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Molecular Dynamics of Yukawa System (Dust Plasma) with Deformable Periodic Boundary Conditions: Formulation

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Molecular dynamics of the Yukawa system, the system of particles interacting via the Yukawa or the screened Coulomb potential, are formulated for various statistical ensembles and external conditions. The Yukawa potential smoothly interpolates the long-range Coulomb and the short-range interactions by adjusting a single parameter, the screening length. In order to reduce the effect of boundaries, the periodic boundary conditions are imposed and the deformations of the fundamental vectors of periodicity are taken into account. Ewald-type expressions for interaction energy, force, and kinematic pressure are given explicitly.

1 Introduction

The statistical mechanics of particles interacting via the Yukawa potential has long been studied as models of simple but non trivial system.[1] The potential has two parameters, the charge and the screening length, and the latter gives a well-defined range of force: The long-range (Coulomb) and the short-range forces can be interpolated by changing it. The simplicity of its expression allows us to take advantage of mathematical transformations in evaluating various statistical quantities.

As real systems where interactions are given by the Yukawa potential, we have classical and quantum plasmas and charge stabilized colloidal suspensions. Recent addition to this class is the dust plasma, the system of macroscopic charged particles suspended in plasmas, which appears in plasma processes of semiconductor engineering.[2, 3] In order to transfer minute patterns of integrated circuit onto the surface of substrates, we employ the method of lithography and we have dust plasmas in etching process in reactive plasmas excited by radio-frequency electromagnetic waves. One can take images of particles (dust) in these dust plasmas easily by optical method and formation of lattices has been observed recently.

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Molecular dynamics is a powerful method to analyze dynamic and also static properties of particle systems to microscopic scales. The finiteness of the simulated system, however, is still the main difficulty in interpreting the results and the statistical ensemble and boundary conditions have to be carefully examined.

The purpose of this paper is to describe some mathematical expressions which are indispensable for analyses of Yukawa system by molecular dynamics. They are obtained by straightforward but tedious manipulations and will be useful for related numerical analyses. We first review application of various statistical ensembles and then derive expressions specified to Yukawa system.

As external conditions, we consider both (1) the case of bulk system with constant volume or under constant pressure and (2) that of 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.[4, 5]

2 Formulation of Molecular Dynamics for Microcanonical Ensemble

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

$$\cdot = \frac{d}{dt}. \tag{2.1}$$

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

$$\mathbf{r} = \mathsf{h} \cdot \mathbf{x} \tag{2.2}$$

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

$$\mathsf{h} = (\mathbf{a}, \mathbf{b}, \mathbf{c}). \tag{2.3}$$

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

$$\mathbf{r} = (\mathbf{R}, z) \tag{2.4}$$

or

$$\mathbf{r} = \mathbf{R} + z\hat{z} \tag{2.5}$$

as

$$\mathbf{R} = \mathsf{h} \cdot \mathbf{X}. \tag{2.6}$$

2.1 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

$$\mathcal{L}(\{\mathbf{r}_i, \dot{\mathbf{r}}_i\}) = \sum_{i=1}^{N} \frac{m_i}{2} \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i - U(\{\mathbf{r}_i\}), \tag{2.7}$$

where $U(\{\mathbf{r}_i\})$ is the potential energy, and we have naturally

$$\dot{\mathbf{r}}_i = \mathsf{h} \cdot \dot{\mathbf{x}}_i. \tag{2.8}$$

Equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \mathbf{r}_i} = 0, \tag{2.9}$$

or

$$m_i \frac{d^2}{dt^2}\mathbf{r}_i = -\frac{\partial}{\partial \mathbf{r}_i}U. \tag{2.10}$$

The momentum is defined by

$$\mathbf{p}_i = m_i \dot{\mathbf{r}}_i \tag{2.11}$$

and the Hamiltonian is given by

$$\mathcal{H} = \sum_i \frac{1}{2m_i}\mathbf{p}_i \cdot \mathbf{p}_i + U(\{\mathbf{r}_i\}). \tag{2.12}$$

We have the conservation of total energy in the form

$$\frac{d}{dt}\mathcal{H} = 0. \tag{2.13}$$

2.2 Dynamics with deformable periodic boundaries

2.2.1 Periodicity in three dimensions

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

$$\mathcal{L}(\{\mathbf{x}_i, \dot{\mathbf{x}}_i\}, \mathsf{h}, \dot{\mathsf{h}}) = \sum_{i=1}^{N} \frac{m_i}{2}\dot{\mathbf{x}}_i^t \cdot \mathsf{G} \cdot \dot{\mathbf{x}}_i - U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{W}{2}\mathbf{Tr}\left[\dot{\mathsf{h}}^t \cdot \dot{\mathsf{h}}\right], \tag{2.14}$$

where

$$\mathsf{G} = \mathsf{h}^t \cdot \mathsf{h}. \tag{2.15}$$

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

$$\mathbf{v}_i \equiv \mathsf{h} \cdot \dot{\mathbf{x}}_i. \tag{2.16}$$

The equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \mathbf{x}_i} = 0 \tag{2.17}$$

and

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{h}_{\alpha\beta}}\right) - \frac{\partial \mathcal{L}}{\partial h_{\alpha\beta}} = 0, \tag{2.18}$$

or

$$m_i \frac{d}{dt}\mathsf{G} \cdot \frac{d}{dt}\mathbf{x}_i = -\frac{\partial}{\partial \mathbf{x}_i}U \tag{2.19}$$

and

$$W\frac{d^2}{dt^2}\mathsf{h} = \Pi \cdot \sigma. \tag{2.20}$$

Tensors Π and σ are given respectively by

$$\Pi = \frac{1}{V_0}\left\{\sum_{i=1}^{N} m_i \left(\mathsf{h}\cdot\dot{\mathbf{x}}_i\right)\left(\mathsf{h}\cdot\dot{\mathbf{x}}_i\right) - \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\sum_{\mathbf{p}} \frac{(\mathbf{r}_{ij}-\mathbf{p})(\mathbf{r}_{ij}-\mathbf{p})}{|\mathbf{r}_{ij}-\mathbf{p}|}\frac{\partial v\left(|\mathbf{r}_{ij}-\mathbf{p}|\right)}{\partial|\mathbf{r}_{ij}-\mathbf{p}|}\right\} + \Pi_0, \tag{2.21}$$

$$\Pi_0 = -\frac{N}{2V_0}\sum_{\mathbf{p}}{}' \frac{\mathbf{p}\mathbf{p}}{p}\frac{\partial v\left(p\right)}{\partial p}, \tag{2.22}$$

and

$$\sigma = V_0\left(\mathsf{h}^t\right)^{-1}. \tag{2.23}$$

Here V_0 is the volume of the unit cell and $v(r)$ is the interaction potential.

The momenta are defined by

$$\mathbf{p}_i = m_i \mathsf{G}\cdot\dot{\mathbf{x}}_i \tag{2.24}$$

and

$$\mu = W\dot{\mathsf{h}}, \tag{2.25}$$

and the Hamiltonian is given by

$$\mathcal{H} = \sum_i \frac{1}{2m_i}(\mathsf{G}^{-1}\cdot\mathbf{p}_i)\cdot\mathbf{p}_i + U(\mathsf{h},\{\mathbf{x}_i\}) + \frac{1}{2W}\mathbf{Tr}(\mu^t\cdot\mu). \tag{2.26}$$

The conservation of Hamiltonian is written as

$$\frac{d}{dt}\mathcal{H} = 0. \tag{2.27}$$

2.2.2 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

$$\mathcal{L}(\{\mathbf{X}_i, z_i, \dot{\mathbf{X}}_i, \dot{z}_i\},\mathsf{h},\dot{\mathsf{h}}) = \sum_{i=1}^{N}\frac{m_i}{2}\dot{\mathbf{X}}_i^t\cdot\mathsf{G}\cdot\dot{\mathbf{X}}_i + \sum_{i=1}^{N}\frac{m_i}{2}\dot{z}_i\dot{z}_i - U(\mathsf{h},\{\mathbf{X}_i, z_i\}) + \frac{W}{2}\mathbf{Tr}\left[\dot{\mathsf{h}}^t\cdot\dot{\mathsf{h}}\right]. \tag{2.28}$$

Velocities in two dimensions are *defined* by

$$\dot{\mathbf{R}}_i \equiv \mathsf{h}\cdot\dot{\mathbf{X}}_i. \tag{2.29}$$

Equations of motion are given by

$$\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{X}}_i}\right) - \frac{\partial\mathcal{L}}{\partial\mathbf{X}_i} = 0, \tag{2.30}$$

$$\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{z}_i}\right) - \frac{\partial\mathcal{L}}{\partial z_i} = 0, \tag{2.31}$$

and

$$\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{h}_{\alpha\beta}}\right) - \frac{\partial\mathcal{L}}{\partial h_{\alpha\beta}} = 0, \tag{2.32}$$

or

$$m_i\frac{d}{dt}\mathsf{G}\cdot\frac{d}{dt}\mathbf{X}_i = -\frac{\partial}{\partial\mathbf{X}_i}U, \tag{2.33}$$

$$m_i \frac{d^2}{dt^2} z_i = -\frac{\partial}{\partial z_i} U, \tag{2.34}$$

and

$$W \frac{d^2}{dt^2} \mathsf{h} = \Pi \cdot \sigma. \tag{2.35}$$

Here Π is defined by

$$\Pi = \frac{1}{V_0} \left\{ \sum_{i=1}^{N} m_i \left(\mathsf{h} \cdot \dot{\mathbf{X}}_i \right) \left(\mathsf{h} \cdot \dot{\mathbf{X}}_i \right) - \frac{1}{2} \sum_{i \neq j} \sum_{\mathbf{P}} \frac{(\mathbf{R}_{ij} - \mathbf{P})(\mathbf{R}_{ij} - \mathbf{P})}{|\mathbf{r}_{ij} - \mathbf{P}|} \frac{\partial}{\partial |\mathbf{r}_{ij} - \mathbf{P}|} v\left(|\mathbf{r}_{ij} - \mathbf{P}| \right) \right\} + \Pi_0 \tag{2.36}$$

and

$$\Pi_0 = -\frac{N}{2V_0} \sum_{\mathbf{P} \neq 0} \frac{\mathbf{P}\mathbf{P}}{P} \frac{\partial}{\partial P} v(P). \tag{2.37}$$

3 Dynamics with Deformable Periodic Boundaries under External Pressure

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

$$-\, p_{ext}(t) \det \mathsf{h} \tag{3.1}$$

to the Lagrangian. Here $\det \mathsf{h}$ is the volume of our unit cell. The Lagrangian is then written as

$$\mathcal{L}(\{\mathbf{x}_i, \dot{\mathbf{x}}_i\}, \mathsf{h}, \dot{\mathsf{h}}, t) = \sum_{i=1}^{N} \frac{m_i}{2} \dot{\mathbf{x}}_i^t \cdot \mathsf{G} \cdot \dot{\mathbf{x}}_i - U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{W}{2} \mathbf{Tr} \left[\dot{\mathsf{h}}^t \cdot \dot{\mathsf{h}} \right] - p_{ext}(t) \det \mathsf{h}. \tag{3.2}$$

Equations of motion are given by

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}_i} \right) - \frac{\partial \mathcal{L}}{\partial \mathbf{x}_i} = 0 \tag{3.3}$$

and

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{h}_{\alpha\beta}} \right) - \frac{\partial \mathcal{L}}{\partial h_{\alpha\beta}} = 0, \tag{3.4}$$

or

$$m_i \frac{d}{dt} \mathsf{G} \cdot \frac{d}{dt} \mathbf{x}_i = -\frac{\partial}{\partial \mathbf{x}_i} U \tag{3.5}$$

and

$$W \frac{d^2}{dt^2} \mathsf{h} = \left[\Pi - p_{ext}(t) \mathsf{I} \right] \cdot \sigma. \tag{3.6}$$

The momenta are defined by

$$\mathbf{p}_i = m_i \mathsf{G} \cdot \dot{\mathbf{x}}_i \tag{3.7}$$

and

$$\mu = W \dot{\mathsf{h}}, \tag{3.8}$$

and the Hamiltonian is given by

$$\mathcal{H} = \sum_i \frac{1}{2m_i} (\mathsf{G}^{-1} \cdot \mathbf{p}_i) \cdot \mathbf{p}_i + U(\mathsf{h}, \{\mathbf{x}_i\}) + \frac{1}{2W} \mathbf{Tr}(\mu^t \cdot \mu) + p_{ext}(t) \det \mathsf{h}. \tag{3.9}$$

In this case, the conservation of Hamiltonian is written as

$$\frac{d}{dt} \mathcal{H} = \det \mathsf{h}\, \frac{d}{dt} p_{ext}(t). \tag{3.10}$$

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

In order to simulate the canonical ensemble, we define the virtual time t' by

$$t = \int^{t'} \frac{dt'}{s} \tag{4.1}$$

or

$$dt = \frac{dt'}{s} \tag{4.2}$$

and consider the dynamics of a virtual system[6, 7] whose Lagrangian $\mathcal{L}'$ is given by

$$\mathcal{L}'(\{\mathbf{x}'_i, \dot{\mathbf{x}'}_i\}, \mathsf{h}', \dot{\mathsf{h}}', s', \dot{s}', t') = \sum_{i=1}^{N} \frac{m_i}{2} s'^2 \dot{\mathbf{x}'}_i^t \cdot \mathsf{G}' \cdot \dot{\mathbf{x}'}_i + \frac{W}{2} s'^2 \mathbf{Tr}\left[\dot{\mathsf{h}}'^t \cdot \dot{\mathsf{h}}'\right]$$

$$+ \frac{Q}{2}\dot{s'}^2 - U(\mathsf{h}', \{\mathbf{x}'_i\}) - p_{ext}(t') \det \mathsf{h}' - g k_B T \ln s'. \tag{4.3}$$

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. According to whether the time average is taken over the virtual time or the real time, we set the parameter g to be equal to $3N + 9 + 1$ or $3N + 9$, N being the number of particles in the unit cell.

5 Ewald-Type Formulae for Yukawa Lattice Sum

In this section, we summarize some Ewald-type expressions for lattice sums[8] in the Yukawa system. In order to take the deformaton of fundamental vectors, we calculate the pressure tensor in addition to interaction energy and force.

5.1 Interaction energy

5.1.1 Periodicity in three dimensions

We rewrite the Yukawa potential into

$$\frac{q^2}{r}\exp(-\kappa r) = \frac{2}{\sqrt{\pi}} q^2 \left(\int_0^G + \int_G^\infty\right) d\rho \exp\left(-r^2\rho^2 - \frac{\kappa^2}{4\rho^2}\right), \tag{5.1}$$

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

$$\sum_{\mathbf{p}} \frac{1}{|\mathbf{p}-\mathbf{r}|} \exp\left(-\kappa|\mathbf{p}-\mathbf{r}|\right)$$

$$= \sum_{\mathbf{p}} \frac{2}{\sqrt{\pi}} \left(\int_0^G + \int_G^\infty\right) d\rho \exp\left(-|\mathbf{p}-\mathbf{r}|^2\rho^2 - \frac{\kappa^2}{4\rho^2}\right)$$

$$= \sum_{\mathbf{p}} \frac{1}{2|\mathbf{p}-\mathbf{r}|} \left\{\exp\left(\kappa|\mathbf{p}-\mathbf{r}|\right) \operatorname{erfc}\left(G|\mathbf{p}-\mathbf{r}| + \frac{\kappa}{2G}\right)\right.$$

$$\left. + \exp\left(-\kappa|\mathbf{p}-\mathbf{r}|\right) \operatorname{erfc}\left(G|\mathbf{p}-\mathbf{r}| - \frac{\kappa}{2G}\right)\right\} + \frac{1}{V_0}\sum_{\mathbf{g}} \frac{4\pi}{g^2+\kappa^2} \exp\left(-\frac{g^2+\kappa^2}{4G^2} + i\mathbf{g}\cdot\mathbf{r}\right). \tag{5.2}$$

Here $\{\mathbf{g}\}$ is the reciprocal lattice. The interaction energy between a particle and its own image or the Madelung energy of lattice $\{\mathbf{p}\}$ is given by

$$\begin{aligned}\frac{\phi_0}{e^2} &= \lim_{r\to 0}\left[\sum_{\mathbf{p}}\frac{1}{|\mathbf{p}-\mathbf{r}|}\exp\left(-\kappa|\mathbf{p}-\mathbf{r}|\right)-\frac{1}{r}\exp\left(-\kappa r\right)\right] \\ &= \sum_{\mathbf{p}}{}'\frac{1}{2p}\left\{\exp\left(\kappa p\right)\operatorname{erfc}\left(Gp+\frac{\kappa}{2G}\right)+\exp\left(-\kappa p\right)\operatorname{erfc}\left(Gp-\frac{\kappa}{2G}\right)\right\} \\ &+\frac{1}{V_0}\sum_{\mathbf{g}}\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)+\kappa\operatorname{erfc}\left(\frac{\kappa}{2G}\right)-\frac{2}{\sqrt{\pi}}G\exp\left(-\frac{\kappa^2}{4G^2}\right).\end{aligned} \tag{5.3}$$

The interaction energy U is thus given by

$$\begin{aligned}\frac{U}{e^2} &= \frac{1}{2}\sum_{i\neq j}^{N}\sum_{\mathbf{p}}\frac{1}{|\mathbf{r}_{ij}-\mathbf{p}|}\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{p}|)+\frac{N}{2}\phi_0 \\ &= \frac{1}{2}\sum_{i\neq j}^{N}\sum_{\mathbf{p}}\frac{1}{2|\mathbf{r}_{ij}-\mathbf{p}|}\left\{\exp\left(\kappa|\mathbf{r}_{ij}-\mathbf{p}|\right)\operatorname{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|+\frac{\kappa}{2G}\right)\right. \\ &\left.+\exp\left(-\kappa|\mathbf{r}_{ij}-\mathbf{p}|\right)\operatorname{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|-\frac{\kappa}{2G}\right)\right\} \\ &+\frac{1}{2V_0}\sum_{\mathbf{g}}\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\sum_{i,j}^{N}\exp\left(i\mathbf{g}\cdot\mathbf{r}_{ij}\right) \\ &+\frac{N}{2}\sum_{\mathbf{p}}{}'\frac{1}{2p}\left\{\exp\left(\kappa p\right)\operatorname{erfc}\left(Gp+\frac{\kappa}{2G}\right)+\exp\left(-\kappa p\right)\operatorname{erfc}\left(Gp-\frac{\kappa}{2G}\right)\right\} \\ &+\frac{N}{2}\left[\kappa\operatorname{erfc}\left(\frac{\kappa}{2G}\right)-\frac{2}{\sqrt{\pi}}G\exp\left(-\frac{\kappa^2}{4G^2}\right)\right].\end{aligned} \tag{5.4}$$

5.1.2 Periodicity in two dimensions

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

$$\begin{aligned}&\sum_{\mathbf{P}}\frac{1}{|\mathbf{P}-\mathbf{r}|}\exp\left(-\kappa|\mathbf{P}-\mathbf{r}|\right) \\ &=\sum_{\mathbf{P}}\frac{1}{2|\mathbf{P}-\mathbf{r}|}\left\{\exp\left(\kappa|\mathbf{P}-\mathbf{r}|\right)\operatorname{erfc}\left(G|\mathbf{P}-\mathbf{r}|+\frac{\kappa}{2G}\right)\right. \\ &\left.+\exp\left(-\kappa|\mathbf{P}-\mathbf{r}|\right)\operatorname{erfc}\left(G|\mathbf{P}-\mathbf{r}|-\frac{\kappa}{2G}\right)\right\} \\ &+\frac{1}{S_0}\sum_{\mathbf{K}}\frac{\pi}{\sqrt{K^2+\kappa^2}}\exp(i\mathbf{K}\cdot\mathbf{R}) \\ &\times\left(\exp(\sqrt{K^2+\kappa^2}|z|)\operatorname{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+G|z|)\right. \\ &\left.+\exp(-\sqrt{K^2+\kappa^2}|z|)\operatorname{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-G|z|)\right).\end{aligned} \tag{5.5}$$

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 a particle and its own image or the Madelung energy of two-dimensional lattice $\{\mathbf{P}\}$ is given by

$$\frac{\phi_0}{e^2}=\lim_{r\to 0}\{\sum_{\mathbf{P}}\frac{1}{|\mathbf{P}-\mathbf{r}|}\exp\left(-\kappa|\mathbf{P}-\mathbf{r}|\right)-\frac{1}{r}\exp(-\kappa r)\}$$

$$= \sum_{\mathbf{P}}{}' \frac{1}{2P} \left\{ \exp(\kappa P) \mathrm{erfc}\left(GP + \frac{\kappa}{2G} \right) + \exp(-\kappa P) \mathrm{erfc}\left(GP - \frac{\kappa}{2G} \right) \right\}$$
$$+ \frac{1}{S_0} \sum_{\mathbf{K}} \frac{2\pi}{\sqrt{K^2+\kappa^2}} \mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G} \right) + \kappa\, \mathrm{erfc}\left(\frac{\kappa}{2G} \right) - \frac{2}{\sqrt{\pi}} G \exp\left(-\frac{\kappa^2}{4G^2} \right). \quad (5.6)$$

The interaction energy U is given by

$$\frac{U}{e^2} = \frac{1}{2} \sum_{i \neq j}^{N} \sum_{\mathbf{P}} \frac{1}{|\mathbf{r}_{ij} - \mathbf{P}|} \exp(-\kappa |\mathbf{r}_{ij} - \mathbf{P}|) + \frac{N}{2} \phi_0$$
$$= \frac{1}{2} \sum_{i \neq j} \sum_{\mathbf{P}} \frac{1}{2|\mathbf{P} - \mathbf{r}_{ij}|} \left\{ \exp(\kappa |\mathbf{P} - \mathbf{r}_{ij}|) \,\mathrm{erfc}\left(G|\mathbf{P} - \mathbf{r}_{ij}| + \frac{\kappa}{2G} \right) \right.$$
$$\left. + \exp(-\kappa |\mathbf{P} - \mathbf{r}_{ij}|) \,\mathrm{erfc}\left(G|\mathbf{P} - \mathbf{r}_{ij}| - \frac{\kappa}{2G} \right) \right\}$$
$$+ \frac{1}{2S_0} \sum_{i,j} \sum_{\mathbf{K}} \frac{\pi}{\sqrt{K^2+\kappa^2}} \exp(i\mathbf{K} \cdot \mathbf{R}_{ij})$$
$$\times \left(\exp(\sqrt{K^2+\kappa^2}|z_{ij}|) \mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G} + G|z_{ij}| \right) \right.$$
$$\left. + \exp(-\sqrt{K^2+\kappa^2}|z_{ij}|) \mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G} - G|z_{ij}| \right) \right)$$
$$+ \frac{N}{2} \sum_{\mathbf{P}}{}' \frac{1}{2P} \left\{ \exp(\kappa P) \mathrm{erfc}\left(GP + \frac{\kappa}{2G} \right) + \exp(-\kappa P) \mathrm{erfc}\left(GP - \frac{\kappa}{2G} \right) \right\}$$
$$+ \frac{N}{2} \left[\kappa\, \mathrm{erfc}\left(\frac{\kappa}{2G} \right) - \frac{2}{\sqrt{\pi}} G \exp\left(-\frac{\kappa^2}{4G^2} \right) \right]. \quad (5.7)$$

5.2 Force

5.2.1 Periodicity in three dimensions

We first note that

$$\frac{\partial}{\partial \mathbf{x}_i} U = \mathsf{h}^t \cdot \frac{\partial}{\partial \mathbf{r}_i} U. \quad (5.8)$$

The second factor is calculated as

$$-\frac{\partial}{\partial \mathbf{r}_i} \frac{U}{e^2} = \sum_{j(\neq i)} \sum_{\mathbf{P}} \frac{(\mathbf{r}_i - \mathbf{r}_j - \mathbf{p})}{|\mathbf{r}_{ij} - \mathbf{p}|^3}$$
$$\times \left[\frac{1}{2} (1 - \kappa |\mathbf{r}_{ij} - \mathbf{p}|) \exp(\kappa |\mathbf{r}_{ij} - \mathbf{p}|) \,\mathrm{erfc}\left(G|\mathbf{r}_{ij} - \mathbf{p}| + \frac{\kappa}{2G} \right) \right.$$
$$+ \frac{1}{2} (1 + \kappa |\mathbf{r}_{ij} - \mathbf{p}|) \exp(-\kappa |\mathbf{r}_{ij} - \mathbf{p}|) \,\mathrm{erfc}\left(G|\mathbf{r}_{ij} - \mathbf{p}| - \frac{\kappa}{2G} \right)$$
$$\left. + \frac{2}{\sqrt{\pi}} G |\mathbf{r}_{ij} - \mathbf{p}| \exp\left(-G^2 |\mathbf{r}_{ij} - \mathbf{p}|^2 - \frac{\kappa^2}{4G^2} \right) \right]$$
$$- \frac{1}{2V_0} \sum_{\mathbf{g}} \frac{8\pi}{g^2+\kappa^2} i\mathbf{g} \exp\left(-\frac{g^2+\kappa^2}{4G^2} \right) \left[\sum_{j}^{N} \exp(i\mathbf{g} \cdot \mathbf{r}_{ij}) \right]. \quad (5.9)$$

5.2.2 Periodicity in two dimensions

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

$$\frac{\partial}{\partial \mathbf{X}_i} U = \mathsf{h}^t \cdot \frac{\partial}{\partial \mathbf{R}_i} U, \quad (5.10)$$

$$
\begin{aligned}
-\frac{\partial}{\partial \mathbf{R}_i}\frac{U}{e^2} = & \sum_{j(\neq i)}\sum_{\mathbf{P}} \frac{(\mathbf{r}_i - \mathbf{r}_j - \mathbf{P})}{|\mathbf{r}_{ij} - \mathbf{P}|^3} \\
& \times\left[\frac{1}{2}(1-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|+\frac{\kappa}{2G}\right)\right. \\
& +\frac{1}{2}(1+\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|-\frac{\kappa}{2G}\right) \\
& \left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}_{ij}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}_{ij}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right)\right] \\
& -\frac{1}{S_0}\sum_{\mathbf{K}}\frac{\pi}{\sqrt{K^2+\kappa^2}}i\mathbf{K}\sum_{j}^{N}\exp(i\mathbf{K}\cdot\mathbf{R}_{ij}) \\
& \times\left(\exp(\sqrt{K^2+\kappa^2}|z_{ij}|)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+G|z_{ij}|)\right. \\
& \left.+\exp(-\sqrt{K^2+\kappa^2}|z_{ij}|)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-G|z_{ij}|)\right), \qquad (5.11)
\end{aligned}
$$

and

$$
\begin{aligned}
-\frac{\partial}{\partial z_i}\frac{U}{e^2} = & \sum_{j(\neq i)}\sum_{\mathbf{P}} \frac{z_{ij}}{|\mathbf{r}_{ij} - \mathbf{P}|^3} \\
& \times\left[\frac{1}{2}(1-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|+\frac{\kappa}{2G}\right)\right. \\
& +\frac{1}{2}(1+\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{P}|-\frac{\kappa}{2G}\right) \\
& \left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}_{ij}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}_{ij}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right)\right] \\
& -\frac{1}{S_0}\sum_{\mathbf{K}}\pi\sum_{j}^{N}\mathrm{sign}(z_{ij})\exp(i\mathbf{K}\cdot\mathbf{R}_{ij}) \\
& \times\left(\exp(\sqrt{K^2+\kappa^2}|z_{ij}|)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+G|z_{ij}|)\right. \\
& \left.-\exp(-\sqrt{K^2+\kappa^2}|z_{ij}|)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-G|z_{ij}|)\right). \qquad (5.12)
\end{aligned}
$$

5.3 Pressure Tensors

5.3.1 Periodicity in three dimensions

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

$$
\begin{aligned}
& \sum_{\mathbf{P}}\frac{(\mathbf{r}-\mathbf{p})(\mathbf{r}-\mathbf{p})}{|\mathbf{r}-\mathbf{p}|}\left\{\frac{\partial}{\partial|\mathbf{r}-\mathbf{p}|}\frac{1}{|\mathbf{r}-\mathbf{p}|}\exp(-\kappa|\mathbf{r}-\mathbf{p}|)\right\} \\
= & -\sum_{\mathbf{P}}\frac{(\mathbf{r}-\mathbf{p})(\mathbf{r}-\mathbf{p})}{|\mathbf{r}-\mathbf{p}|^3}\left\{\frac{1}{2}(1-\kappa|\mathbf{r}-\mathbf{p}|)\exp(\kappa|\mathbf{r}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{p}|+\frac{\kappa}{2G}\right)\right. \\
& +\frac{1}{2}(1+\kappa|\mathbf{r}-\mathbf{p}|)\exp(-\kappa|\mathbf{r}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{p}|-\frac{\kappa}{2G}\right) \\
& \left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}-\mathbf{p}|\exp\left(-G^2|\mathbf{r}-\mathbf{p}|^2-\frac{\kappa^2}{4G^2}\right)\right\}
\end{aligned}
$$

$$+\frac{1}{V_0}\sum_{\mathbf{g}}\mathbf{g}\mathbf{g}\frac{8\pi}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right)$$
$$-\mathsf{I}\frac{1}{V_0}\sum_{\mathbf{g}}\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right), \tag{5.13}$$

$$\sum_{\mathbf{p}\neq 0}\frac{\mathbf{p}\mathbf{p}}{p}\left\{\frac{\partial}{\partial p}\frac{1}{p}\exp(-\kappa p)\right\}$$
$$=-\sum_{\mathbf{p}\neq 0}\frac{\mathbf{p}\mathbf{p}}{p^3}\left\{\frac{1}{2}(1-\kappa p)\exp(\kappa p)\,\mathrm{erfc}\left(Gp+\frac{\kappa}{2G}\right)\right.$$
$$\left.+\frac{1}{2}(1+\kappa p)\exp(-\kappa p)\,\mathrm{erfc}\left(Gp-\frac{\kappa}{2G}\right)+\frac{2}{\sqrt{\pi}}Gp\exp\left(-G^2p^2-\frac{\kappa^2}{4G^2}\right)\right\}$$
$$+\frac{1}{V_0}\sum_{\mathbf{g}}\mathbf{g}\mathbf{g}\frac{8\pi}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)$$
$$-\mathsf{I}\frac{1}{V_0}\sum_{\mathbf{g}}\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right). \tag{5.14}$$

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

$$V_0\mathsf{\Pi}=\sum_{i=1}^{N}m_i\left(\mathsf{h}\cdot\dot{\mathbf{x}}_i\right)\left(\mathsf{h}\cdot\dot{\mathbf{x}}_i\right)$$
$$-\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\sum_{\mathbf{p}}\frac{(\mathbf{r}_{ij}-\mathbf{p})(\mathbf{r}_{ij}-\mathbf{p})}{|\mathbf{r}_{ij}-\mathbf{p}|}\frac{\partial v\left(|\mathbf{r}_{ij}-\mathbf{p}|\right)}{\partial|\mathbf{r}_{ij}-\mathbf{p}|}+V_0\mathsf{\Pi}_0$$
$$=\sum_{i=1}^{N}m_i\left(\mathsf{h}\cdot\dot{\mathbf{x}}_i\right)\left(\mathsf{h}\cdot\dot{\mathbf{x}}_i\right)$$
$$+\frac{1}{2}\sum_{i\neq j}\sum_{\mathbf{p}}\frac{(\mathbf{r}_{ij}-\mathbf{p})(\mathbf{r}_{ij}-\mathbf{p})}{|\mathbf{r}_{ij}-\mathbf{p}|^3}\left\{\frac{1}{2}(1-\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\exp(\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|+\frac{\kappa}{2G}\right)\right.$$
$$+\frac{1}{2}(1+\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\exp(-\kappa|\mathbf{r}_{ij}-\mathbf{p}|)\,\mathrm{erfc}\left(G|\mathbf{r}_{ij}-\mathbf{p}|-\frac{\kappa}{2G}\right)$$
$$\left.+\frac{2}{\sqrt{\pi}}G|\mathbf{r}_{ij}-\mathbf{p}|\exp\left(-G^2|\mathbf{r}_{ij}-\mathbf{p}|^2-\frac{\kappa^2}{4G^2}\right)\right\}$$
$$+\frac{N}{2}\sum_{\mathbf{p}\neq 0}\frac{\mathbf{p}\mathbf{p}}{p^3}\left\{\frac{1}{2}(1-\kappa p)\exp(\kappa p)\,\mathrm{erfc}\left(Gp+\frac{\kappa}{2G}\right)\right.$$
$$+\frac{1}{2}(1+\kappa p)\exp(-\kappa p)\,\mathrm{erfc}\left(Gp-\frac{\kappa}{2G}\right)$$
$$\left.+\frac{2}{\sqrt{\pi}}Gp\exp\left(-G^2p^2-\frac{\kappa^2}{4G^2}\right)\right\}$$
$$-\frac{1}{2V_0}\sum_{\mathbf{g}}\mathbf{g}\mathbf{g}\frac{8\pi}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\sum_{i,j}\exp\left(i\mathbf{g}\cdot\mathbf{r}_{ij}\right)$$
$$+\mathsf{I}\frac{1}{2V_0}\sum_{\mathbf{g}}\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right)\sum_{i,j}\exp\left(i\mathbf{g}\cdot\mathbf{r}_{ij}\right). \tag{5.15}$$

5.3.2 Periodicity in two dimensions

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

$$
\begin{aligned}
&\sum_{\mathbf{P}} \frac{(\mathbf{r}-\mathbf{P})(\mathbf{r}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|} \left\{ \frac{\partial}{\partial|\mathbf{r}-\mathbf{P}|} \frac{1}{|\mathbf{r}-\mathbf{P}|} \exp\left(-\kappa|\mathbf{r}-\mathbf{P}|\right) \right\} \\
&= -\sum_{\mathbf{P}} \frac{(\mathbf{r}-\mathbf{P})(\mathbf{r}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|^3} \left\{ \frac{1}{2}(1-\kappa|\mathbf{r}-\mathbf{P}|)\exp(\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|+\frac{\kappa}{2G}\right) \right. \\
&+\frac{1}{2}(1+\kappa|\mathbf{r}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|-\frac{\kappa}{2G}\right) \\
&\left. +\frac{2}{\sqrt{\pi}}G|\mathbf{r}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right) \right\} \\
&+\frac{1}{S_0}\sum_{\mathbf{K}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dg_z \mathbf{g}\mathbf{g} \frac{8\pi}{(g^2+\kappa^2)^2} \left(\frac{g^2+\kappa^2}{4G^2}+1\right) \exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
&-\frac{1}{S_0}\sum_{\mathbf{K}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dg_z \frac{4\pi}{g^2+\kappa^2} \exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right),
\end{aligned}
\tag{5.16}
$$

where

$$
\mathbf{g} = \mathbf{K} + g_z \hat{z} \tag{5.17}
$$

and

$$
\mathbf{g}\mathbf{g} = \mathbf{K}\mathbf{K} + \mathbf{K} g_z \hat{z} + g_z \hat{z} \mathbf{K} + g_z^2 \hat{z}\hat{z}. \tag{5.18}
$$

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

$$
\begin{aligned}
&\sum_{\mathbf{P}} \frac{(\mathbf{R}-\mathbf{P})(\mathbf{R}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|} \left\{ \frac{\partial}{\partial|\mathbf{r}-\mathbf{P}|} \frac{1}{|\mathbf{r}-\mathbf{P}|} \exp\left(-\kappa|\mathbf{r}-\mathbf{P}|\right) \right\} \\
&= -\sum_{\mathbf{P}} \frac{(\mathbf{R}-\mathbf{P})(\mathbf{R}-\mathbf{P})}{|\mathbf{r}-\mathbf{P}|^3} \left\{ \frac{1}{2}(1-\kappa|\mathbf{r}-\mathbf{P}|)\exp(\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|+\frac{\kappa}{2G}\right) \right. \\
&+\frac{1}{2}(1+\kappa|\mathbf{r}-\mathbf{P}|)\exp(-\kappa|\mathbf{r}-\mathbf{P}|)\,\mathrm{erfc}\left(G|\mathbf{r}-\mathbf{P}|-\frac{\kappa}{2G}\right) \\
&\left. +\frac{2}{\sqrt{\pi}}G|\mathbf{r}-\mathbf{P}|\exp\left(-G^2|\mathbf{r}-\mathbf{P}|^2-\frac{\kappa^2}{4G^2}\right) \right\} \\
&+\frac{1}{S_0}\sum_{\mathbf{K}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dg_z \mathbf{K}\mathbf{K} \frac{8\pi}{(g^2+\kappa^2)^2} \left(\frac{g^2+\kappa^2}{4G^2}+1\right) \exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
&-\frac{1}{S_0}\sum_{\mathbf{K}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dg_z \frac{4\pi}{g^2+\kappa^2} \exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right).
\end{aligned}
\tag{5.19}
$$

The integrations with respect to g_z give

$$
\begin{aligned}
&\frac{1}{S_0}\sum_{\mathbf{K}} \frac{1}{2\pi} \int_{-\infty}^{\infty} dg_z \frac{4\pi}{g^2+\kappa^2} \exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
&= \frac{1}{S_0}\sum_{\mathbf{K}} \frac{\pi}{\sqrt{K^2+\kappa^2}} \exp(i\mathbf{K}\cdot\mathbf{R}) \times \left[\exp(\sqrt{K^2+\kappa^2}|z|)\mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G}+G|z|\right) \right. \\
&\left. +\exp(-\sqrt{K^2+\kappa^2}|z|)\mathrm{erfc}\left(\frac{\sqrt{K^2+\kappa^2}}{2G}-G|z|\right) \right],
\end{aligned}
\tag{5.20}
$$

and

$$
\begin{aligned}
&\frac{1}{S_0}\sum_{\mathbf{K}}\frac{1}{2\pi}\int_{-\infty}^{\infty} dg_z \frac{8\pi}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}+i\mathbf{g}\cdot\mathbf{r}\right) \\
&= \frac{1}{S_0}\sum_{\mathbf{K}}\frac{\pi}{(K^2+\kappa^2)^{3/2}}\exp(i\mathbf{K}\cdot\mathbf{R})\left[(1-\sqrt{K^2+\kappa^2}|z|)\exp(\sqrt{K^2+\kappa^2}|z|)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}+G|z|)\right. \\
&\quad +(1+\sqrt{K^2+\kappa^2}|z|)\exp(-\sqrt{K^2+\kappa^2}|z|)\mathrm{erfc}(\frac{\sqrt{K^2+\kappa^2}}{2G}-G|z|) \\
&\quad \left.+\frac{2}{\sqrt{\pi}}\frac{\sqrt{K^2+\kappa^2}}{G}\exp(-\frac{K^2+\kappa^2}{4G^2}-G^2z^2)\right]. \qquad (5.21)
\end{aligned}
$$

The tensor related to the Madelung energy is similarly calculated as

$$
\begin{aligned}
&\sum_{\mathbf{P}\neq 0}\frac{\mathbf{PP}}{P}\frac{\partial}{\partial P}\frac{1}{P}\exp(-\kappa P) \\
&= -\sum_{\mathbf{P}\neq 0}\frac{\mathbf{PP}}{P^3}\left\{\frac{1}{2}(1-\kappa P)\exp(\kappa P)\mathrm{erfc}\left(GP+\frac{\kappa}{2G}\right)\right. \\
&\quad +\frac{1}{2}(1+\kappa P)\exp(-\kappa P)\mathrm{erfc}\left(GP-\frac{\kappa}{2G}\right) \\
&\quad \left.+\frac{2}{\sqrt{\pi}}GP\exp\left(-G^2P^2-\frac{\kappa^2}{4G^2}\right)\right\} \\
&\quad +\frac{1}{S_0}\sum_{\mathbf{K}}\frac{1}{2\pi}\int_{-\infty}^{\infty} dg_z\mathbf{KK}\frac{8\pi}{(g^2+\kappa^2)^2}\left(\frac{g^2+\kappa^2}{4G^2}+1\right)\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right) \\
&\quad -\mathrm{I}\frac{1}{S_0}\sum_{\mathbf{K}}\frac{1}{2\pi}\int_{-\infty}^{\infty} dg_z\frac{4\pi}{g^2+\kappa^2}\exp\left(-\frac{g^2+\kappa^2}{4G^2}\right). \qquad (5.22)
\end{aligned}
$$

6 Conclusion

We have summarized mathematical expressions which are necessary for molecular dynamics of Yukawa system with deformable periodic boundary conditions in three or two dimensions. As statistical ensemble, both microcanonical and canonical ensembles are considered with constant volume or under constant pressure. Simulations of bulk system[9] and those of finite system in external potential are in progress.

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