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Equilibration of energies in a two-dimensional harmonic graphene lattice

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We study dynamical phenomena in a harmonic graphene (honeycomb) lattice, consisting of equal particles connected by linear and angular springs. Equations of in-plane motion for the lattice are derived. Initial conditions typical for molecular dynamic modelling are considered. Particles have random initial velocities and zero displacements. In this case, the lattice is far from thermal equilibrium. In particular, initial kinetic and potential energies are not equal. Moreover, initial kinetic energies (and temperatures), corresponding to degrees of freedom of the unit cell, are generally different. The motion of particles leads to equilibration of kinetic and potential energies and redistribution of kinetic energy among degrees of freedom. During equilibration, the kinetic energy performs decaying high-frequency oscillations. We show that these oscillations are accurately described by an integral depending on dispersion relation and polarization matrix of the lattice. At large times, kinetic and potential energies tend to equal values. Kinetic energy is partially redistributed among degrees of freedom of the unit cell. Equilibrium distribution of the kinetic energies is accurately predicted by the non-equipartition theorem. Presented results may serve for better understanding of the approach to thermal equilibrium in graphene.

This article is part of the theme issue 'Modelling of dynamic phenomena and localization in structured media (part 2)'.

1. Introduction

Two-dimensional materials attract significant interest from researchers due to their extraordinary physical properties [1,2]. The best-known two-dimensional material is graphene, a monolayer of carbon atoms forming a perfect hexagonal (honeycomb) lattice [3,4]. Recent advances in nanoscale manufacturing allow the fabrication of single-layer graphene of submicrometre size [5]. The perfect structure of graphene yields unique physical properties. A review of theoretical and experimental studies of graphene's mechanical and thermal properties can be found in [6,7]. In particular, in paper [8], it is shown that the strength of graphene is close to the so-called theoretical strength. Graphene also shows extraordinary heat-conducting properties, including high thermal conductivity (above 3000 W m K^{-1} , [9]). Also, although in-plane elastic properties of graphene are isotropic [10], heat transport is anisotropic [11,12].

The low concentration of defects in graphene makes it a promising candidate for investigation of the ballistic heat transport [13–16]. In contrast with conventional diffusive heat transport, in the ballistic regime, the heat is carried by waves, travelling with velocities close to the speed of sound. This phenomenon is of great interest from both theoretical and applied points of view [13]. However, a theory of ballistic heat transport is still under development. In ballistic heat transport experiments, an initial temperature distribution can be generated by ultrashort laser excitation [17–21]. Laser excitation creates a strongly non-equilibrium state in the material. Therefore, it is important to develop mathematical models describing the transition from the non-equilibrium state to thermal equilibrium.

A convenient model for the description of thermal properties of solids is a harmonic crystal, i.e. a set of particles forming a perfect lattice and interacting via linearized forces. An approach to thermal equilibrium in harmonic crystals is considered in many works [22–32]. In particular, in a pioneering paper by Klein & Prigogine [26], the behaviour of kinetic temperature, proportional to kinetic energy of thermal motion, in a one-dimensional harmonic chain with random initial conditions. An expression for the temperature is obtained using an exact analytical solution of equations of motion. Another approach based on analysis of covariances of particle velocities is proposed by Krivtsov [27]. In papers [28–30,33–36], this approach is applied to crystals with monoatomic lattice. It is shown that the approach to thermal equilibrium is accompanied by two physical processes: equilibration of kinetic and potential energies and redistribution of energy among degrees of freedom of the unit cell. Generalization for the case of complex lattices with an arbitrary number of particles per unit cell is carried out in paper [37]. In the present paper, an approach to thermal equilibrium in a two-dimensional graphene lattice is considered.

The main goal of the present paper is to investigate peculiarities of thermal equilibration in graphene. The paper is organized as follows. In §2, the geometry of the lattice is described. In §3, equations of motion of the graphene lattice are derived using the Lagrange–Euler formalism. Equations of motion are obtained using a two-parametric model. In the framework of this model, atoms interact via longitudinal and angular springs. It is the simplest model allowing a correct description of in-plane elastic properties of graphene [38] as well as other honeycomb structures [39]. Random initial conditions, typical for molecular dynamics modelling of thermal processes, are discussed in §4. In §5, a dispersion relation is derived. Exact formulae, describing the time evolution of kinetic and potential energies, are presented in §6. In §7, analytical predictions are compared with results of numerical solution of equations of motion. Redistribution of kinetic energy between degrees of freedom of the unit cell¹ is investigated in §8.

2. Geometry of the lattice

Graphene has a regular honeycomb lattice shown in figure 1*a*. Its unit cell contains two carbon atoms (figure 1*b*). Unit cells are numbered by pairs of indices $\{n, m\}$. Displacements of atoms from

¹Exchange between energies corresponding to motion of particles in different spacial directions is considered. There is no energy exchange between the normal modes.

Figure 1. Graphene structure: (a) honeycomb lattice, (b) unit cell (rhombus). (Online version in colour.)

unit cell $\{n, m\}$ are denoted as $\mathbf{U}_{n,m}$, $\mathbf{V}_{n,m}$. Position vectors of unit cells $\{n, m\}$ and $\{s, p\}$ in the reference configuration are related as

$$\mathbf{r}_{n,m} = \mathbf{r}_{s,p} + (n-s)\mathbf{e}_1 + (m-p)\mathbf{e}_2. \quad (2.1)$$

Here, primitive vectors of the lattice, $\mathbf{e}_1$, $\mathbf{e}_2$, are represented in Cartesian basis as

$$\mathbf{e}_1 = a \frac{\sqrt{3}}{2} (\mathbf{i} + \sqrt{3}\mathbf{j}) \quad \text{and} \quad \mathbf{e}_2 = a \frac{\sqrt{3}}{2} (-\mathbf{i} + \sqrt{3}\mathbf{j}), \quad (2.2)$$

where a is an equilibrium bond length in graphene; in figure 1b, vector $\mathbf{i}$ is horizontal, vector $\mathbf{j}$ is vertical.

Vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$ connect atoms with the displacements $\mathbf{U}_{n,m}$ and $\mathbf{V}_{n,m}$ with their nearest neighbours (figure 1). The vectors satisfy relations $\mathbf{a}_4 = -\mathbf{a}_1$, $\mathbf{a}_5 = -\mathbf{a}_2$, $\mathbf{a}_6 = -\mathbf{a}_3$.

3. Equations of motion

In this section, the equations of motion for two atoms in a unit cell are derived using the Lagrange–Euler formalism. Each atom has 2 d.f., i.e. in-plane motions are considered. Since in harmonic approximation in-plane and out-of-plane motions are decoupled, the latter can be considered separately (see [37,40]).

The following model of interactions in graphene is considered. Each atom is connected with three nearest neighbours by linear springs (bonds) with stiffness c . Additionally, the nearest bonds between particles are connected by angular springs with stiffness g .

In the framework of the Lagrange–Euler formalism, equations of motion of the unit cell have the form:

$$\frac{d}{dt} \frac{\partial K}{\partial \dot{q}_{n,m}^i} - \frac{\partial K}{\partial q_{n,m}^i} = - \frac{\partial W}{\partial q_{n,m}^i}, \quad \mathbf{q}_{n,m} = \begin{bmatrix} U_{n,m}^x & U_{n,m}^y & V_{n,m}^x & V_{n,m}^y \end{bmatrix}^T, \quad (3.1)$$

where $U_{n,m}^x, U_{n,m}^y, V_{n,m}^x, V_{n,m}^y$ are components of displacement vectors $\mathbf{U}_{n,m}, \mathbf{V}_{n,m}$ in Cartesian basis; $q_{n,m}^i, i = 1, 2, 3, 4$ is the i -th component of column $\mathbf{q}_{n,m}$; K is the total kinetic energy of the unit cell; W is contribution of particles with displacements $\mathbf{U}_{n,m}, \mathbf{V}_{n,m}$ to the total potential energy of the lattice (see formulae (3.3), (3.4), (3.5)); $\top$ stands for the transpose sign. Here and below matrices are denoted by bold italic symbols, while invariant vectors, e.g. displacements, are denoted by bold symbols.

The total kinetic energy of the unit cell is calculated as

$$K = \frac{1}{2}M(\dot{\mathbf{U}}_{n,m}^2 + \dot{\mathbf{V}}_{n,m}^2), \quad (3.2)$$

where M is particle mass.

Potential energy, W , is equal to the sum of energies of all linear and angular springs connected with particles from the unit cell $\{n, m\}$:

$$W = W^s + W^b. \quad (3.3)$$

Here, W^s and W^b stand for contributions of linear and angular springs respectively. The expression for W^s in harmonic approximation has the form

$$W^s = \frac{c}{2a^2} \left[(a_1 \cdot (\mathbf{V}_{n+1,m} - \mathbf{U}_{n,m}))^2 + (a_2 \cdot (\mathbf{V}_{n,m+1} - \mathbf{U}_{n,m}))^2 + (a_3 \cdot (\mathbf{V}_{n,m} - \mathbf{U}_{n,m}))^2 + (a_4 \cdot (\mathbf{U}_{n-1,m} - \mathbf{V}_{n,m}))^2 + (a_5 \cdot (\mathbf{U}_{n,m-1} - \mathbf{V}_{n,m}))^2 \right]. \quad (3.4)$$

Here, dot stands for the scalar product; a is an equilibrium length of linear springs defined by formula (2.2).

The angular part of the potential energy, W^b , depends on the change of 14 angles shown in figure 2. The following expression for W^b is used

$$W^b = \sum_{i=1}^{14} \Pi_i^b \quad \text{and} \quad \Pi_i^b = \frac{1}{2}ga^2(\Theta_i - \Theta_i^0)^2. \quad (3.5)$$

Since calculation of forces in the case of multibody interactions is not trivial [41], we show detailed derivation for a single angular spring.

Consider, for example, angular spring number 2 connecting bonds with vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ (figures 1 and 2). Change of angle Θ_2 between the bonds is caused by relative rotation of vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ due to motion of particles. In a deformed state, these vectors turn into vectors $\mathbf{a}_1 + \mathbf{V}_{n+1,m} - \mathbf{U}_{n,m}$ and $\mathbf{a}_2 + \mathbf{V}_{n,m+1} - \mathbf{U}_{n,m}$. Corresponding rotation angles are denoted ϕ_1, ϕ_2 . The angles are calculated as

$$\begin{aligned} \sin \phi_1 &= \frac{(\mathbf{a}_1 \times (\mathbf{V}_{n+1,m} - \mathbf{U}_{n,m})) \cdot \mathbf{n}}{|\mathbf{a}_1| |\mathbf{a}_1 + \mathbf{V}_{n+1,m} - \mathbf{U}_{n,m}|}, & \sin \phi_2 &= \frac{(\mathbf{a}_2 \times (\mathbf{V}_{n,m+1} - \mathbf{U}_{n,m})) \cdot \mathbf{n}}{|\mathbf{a}_2| |\mathbf{a}_2 + \mathbf{V}_{n,m+1} - \mathbf{U}_{n,m}|} \Rightarrow \\ &\Rightarrow \phi_1 \approx \frac{1}{a^2} (\mathbf{n} \times \mathbf{a}_1) \cdot (\mathbf{V}_{n+1,m} - \mathbf{U}_{n,m}), & \phi_2 &\approx \frac{1}{a^2} (\mathbf{n} \times \mathbf{a}_2) \cdot (\mathbf{V}_{n,m+1} - \mathbf{U}_{n,m}), \end{aligned} \quad (3.6)$$

where $\mathbf{n} = \mathbf{i} \times \mathbf{j}$ is a unit vector, normal to graphene plane; $\times$ stands for the cross product. Then a change of angle Θ_2 is calculated as the angle of relative rotation $\phi_1 - \phi_2$. Therefore, the expression for the potential energy of the angular spring number 2 takes the form

$$\Pi_2^b = \frac{g}{2a^2} [(\mathbf{n} \times \mathbf{a}_1) \cdot (\mathbf{V}_{n+1,m} - \mathbf{U}_{n,m}) - (\mathbf{n} \times \mathbf{a}_2) \cdot (\mathbf{V}_{n,m+1} - \mathbf{U}_{n,m})]^2. \quad (3.7)$$

Energies of other angular springs are calculated similarly.

Figure 2. Numbering of angles for the given unit cell.

Substituting expressions for kinetic and potential energies into the Lagrange–Euler equation (3.1), yields equations of motion for the unit cell

$$\left. \begin{aligned}
 \ddot{M}u_{n,m}^x &= \frac{c\sqrt{3}}{4} \left[\sqrt{3}V_{n+1,m}^x + V_{n+1,m}^y - 2\sqrt{3}u_{n,m}^x + \sqrt{3}V_{n,m+1}^x - V_{n,m+1}^y \right] \\
 &+ \frac{g}{4} \left[2 \left(-u_{n-1,m}^x + \sqrt{3}u_{n-1,m}^y - u_{n,m-1}^x - \sqrt{3}u_{n,m-1}^y \right) + u_{n+1,m-1}^x \right. \\
 &+ \sqrt{3}u_{n+1,m-1}^y + u_{n-1,m+1}^x - \sqrt{3}u_{n-1,m+1}^y - 2 \left(u_{n+1,m}^x + u_{n,m+1}^x \right) \\
 &\left. + 6 \left(V_{n+1,m}^x - \sqrt{3}V_{n+1,m}^y - 5u_{n,m}^x + 4V_{n,m}^x + V_{n,m+1}^x + \sqrt{3}V_{n,m+1}^y \right) \right], \\
 \ddot{M}u_{n,m}^y &= \frac{c}{4} \left[\sqrt{3}V_{n+1,m}^x + V_{n+1,m}^y - 6u_{n,m}^y + 4V_{n,m}^y - \sqrt{3}V_{n,m+1}^x + V_{n,m+1}^y \right] \\
 &+ \frac{\sqrt{3}g}{4} \left[u_{n-1,m+1}^x - \sqrt{3}u_{n-1,m+1}^y - u_{n+1,m-1}^x - \sqrt{3}u_{n+1,m-1}^y + 2u_{n+1,m}^x \right. \\
 &\left. - 2u_{n,m+1}^x - 10\sqrt{3}u_{n,m}^y + 6 \left(V_{n,m+1}^x + \sqrt{3}V_{n,m+1}^y - V_{n+1,m}^x + \sqrt{3}V_{n+1,m}^y \right) \right]
 \end{aligned} \right\} \quad (3.8)$$

and

$$\left. \begin{aligned}
 M\ddot{V}_{n,m}^x &= \frac{\sqrt{3}c}{4} \left[\sqrt{3}U_{n-1,m}^x + U_{n-1,m}^y - 2\sqrt{3}V_{n,m}^x + \sqrt{3}U_{n,m-1}^x - U_{n,m-1}^y \right] \\
 &\quad + \frac{g}{4} \left[6 \left(U_{n-1,m}^x - \sqrt{3}U_{n-1,m}^y + U_{n,m-1}^x + \sqrt{3}U_{n,m-1}^y + 4U_{n,m}^x \right) \right. \\
 &\quad \left. - 2 \left(V_{n+1,m}^x - \sqrt{3}V_{n+1,m}^y + V_{n,m+1}^x + \sqrt{3}V_{n,m+1}^y \right) + V_{n+1,m-1}^x - \sqrt{3}V_{n+1,m-1}^y \right. \\
 &\quad \left. + V_{n-1,m+1}^x + \sqrt{3}V_{n-1,m+1}^y - 30V_{n,m}^x - 2 \left(V_{n,m-1}^x + V_{n-1,m}^x \right) \right], \\
 M\ddot{V}_{n,m}^y &= \frac{c}{4} \left[\sqrt{3}U_{n-1,m}^x + U_{n-1,m}^y + 4U_{n,m}^y - 6V_{n,m}^y - \sqrt{3}U_{n,m-1}^x + U_{n,m-1}^y \right] \\
 &\quad + \frac{\sqrt{3}g}{4} \left[2\sqrt{3} \left(-\sqrt{3}U_{n-1,m}^x + 3U_{n-1,m}^y - 5V_{n,m}^y + \sqrt{3}U_{n,m-1}^x + 3U_{n,m-1}^y \right) \right. \\
 &\quad \left. + V_{n+1,m-1}^x - \sqrt{3}V_{n+1,m-1}^y - V_{n-1,m+1}^x - \sqrt{3}V_{n-1,m+1}^y - 2 \left(V_{n,m-1}^x - V_{n-1,m}^x \right) \right].
 \end{aligned} \right\} \quad (3.9)$$

In further calculations, we use the following values of parameters for graphene [42]:

$$c = 730.2 \text{ N m}^{-1} \quad g = 66.9 \text{ N m}^{-1}, \quad a = 0.142 \text{ nm}. \quad (3.10)$$

Thus equations of motion of the unit cell are given by the formulae (3.8), (3.9), (3.10). In §5, equations (3.8), (3.9) are employed for derivation of the dispersion relation.

4. Initial conditions

In this section, we introduce initial conditions typical for molecular dynamics modelling of thermal processes in lattices [27,28,37]. Initially, particles have random velocities and zero displacements. Under these initial conditions, the system is far from thermal equilibrium.

The initial conditions have the forms

$$\mathbf{q}_{n,m} = 0 \quad \text{and} \quad \dot{\mathbf{q}}_{n,m} = \dot{\mathbf{q}}_{n,m}^0. \quad (4.1)$$

Here, $\dot{\mathbf{q}}_{n,m}^0$ is a column of random initial velocities of particles from unit cell $\{n, m\}$ such that

$$\langle \dot{\mathbf{q}}_{n,m}^0 \rangle = 0 \quad \text{and} \quad \langle \dot{\mathbf{q}}_{n,m}^0 \dot{\mathbf{q}}_{s,p}^0 \rangle = \mathbf{A} \delta_D(n-m) \delta_D(s-p), \quad (4.2)$$

where $\langle \dots \rangle$ stands for mathematical expectation (in computer simulations, mathematical expectation is approximated by average over realizations with different random initial conditions); $\delta_D(0) = 1$; $\delta_D(n-m) = 0$ for $n \neq m$; $\mathbf{A}$ is a constant matrix independent of n and m . In other words, components of $\dot{\mathbf{q}}_{n,m}^0$ are random numbers with zero mean and generally different variances given by diagonal elements of matrix $\mathbf{A}$. Off-diagonal elements of matrix $\mathbf{A}$ are equal to covariances of initial velocities, corresponding to different degrees of freedom of the unit cell. Initial velocities of particles from different unit cells are statistically independent. An example of initial conditions (4.1), (4.2) is given by formula (7.1).

From a macroscopic point of view, initial conditions (4.1), (4.2) correspond to *uniform* spatial distribution of kinetic temperature, proportional to the kinetic energy of thermal motion. Under these initial conditions, initial kinetic and potential energies are not equal (potential energy is equal to zero). Moreover, kinetic energies, corresponding to different degrees of freedom of the unit cell, are generally different. Time evolution of the energy is considered in §6, 7, 8.

5. Bloch's theorem and dispersion relation

In the present section, we derive the dispersion relation for graphene lattice described by equations of motion (3.8), (3.9).

Figure 3. Dispersion surfaces for graphene: (a) ω_1 (acoustic), (b) ω_2 (acoustic), (c) ω_3 (optical), (d) ω_4 (optical). Frequencies are normalized by $\sqrt{c/M}$. (Online version in colour.)

We seek for the solution of equations of motion (3.8), (3.9) in a form of propagating plane waves:

$$\mathbf{U}_{n,m} = \mathbf{U}(\mathbf{k})e^{i(\mathbf{k} \cdot \mathbf{r}_{n,m} - \omega t)} \quad \text{and} \quad \mathbf{V}_{n,m} = \mathbf{V}(\mathbf{k})e^{i(\mathbf{k} \cdot \mathbf{r}_{n,m} - \omega t)}, \quad (5.1)$$

where $\mathbf{U}(\mathbf{k}), \mathbf{V}(\mathbf{k})$ are amplitudes of the waves; ω is a frequency; $\mathbf{k}$ is a wave vector; $\mathbf{r}_{n,m}$ stands for position vector of the unit cell. The Bloch (or the Bloch-Floquet) theorem states that the displacements of the atoms in a unit cell identified by the integer pair $\{n + s, m + p\}$ (figure 1) satisfy the relation [43]

$$\mathbf{U}_{n+s, m+p} = \mathbf{U}_{n,m} e^{ik \cdot (se_1 + pe_2)} \quad \text{and} \quad \mathbf{V}_{n+s, m+p} = \mathbf{V}_{n,m} e^{ik \cdot (se_1 + pe_2)}. \quad (5.2)$$

As a consequence of the theorem, the proportionate change in the wave amplitude across a unit cell due to a wave propagation does not depend on the location of the unit cell within the lattice. The theorem is widely used in solid-state physics [44] and in engineering analysis of periodic structures [45,46]. Hence, we study wave propagation in the entire lattice by considering motion within a single unit cell.

Using a formula (5.2), we represent equations of motion (3.8), (3.9) in the form

$$\mathbf{M}\ddot{\mathbf{q}}_{n,m} + \mathbf{C}\mathbf{q}_{n,m} = 0, \quad \mathbf{M} = \mathbf{M}\mathbf{E}, \quad (5.3)$$

where $\mathbf{C}$ and $\mathbf{M}$ are 4×4 stiffness and mass matrices; $\mathbf{E}$ is 4×4 identity matrix; vector $\mathbf{q}_{n,m}$ is defined by formula (3.1).

Figure 4. First Brillouin zone of graphene lattice. (Online version in colour.)

We represent wave vector, $\mathbf{k}$, in reciprocal basis $\tilde{\mathbf{e}}_i$ such that $\tilde{\mathbf{e}}_i \cdot \mathbf{e}_j = 2\pi \delta_{ij}$:

$$\mathbf{k} = k_1 \tilde{\mathbf{e}}_1 + k_2 \tilde{\mathbf{e}}_2, \quad \tilde{\mathbf{e}}_1 = \frac{2\pi}{3a} (\sqrt{3}\mathbf{i} + \mathbf{j}), \quad \tilde{\mathbf{e}}_2 = \frac{2\pi}{3a} (-\sqrt{3}\mathbf{i} + \mathbf{j}). \quad (5.4)$$

Here and below $k_1, k_2 \in [0; 1]$ are dimensionless components of the wave vector. Taking these relations into account, we substitute (5.1) into (5.3) and obtain a homogeneous system of linear equations with respect to $\mathbf{q}_{n,m}$:

$$\left(\mathbf{C}(k_1, k_2) - \omega^2 \mathbf{M} \right) \mathbf{q}_{n,m} = 0. \quad (5.5)$$

The system has non-trivial solutions under the following condition:

$$\det \left(\boldsymbol{\Omega}(k_1, k_2) - \omega^2 \mathbf{E} \right) = 0 \quad \text{and} \quad \boldsymbol{\Omega}(k_1, k_2) = \frac{1}{M} \mathbf{C}, \quad (5.6)$$

where $\boldsymbol{\Omega}$ is referred to as the dynamical matrix [47]. The solution of the fourth order equation (5.6) with respect to ω^2 yields dispersion surfaces $\omega_i(k_1, k_2)$, $i = 1, 2, 3, 4$. Two acoustic (ω_1, ω_2) and two optical (ω_3, ω_4) surfaces obtained by numerical solution of equation (5.6) are shown in figure 3. The dispersion surfaces are periodic with a unit periodic cell corresponding to the first Brillouin zone shown in figure 4.

Due to the symmetry of the lattice, the irreducible zone, limited by path $\boldsymbol{\gamma} - K - M - \boldsymbol{\gamma}$, covers all possible values of wave frequencies. In the following section, it is shown that dispersion relation and dynamic matrix determine time evolution of kinetic and potential energies during the approach to thermal equilibrium.

6. Time evolution of kinetic energies: an exact solution

In this section, we consider the time evolution of kinetic energies, corresponding to different degrees of freedom of the unit cell. Initially, particle displacements are equal to zero. Therefore, potential energy is equal to zero, while kinetic energy is equal to the total energy. Motion of particles causes two physical processes: redistribution of energy among kinetic and potential forms and redistribution of kinetic energy among degrees of freedom of the unit cell. An analytical description of these processes is presented below. Note that these processes are present in both harmonic and anharmonic systems [26–29, 37]. In particular, redistribution of kinetic energy among degrees of freedom of the unit cell is caused by coupling between four equations of motion (3.8), (3.9). The effect of anharmonicity is discussed in §9.

Following paper [37], we introduce the following matrix, characterizing mathematical expectation of kinetic energies of the unit cell:

$$\mathbf{K} = \frac{M}{2} \langle \dot{\mathbf{q}}_{n,m} \dot{\mathbf{q}}_{n,m}^\top \rangle \quad \text{and} \quad \dot{\mathbf{q}}_{n,m} = \begin{bmatrix} \dot{U}_{n,m}^x & \dot{U}_{n,m}^y & \dot{V}_{n,m}^x & \dot{V}_{n,m}^y \end{bmatrix}^\top. \quad (6.1)$$

Diagonal elements of matrix $\mathbf{K}$ are equal to kinetic energies, corresponding to degrees of freedom of the unit cell:

$$K_{11} = \frac{1}{2}M\langle(\dot{U}_{n,m}^x)^2\rangle, \quad K_{22} = \frac{1}{2}M\langle(\dot{U}_{n,m}^y)^2\rangle, \quad K_{33} = \frac{1}{2}M\langle(\dot{V}_{n,m}^x)^2\rangle \quad \text{and} \quad K_{44} = \frac{1}{2}M\langle(\dot{V}_{n,m}^y)^2\rangle. \quad (6.2)$$

Off-diagonal elements of matrix $\mathbf{K}$ characterize the correlation between different degrees of freedom. Since initial conditions are spatially homogeneous, $\mathbf{K}$ is independent of n, m .

In paper [37], it is shown that the time evolution of matrix $\mathbf{K}$ is exactly described by the formula

$$\mathbf{K} = \int_0^1 \int_0^1 \mathbf{P}\mathbf{K}'\mathbf{P}^{*\top} dk_1 dk_2 \quad \text{and} \quad K'_{ij} = \frac{1}{2}\{\mathbf{P}^{*\top}\mathbf{K}_0\mathbf{P}\}_{ij} [\cos((\omega_i - \omega_j)t) + \cos((\omega_i + \omega_j)t)]. \quad (6.3)$$

Here, $\mathbf{K}_0$ is an initial value of matrix $\mathbf{K}$; $\{\dots\}_{ij}$ is element i, j of the matrix; $\omega_i(\mathbf{k}) \geq 0, i = 1, \dots, 4$ are branches of dispersion relation; $\mathbf{P}(\mathbf{k})$ stands for the polarization matrix, composed of normalized eigenvectors of the dynamic matrix (5.6); * stands for complex conjugate; k_1, k_2 are dimensionless components of the wave vector (5.4).

If initial kinetic energies, corresponding to all degrees of freedom of the unit cell, are equal then the total kinetic energy of the cell has the form

$$K = \text{tr}\mathbf{K} = \frac{K_0}{2} \left[1 + \frac{1}{4} \sum_{j=1}^4 \int_0^1 \int_0^1 \cos(2\omega_j(k_1, k_2)t) dk_1 dk_2 \right]. \quad (6.4)$$

Here K_0 is an initial value of the total kinetic energy of the unit cell. Given the known kinetic energy, the potential energy per unit cell can be calculated as $\Pi = K_0 - K$. At large times, the integral in the right side of formula (6.4) tends to zero. Kinetic energy tends to half of its initial value. Therefore, at large times, mathematical expectations of kinetic and potential energies are equal. This fact is in a good agreement with the results presented in paper [48].

Oscillations of the kinetic energies, described by formulae (6.3), (6.4), decay in time. At large times, the system tends to thermal equilibrium, i.e. to a state with spatially and temporary uniform distribution of kinetic temperature [37]. Kinetic and potential energies tend to some equilibrium values and $\mathbf{K}$ tends to $\mathbf{K}_{eq}$. Equilibrium kinetic energies can be calculated using the *non-equipartition theorem*, derived in paper [37]:

$$\mathbf{K}_{eq} = \frac{1}{2} \int_0^1 \int_0^1 \mathbf{P} \text{diag}(\mathbf{P}^{*\top}\mathbf{K}_0\mathbf{P}) \mathbf{P}^{*\top} dk_1 dk_2, \quad (6.5)$$

where $\text{diag}(\dots)$ stands for the diagonal part of the matrix. The theorem relates equilibrium distribution of kinetic energy among degrees of freedom with initial conditions.

In the following sections, formulae (6.3), (6.4), (6.5) are employed for investigation of redistribution of energy among kinetic and potential forms and redistribution of kinetic energy among degrees of freedom of the unit cell.

7. Equilibration of kinetic and potential energies

In this section, we consider behaviour of the total kinetic energy of the unit cell. Time evolution of the energy is caused by redistribution of energy among kinetic and potential forms.

To check formulae (6.3), (6.4), we compare them with results of the numerical solution of lattice dynamics equations (3.8), (3.9) with the following initial conditions:

$$\left. \begin{aligned} \mathbf{U}_{n,m} = \mathbf{V}_{n,m} = 0, \quad \dot{U}_{n,m}^x &= \beta_{n,m}^x \sqrt{\frac{2K_{11}^0}{M}}, \quad \dot{U}_{n,m}^y = \beta_{n,m}^y \sqrt{\frac{2K_{22}^0}{M}} \\ \text{and} \quad \dot{V}_{n,m}^x &= \gamma_{n,m}^x \sqrt{\frac{2K_{33}^0}{M}}, \quad \dot{V}_{n,m}^y = \gamma_{n,m}^y \sqrt{\frac{2K_{44}^0}{M}}, \end{aligned} \right\} \quad (7.1)$$

Figure 5. Dependence of the total kinetic energy K/K_0 of a graphene sheet on time t/τ_* . Analytical solution (6.4) (solid line), and results of numerical simulations (dots). (Online version in colour.)

where K_{ii}^0 , $i = 1, 2, 3, 4$ are proportional to mathematical expectations of initial kinetic energies, corresponding to degrees of freedom of the unit cell; $\beta_{n,m}^x, \beta_{n,m}^y, \gamma_{n,m}^x, \gamma_{n,m}^y$ are uncorrelated random values with zero mean and unit variance (in computer simulations, these values are uniformly distributed in the interval $[-1; 1]$). Corresponding matrix K_0 is diagonal. In simulations, the graphene sheet consists of 500×500 unit cells under fixed boundary conditions. Since we are interested in the behaviour of energies at relatively short times, boundary conditions are not important. Numerical integration of equations of motion is carried out using a symplectic leap-frog integrator with time-step $5 \times 10^{-3} \tau_*$, where $\tau_* = 2\pi\sqrt{M/c}$. During the simulation, kinetic energies, corresponding to degrees of freedom of the unit cell, for the whole sheet are calculated. In this case, averaging over realizations is not necessary.

Consider the case where initial kinetic energies corresponding to all degrees of freedom of the unit cell are equal ($K_{11}^0 = K_{22}^0 = K_{33}^0 = K_{44}^0$). It can be shown that under these initial conditions, the kinetic energies remain equal at any moment in time, i.e. matrix K remains spherical. Then behaviour of kinetic energy is described by formula (6.4). Comparison with the results of numerical simulations is shown in figure 5. It is seen that analytical solution (6.4) practically coincides with the results of the numerical integration of lattice dynamics equations. The kinetic energy of the system oscillates in time and tends to half of the initial value. Since the total energy of the system is conserved, then at large times kinetic and potential energies become equal.

The oscillations of kinetic energy, shown in figure 5, are quite complicated and contain multiple frequencies. Formula (6.4) allows us to simplify analysis of the oscillations. It shows individual contributions of branches of the dispersion relation. Rewriting formula (6.4), yields

$$K = \frac{K_0}{2} + \sum_{j=1}^4 I_j \quad \text{and} \quad I_j = \frac{K_0}{8} \int_0^1 \int_0^1 \cos(2\omega_j(k_1, k_2)t) dk_1 dk_2. \quad (7.2)$$

Contributions I_j are presented in figure 6. It is seen that oscillations shown in figure 5 have six main frequencies. Contributions, I_1, I_2 , of acoustic branches, ω_1, ω_2 , have one main frequency each, while contributions, I_3, I_4 , of optical branches, ω_3, ω_4 , have a form of beats (two close main frequencies). Note that all main frequencies are larger than $\sqrt{c/M}$. Particular expressions for the frequencies can be derived from asymptotic analysis of corresponding integrals (see e.g. paper [49]). The analysis is beyond the scope of the present paper.

Analysis of formula (6.3) and numerical results also show that behaviour of the total kinetic energy is independent on initial distribution of kinetic energy among degrees of freedom of the unit cell.

Figure 6. Contributions of branches of dispersion relation to oscillations of the total kinetic energy in graphene. Here, $I_j, j = 1, 2, 3, 4$ stands for contribution of branch ω_j (see formula (6.4)). (Online version in colour.)

Thus equilibration of kinetic and potential energies in graphene is accurately described by formula (6.4) for any distribution of the initial kinetic energy among degrees of freedom of the unit cell.

8. Redistribution of kinetic energy among degrees of freedom

In the present section, we consider the behaviour of kinetic energies K_{11} , K_{22} , K_{33} , K_{44} , corresponding to degrees of freedom of the unit cell (see formula (6.2)).

We investigate two processes. Firstly, we consider redistribution of the kinetic energy among two sublattices. Initial conditions are such that one sublattice is motionless, i.e. $K_{11}^0 = K_{22}^0 = \frac{1}{2}K_0$, $K_{33}^0 = K_{44}^0 = 0$. Here, K_0 is the total initial kinetic energy of the unit cell. We calculate equilibrium kinetic energies by numerical evaluation of the integral in formula (6.5). Calculation yields the following values:

$$K_{11}^{\text{eq}} = K_{22}^{\text{eq}} = K_{33}^{\text{eq}} = K_{44}^{\text{eq}} = 0.125K_0. \quad (8.1)$$

Remaining elements of matrix $\mathbf{K}_{eq}$ are negligible. Dependencies of kinetic energies on time, obtained by numerical solution of equations of motion and by numerical evaluation of integral (6.3) are presented in figure 7. The figure shows that kinetic energies of sublattices oscillate in time and tend to equal equilibrium values (8.1), predicted by the non-equipartition theorem (6.5). Therefore, in this case, energy is equally distributed between degrees of freedom of the unit cell. Note that kinetic energies K_{11} , K_{22} and K_{33} , K_{44} remain equal at any moment in time.

Consider redistribution of the kinetic energy among spatial directions. Initial conditions are such that particle velocities are directed along the x axis. In this case, $K_{11}^0 = K_{33}^0 = \frac{1}{2}K_0$, $K_{22}^0 = 0$, $K_{44}^0 = 0$. We calculate equilibrium kinetic energies, K_{ii}^{eq} , by numerical evaluation of the integral in formula (6.5):

$$K_{11}^{\text{eq}} = K_{33}^{\text{eq}} = 0.1819K_0 \quad \text{and} \quad K_{22}^{\text{eq}} = K_{44}^{\text{eq}} = 0.0681K_0. \quad (8.2)$$

Note that in this case some off-diagonal elements of matrix $\mathbf{K}_{eq}$ are not equal to zero, notably:

$$K_{13}^{\text{eq}} = K_{31}^{\text{eq}} = -0.0073K_0 \quad K_{24}^{\text{eq}} = K_{42}^{\text{eq}} = -0.0026K_0. \quad (8.3)$$

Therefore, velocities of two particles in a unit cell are correlated. Time dependencies of kinetic energies, obtained by numerical solution of equations of motion and by numerical evaluation of integral (6.3) are presented in figure 8. The figure shows that analytical and numerical results practically coincide.

Figure 7. Redistribution of kinetic energy among sublattices in graphene ($K_{11}^0 = K_{22}^0 = \frac{1}{2}K_0$, $K_{33}^0 = K_{44}^0 = 0$). Subplots show kinetic energies $K_{11} = K_{22}$ (a) and $K_{33} = K_{44}$ (b). Analytical solution (6.3) (line), simulation results (dots) and the equilibrium value (8.1) (dashed line). (Online version in colour.)

Figure 8. Redistribution of kinetic energy among degrees of freedom for two sublattices ($K_{11}^0 = K_{33}^0 = \frac{1}{2}K_0$, $K_{22}^0 = K_{44}^0 = 0$). Subplots show kinetic energies $K_{11} = K_{33}$ (a) and $K_{22} = K_{44}$ (b). Analytical solution (6.3) (line), simulation results (circles) and equilibrium values (8.2) (dashed line). (Online version in colour.)

Figure 9. Redistribution of kinetic energy among degrees of freedom at large times. Analytical solution (6.3) (line) and equilibrium values (8.2) (dashed line). (Online version in colour.)

Note that convergence to equilibrium takes much longer than in the previous example. Figure 9 shows the behaviour of the energies on larger time intervals. It is seen that at large times kinetic energies oscillate with low frequency and tend to equilibrium values predicted by the non-equipartition theorem.

Thus kinetic energy is partially redistributed among degrees of freedom of the unit cell. Equilibrium values of the kinetic energies are generally different. Though in some particular cases they are equal (see e.g. formula (8.1)). Note that off-diagonal elements of matrix $\mathbf{K}$, in general, are not equal to zero, i.e. velocities of particles inside a unit cell are correlated (see formula (8.3)).

9. Conclusion

Time evolution of kinetic energies, corresponding to different degrees of freedom of the unit cell, in graphene lattice with random initial velocities was investigated. It was shown that the evolution is exactly described by formula (6.3). The formula shows that the total kinetic and potential energies of the system oscillate in time and tend to equal equilibrium values. Characteristic frequency of these oscillations is higher than $\sqrt{c/M}$. The oscillations are independent of initial distribution of kinetic energy among degrees of freedom.

If initial kinetic energies, corresponding to degrees of freedom of the unit cell, are different then kinetic energy is partially redistributed. At large times, the energies tend to generally different equilibrium values. Equipartition of energies was observed only in some particular cases. In general, the equilibrium values of the kinetic energies are accurately predicted by the non-equipartition theorem (6.5).

Redistribution of energy among degrees of freedom of the unit cell in harmonic crystals is usually a fast, high-frequency process [29,37,49]. The energies usually oscillate in time and practically reach equilibrium values at times of order of ten periods of atomic vibrations. Characteristic frequency of these oscillations is of order of $\sqrt{c/M}$. It was shown that the oscillations in graphene contain very low frequency of order of $10^{-2}\sqrt{c/M}$.

In the present paper, spatially uniform distribution of kinetic energy (or kinetic temperature) was considered. In the case of non-uniform initial temperature profile, an additional physical process, notably the ballistic heat transport, should be considered. The heat transport is much slower than equilibration of energies considered above [30,50–54]. Therefore, at short times behaviour of kinetic energy at each spatial point can be approximately described by formula (6.5). It was shown that in a spatially uniform case, if initial kinetic energies, corresponding to degrees of freedom of the unit cell, are equal then their equilibrium values are also equal. Note that this fact does not guarantee that kinetic energies will remain equal during heat transport. In particular, in paper [11], it was shown that in heat-conducting harmonic crystals the kinetic energies are generally different even if their initial values are equal.

In the present paper, anharmonic effects were neglected. In paper [29], it is shown numerically that anharmonicity of interatomic interactions causes an additional relaxation process. This process leads, in particular, to equipartition of kinetic energies, corresponding to different degrees of freedom. However, at least in the case of small anharmonicity, the relaxation process is much slower than processes described above. Therefore, we believe that at short times harmonic approximation has reasonable accuracy. Investigation of anharmonic effects would be an interesting extension of the present work.

Thus presented results may serve for better understanding of thermal equilibration and ballistic heat transport in graphene and other two-dimensional materials.

Data accessibility. This article does not contain any additional data.

Authors' contributions. Both authors contributed equally to this study.

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