left\{\frac{1}{2}(1-\kappa p)\exp(\kappa p)\,\mathrm{erfc}\left(Gp+\frac{\kappa}{2G}\right)\right. \\
&\quad \left. +\frac{1}{2}(1+\kappa p)\exp(-\kappa p)\,\mathrm{erfc}\left(Gp-\frac{\kappa}{2G}\right)+\frac{2}{\sqrt{\pi}}Gp\exp\left(-G^2p^2-\frac{\kappa^2}{4G^2}\right)\right\} \\
&\quad +\frac{8\pi}{V_0}\sum_{\mathbf{g}} \mathbf{g}\mathbf{g}\frac{1}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right) \\
&\quad -\mathsf{I}\frac{4\pi}{V_0}\sum_{\mathbf{g}} \frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right). \qquad \text{(A.14)}
\end{aligned}$$

The tensor $\mathsf{\Pi}$ is thus given by

$$\begin{aligned}
V_0\mathsf{\Pi} &= \sum_i m_i(\mathsf{h}\cdot\dot{\mathbf{x}}_i)(\mathsf{h}\cdot\dot{\mathbf{x}}_i) - \frac{1}{2}\sum_{i\neq j} q_i q_j \sum_{\mathbf{p}} \frac{(\mathbf{r}_{ij}-\mathbf{p})(\mathbf{r}_{ij}-\mathbf{p})}{|\mathbf{r}_{ij}-\mathbf{p}|}\frac{\partial v(|\mathbf{r}_{ij}-\mathbf{p}|)}{\partial|\mathbf{r}_{ij}-\mathbf{p}|} + V_0\mathsf{\Pi}_0 \\
&= \sum_i m_i(\mathsf{h}\cdot\dot{\mathbf{x}}_i)(\mathsf{h}\cdot\dot{\mathbf{x}}_i) \\
&\quad +\frac{1}{2}\sum_{i\neq j} q_i q_j \sum_{\mathbf{p}} \frac{(\mathbf{r}_{ij}-\mathbf{p})(\mathbf{r}_{ij}-\mathbf{p})}{|\mathbf{r}_{ij}-\mathbf{p}|^3}\left\{\frac{1}{2}(1-\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\exp(\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|+\frac{\kappa}{2G}\right)\right. \\
&\quad +\frac{1}{2}(1+\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|-\frac{\kappa}{2G}\right) \\
&\quad \left. +\frac{2}{\sqrt{\pi}}G|\mathbf{r}_{ij}-\mathbf{p}|\exp\left(-G^2|\mathbf{r}_{ij}-\mathbf{p}|^2-\frac{\kappa^2}{4G^2}\right)\right\}
\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{2}\left(\sum_i q_i^2\right)\sum_{\mathbf{p}\neq 0}\frac{\mathbf{pp}}{p^3}\left\{\frac{1}{2}(1-\kappa p)\exp(\kappa p)\,\mathrm{erfc}\left(Gp+\frac{\kappa}{2G}\right)\right.\\
&\left.+\frac{1}{2}(1+\kappa p)\exp(-\kappa p)\,\mathrm{erfc}\left(Gp-\frac{\kappa}{2G}\right)+\frac{2}{\sqrt{\pi}}Gp\exp\left(-G^2p^2-\frac{\kappa^2}{4G^2}\right)\right\}\\
&-\frac{4\pi}{V_0}\sum_{\mathbf{g}}\mathbf{gg}\frac{1}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\sum_{i,j}q_iq_j\exp(i\mathbf{g}\cdot\mathbf{r}_{ij})\\
&+\frac{2\pi}{V_0}\sum_{\mathbf{g}}\frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\sum_{i,j}q_iq_j\exp(i\mathbf{g}\cdot\mathbf{r}_{ij}). \qquad \text{(A.15)}
\end{aligned}
$$

A.3.2 Periodicity in two dimensions

For Yukawa system with two-dimensional periodicity $\{\mathbf{P}\}$ we have

$$
\begin{aligned}
&\sum_{\mathbf{P}}\frac{(\mathbf{r}-\mathbf{P})(\mathbf{r}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|}\frac{\partial v(|\mathbf{r}-\mathbf{P}|)}{\partial|\mathbf{r}-\mathbf{P}|}\\
&= -\sum_{\mathbf{P}}\frac{(\mathbf{r}-\mathbf{P})(\mathbf{r}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|^3}\left\{\frac{1}{2}(1-\kappa|\mathbf{r}-\mathbf{P}|)\exp(\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|+\frac{\kappa}{2G}\right)\right.\\
&\quad+\frac{1}{2}(1+\kappa|\mathbf{r}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|-\frac{\kappa}{2G}\right)\\
&\quad\left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right)\right\}\\
&\quad+\frac{4}{S_0}\sum_{\mathbf{K}}\int_{-\infty}^{\infty}dg_z\mathbf{gg}\frac{1}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right)\\
&\quad-\frac{2}{S_0}\sum_{\mathbf{K}}\int_{-\infty}^{\infty}dg_z\frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right), \qquad \text{(A.16)}
\end{aligned}
$$

where

$$\mathbf{g}=\mathbf{K}+g_z\hat{z} \qquad \text{(A.17)}$$

and

$$\mathbf{gg}=\mathbf{KK}+g_z\mathbf{K}\hat{z}+g_z\hat{z}\mathbf{K}+g_z^2\hat{z}\hat{z}. \qquad \text{(A.18)}$$

The equation of motion for h is related to the 2×2 part of the above tensors:

$$
\begin{aligned}
&\sum_{\mathbf{P}}\frac{(\mathbf{R}-\mathbf{P})(\mathbf{R}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|}\frac{\partial v(|\mathbf{r}-\mathbf{P}|)}{\partial|\mathbf{r}-\mathbf{P}|}\\
&= -\sum_{\mathbf{P}}\frac{(\mathbf{R}-\mathbf{P})(\mathbf{R}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|^3}\left\{\frac{1}{2}(1-\kappa|\mathbf{r}-\mathbf{P}|)\exp(\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|+\frac{\kappa}{2G}\right)\right.\\
&\quad+\frac{1}{2}(1+\kappa|\mathbf{r}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|-\frac{\kappa}{2G}\right)\\
&\quad\left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right)\right\}\\
&\quad+\frac{4}{S_0}\sum_{\mathbf{K}}\int_{-\infty}^{\infty}dg_z\mathbf{KK}\frac{1}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right)
\end{aligned}
$$

$$
\begin{aligned}
& -\mathsf{I}\frac{2}{S_0}\sum_{\mathbf{K}}\int_{-\infty}^{\infty} dg_z \frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
= & -\sum_{\mathbf{P}}\frac{(\mathbf{R}-\mathbf{P})(\mathbf{R}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|^3}\left\{\frac{1}{2}(1-\kappa|\mathbf{r}-\mathbf{P}|)\exp(\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|+\frac{\kappa}{2G}\right)\right. \\
& +\frac{1}{2}(1+\kappa|\mathbf{r}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|-\frac{\kappa}{2G}\right) \\
& \left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right)\right\} \\
& +\frac{\pi}{S_0}\sum_{\mathbf{K}}\mathbf{K}\mathbf{K}\frac{1}{(K^2+\kappa^2)^{3/2}}\exp(i\mathbf{K}\cdot\mathbf{R})\left[(1-\sqrt{K^2+\kappa^2}z)\exp(\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz)\right. \\
& +(1+\sqrt{K^2+\kappa^2}z)\exp(-\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz) \\
& \left.+\frac{2}{\sqrt{\pi}}\frac{\sqrt{K^2+\kappa^2}}{G}\exp(-\frac{K^2+\kappa^2}{4G^2}-G^2z^2)\right] \\
& -\mathsf{I}\frac{\pi}{S_0}\sum_{\mathbf{K}}\frac{1}{\sqrt{K^2+\kappa^2}}\exp(i\mathbf{K}\cdot\mathbf{R})\left[\exp(\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz)\right. \\
& \left.+\exp(-\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz)\right]. \qquad \text{(A.19)}
\end{aligned}
$$

Here we have used the relations

$$
\begin{aligned}
& \frac{2}{S_0}\int_{-\infty}^{\infty} dg_z \frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
= & \frac{\pi}{S_0}\frac{1}{\sqrt{K^2+\kappa^2}}\exp(i\mathbf{K}\cdot\mathbf{R})\left[\exp(\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz)\right. \\
& \left.+\exp(-\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz)\right], \qquad \text{(A.20)}
\end{aligned}
$$

and

$$
\begin{aligned}
& \frac{4}{S_0}\int_{-\infty}^{\infty} dg_z \frac{1}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
= & \frac{\pi}{S_0}\frac{1}{(K^2+\kappa^2)^{3/2}}\exp(i\mathbf{K}\cdot\mathbf{R})\left[(1-\sqrt{K^2+\kappa^2}z)\exp(\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+Gz)\right. \\
& +(1+\sqrt{K^2+\kappa^2}z)\exp(-\sqrt{K^2+\kappa^2}z)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-Gz) \\
& \left.+\frac{2}{\sqrt{\pi}}\frac{\sqrt{K^2+\kappa^2}}{G}\exp(-\frac{K^2+\kappa^2}{4G^2}-G^2z^2)\right]. \qquad \text{(A.21)}
\end{aligned}
$$

The tensor related to the Madelung energy is similarly calculated as

$$
\sum_{\mathbf{P}\neq 0}\frac{\mathbf{P}\mathbf{P}}{P}\frac{\partial v(P)}{\partial P}
$$

$$
\begin{aligned}
= & -\sum_{\mathbf{P}\neq 0}\frac{\mathbf{PP}}{P^3}\left\{\frac{1}{2}(1-\kappa P)\exp(\kappa P)\mathrm{erfc}\left(GP+\frac{\kappa}{2G}\right)\right.\\
& \left.+\frac{1}{2}(1+\kappa P)\exp(-\kappa P)\mathrm{erfc}\left(GP-\frac{\kappa}{2G}\right)+\frac{2}{\sqrt{\pi}}GP\exp\left(-G^2P^2-\frac{\kappa^2}{4G^2}\right)\right\}\\
& +\frac{4}{S_0}\sum_{\mathbf{K}}\int_{-\infty}^{\infty}dg_z\mathbf{KK}\frac{1}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\\
& -\mathsf{I}\frac{2}{S_0}\sum_{\mathbf{K}}\int_{-\infty}^{\infty}dg_z\frac{1}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\\
= & -\sum_{\mathbf{P}\neq 0}\frac{\mathbf{PP}}{P^3}\left\{\frac{1}{2}(1-\kappa P)\exp(\kappa P)\mathrm{erfc}\left(GP+\frac{\kappa}{2G}\right)\right.\\
& \left.+\frac{1}{2}(1+\kappa P)\exp(-\kappa P)\mathrm{erfc}\left(GP-\frac{\kappa}{2G}\right)+\frac{2}{\sqrt{\pi}}GP\exp\left(-G^2P^2-\frac{\kappa^2}{4G^2}\right)\right\}\\
& +\frac{2\pi}{S_0}\sum_{\mathbf{K}}\mathbf{KK}\frac{1}{(K^2+\kappa^2)^{3/2}}\left[\mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G}\right)+\frac{1}{\sqrt{\pi}}\frac{\sqrt{K^2+\kappa^2}}{G}\exp\left(-\frac{K^2+\kappa^2}{4G^2}\right)\right]\\
& -\mathsf{I}\frac{2\pi}{S_0}\sum_{\mathbf{K}}\frac{1}{\sqrt{K^2+\kappa^2}}\mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G}\right). \qquad \text{(A.22)}
\end{aligned}
$$

References

[1] For example, M. O. Robbins, K. Kremer, and G. S. Grest, J. Chem. Phys. **88**, 3286(1988).

[2] H. Thomas, G. E. Morfill, V. Demmel, J. Goree, B. Feuerbacher, and D. Möhlmann, Phys. Rev. Lett. **73**, 652(1994).

[3] J. H. Chu and Lin I, Physica A **205**, 183(1994): Phys. Rev. Lett. **72**, 4009(1994).

[4] Y. Hayashi and T. Tachibana, Jpn. J. Appl. Phys. **33** L804(1994).

[5] A. Melzer, T. Trottenberg, and A.Piel, Phys. Lett. A **191** 301(1994).

[6] E. P. Wigner, Phys. Rev. **46** 1002(1934).

[7] H. Totsuji, Y. Inoue, T. Kishimoto, C. Totsuji, and S. Nara, Mem. Fac. Eng. Okayama Univ. **30**, 75(1995).

[8] H. Totsuji, T. Kishimoto, Y. Inoue, C. Totsuji, and S. Nara, Phys. Lett. A **221** 215(1996).

[9] H. Totsuji, T. Kishimoto, and C. Totsuji, Phys. Rev. Lett. **78**, 3113(1997).

[10] T. Kishimoto, C. Totsuji, and H. Totsuji, *Proc. 1996 Int. Conf. Plasma Physics, Nagoya, 1996* (Japan Society of Plasma Science and Nuclear Fusion Research, Nagoya, 1997) Vol. 2, p. 1974.

[11] H. Totsuji, T. Kishimoto, and C. Totsuji, Jpn. J. Appl. Phys. **36**, 4980(1997).

[12] H. Totsuji, T. Kishimoto, and C. Totsuji, *Advances in Dusty plasmas*, eds. P. K. Shukla, D. A. Mendis and T. Desai (World Scientific, Singapore, 1997), p. 377.

[13] H. Totsuji, T. Kishimoto, and C. Totsuji, to appear in *Strongly Coupled Coulomb Systems*, eds. G. J. Kalman, K. Blagoev, and J. M. Rommel (Plenum, New York, 1998).

[14] S. V. Vladimirov and M. Nambu, Phys. Rev. E **52**, 2172(1995).

[15] F. Melandsø and J. Goree, Phys. Rev. E **52**, 5312(1995).

[16] S. V. Vladimirov and O. Ishihara, Phys. Plasmas **3**, 444(1996); O. Ishihara and S. V. Vladimirov, Phys. Plasmas **4**, No.1(1997).

[17] A. Melzer, V. A. Schweigert, I. V. Schweigert, A. Homann, S. Peters, and A. Piel, Phys. Rev. E **54**, R46(1996); V. A. Schweigert, I. V. Schweigert, A. Melzer, A. Homann, and A. Piel, Phys. Rev. E **54**, 4155(1996).

[18] M. Parrinello and A. Rahman, Phys. Rev. Lett. **45**, 1196(1980).

[19] H. Totsuji, H. Shirokoshi, and S. Nara, Phys. Lett. A **162**, 174(1992).

[20] H. C. Anderson, J. Chem. Phys. **72**, 2384(1980).

[21] S. Nosé, J. Chem. Phys. **81**, 511(1984).

[22] For example, J. M. Ziman, *Principles of the Theory of Solids*, 2nd ed. Chap.5, Cam. Univ. Press, (1972).