Interatomic force in systems with multibody interactions

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The system of particles (atoms) interacting via multibody interatomic potential of general form is considered. Possible variants of partition for the total force acting on a single particle into pair contributions are discussed. Two definitions for the force acting between a pair of particles are compared. The forces coincide only if the particles interact via pair or embedded-atom potentials. However in literature both definitions are used in order to determine Cauchy stress tensor. A simplest example of pure shear for perfect square lattice is analyzed. Two methods for stress calculation are considered. It is observed that, at least in the particular case, stresses calculated using classical continuum mechanics definition do not depend on the way of partition for the total force. In contrast, Hardy's definition gives different results depending on the radius of localization function. The differences strongly depend on the way of the partition.

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I. INTRODUCTION

Classical molecular dynamics (MD) [1,2], based on the numerical solution of the Newtonian equations of motion for many interacting particles, has been widely used for physical modeling and simulation for several decades. Interactions between particles are usually described by so-called empirical interatomic potentials. A variety of potentials has been proposed: starting with simple pair potentials [3], more accurate embedded-atom potential [4] and ending with complex bond-order potentials [5–7]. The MD simulation technique requires calculation of the total force acting on every particle. If the potential energy is known, then the total force $\mathbf{F}_i$ acting on particle number i is determined by the following formula [8]:

$$\mathbf{F}_i = -\frac{\partial U(\{\mathbf{R}_i\}_{i=1}^N)}{\partial \mathbf{R}_i}, \tag{1}$$

where $\{\mathbf{R}_i\}_{i=1}^N$ is the set of particle radius-vectors; N is the total number of particles; U is the total potential energy of the system. Thus formula (1) is sufficient for MD simulation. However interpretation and verification of simulation results are not so straightforward. The usual way is to calculate continuum variables, such as stress tensor and heat flux, during MD simulation and compare the results with predictions of continuum theory. This problem was addressed by many authors starting from the late 19th century [9]. Comprehensive reviews on this topic may be found in papers [10,11]. In the majority of approaches it is assumed that the total force can be expressed by the summation of pair contributions $\mathbf{F}_{ij}$ satisfying Newton's third law (see, for example, Hardy's formalism [12])

$$\mathbf{F}_i = \sum_{j\neq i} \mathbf{F}_{ij}, \quad \mathbf{F}_{ij} = -\mathbf{F}_{ji}. \tag{2}$$

Here and below the summation is carried out over all particles in the system. In the paper [11] it was stated that partition [Eq. (2)] can always be carried out. However the physical meaning of $\mathbf{F}_{ij}$ is clear only for pair interactions. Moreover it was stated in [16] that division [Eq. (2)] may be nonunique. Let us explain the reason for the ambiguities. Any system with pair interactions is equivalent to the set of particles connected by longitudinal springs. Therefore $\mathbf{F}_{ij}$ is a force caused by the deformation of the spring. In contrast the simplest system with multibody interactions can be imagined as the set of particles connected by longitudinal and angular springs between the bonds. Every angular spring belongs to three particles and causes the forces acting on all of them. Even in this simple case partition [Eq. (2)] is not straightforward. Note that commonly used multibody potentials, such as Tersoff [6], are even more complex. Several definitions for $\mathbf{F}_{ij}$ were proposed in literature. In the paper [13] the quantity $\mathbf{F}_{ij}$, satisfying Eq. (2), was introduced for systems with three-body forces [5–7]. The generalization for N-body forces was carried out in [14]. Another definition for $\mathbf{F}_{ij}$ was given in papers [15,16]. Both expressions for $\mathbf{F}_{ij}$ mentioned above were used in order to calculate Cauchy stress tensor for a discrete system with multibody interactions [13,16,19]. However the comparison of these approaches for calculation of stresses and the analysis of different definitions for $\mathbf{F}_{ij}$ were not carried out.

In the present paper the problem of the partition for the total force into pair contributions is discussed in detail. Two definitions for the force $\mathbf{F}_{ij}$ acting between a pair of particles (material points [20]) are considered. It is shown that the partition is not unique and does depend on the way the potential energy is represented. The influence of the partition on the value of stresses is analyzed for the simplest example—a pure shear of a square lattice.

II. THEORY

Let us compare possible definitions for the force $\mathbf{F}_{ij}$ acting between two particles. Consider the approach proposed in the paper [13] for the case of three-body interactions. It was shown that both the Stillinger-Weber [5] potential and the Tersoff [6] potential can be expressed in the following form:

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$$U = \frac{1}{2}\sum_i U_i, \quad U_i = \sum_{j\neq i;\ k\neq i,j} U_{ijk}(R_{ij},R_{ik},R_{kj}). \tag{3}$$

Here and below $\mathbf{R}_{ij}=\mathbf{R}_i-\mathbf{R}_j$, $R_{ij}=|\mathbf{R}_{ij}|$. Then using definition [Eq. (1)] the total force acting on the ith particle can be represented in form [Eq. (2)], where the expression for $\mathbf{F}_{ij}$ has form

$$\mathbf{F}_{ij} = -\frac{1}{2}\sum_{k\neq i,j} \frac{\partial(U_{ijk}+U_{kij}+U_{kji}+U_{jik}+U_{ikj}+U_{jki})}{\partial R_{ij}}\mathbf{e}_{ij}. \tag{4}$$

Here and below $\mathbf{e}_{ij}\overset{\text{def}}{=}\mathbf{R}_{ij}/R_{ij}$. The definition for the force $\mathbf{F}_{ij}$ acting between particles i and j arises in a natural way while calculating the derivative. On the other hand in the paper [13] it was shown that the same results can be obtained using the following definition:

$$\mathbf{F}_{ij} \overset{\text{def}}{=} -\frac{\partial U}{\partial R_{ij}}\mathbf{e}_{ij}. \tag{5}$$

One can see that Eqs. (2) are satisfied and furthermore $\mathbf{F}_{ij}$ is central, i.e., parallel to the vector connecting particles i and j. The above mentioned approach was generalized in the paper [14]. Let us assume that the total potential energy depends on all the interatomic distances in the system, i.e.,

$$U = U(\{R_{kn}\}_{k,n>k}). \tag{6}$$

Formula (6) is the most general form for potential energy of the atomic system. According to definition (1) the total force $\mathbf{F}_i$ is

$$\mathbf{F}_i = -\sum_{k,j>k} \frac{\partial U}{\partial R_{kj}}\frac{\partial R_{kj}}{\partial \mathbf{R}_i} = -\sum_{j\neq i}\frac{\partial U}{\partial R_{ij}}\mathbf{e}_{ij}. \tag{7}$$

One can see that again definition (5) naturally follows from the derivation. Thus in general case [Eq. (6)] the total force can be expressed in form Eq. (2).

The partition discussed above requires the potential energy U to be represented as a function of all the interatomic distances in system [Eq. (6)]. The requirement is automatically satisfied in the case of pair potentials [3] and the embedded-atom potential [4]. However representation [Eq. (6)] may be inconvenient in the case of bond-order potentials such as Stillinger-Weber [5] and Tersoff [6], which depend on angles between bonds. Let us consider the approach proposed in papers [15,16]. Assume that the total potential energy of the system has the form

$$U = \sum_i U_i(\{\mathbf{R}_{ij}\}_{j\neq i}). \tag{8}$$

Obviously all potentials mentioned above can be represented in form [Eq. (8)]. In contrast to the previous approach, the geometry of the atomic system should be represented via vectors $\{\mathbf{R}_{ij}\}_{j\neq i}$, but not interatomic distances. At first glance it seems that both approaches are equivalent. Let us show that in general this is not true. Calculating the total force $\mathbf{F}_i$ using definition (1) and expression (8) one obtains

$$\mathbf{F}_i = -\sum_j\sum_{k\neq j}\frac{\partial U_j}{\partial \mathbf{R}_{jk}}\cdot\frac{\partial \mathbf{R}_{jk}}{\partial \mathbf{R}_i} = \sum_{j\neq i}\left(\frac{\partial U_j}{\partial \mathbf{R}_{ji}} - \frac{\partial U_i}{\partial \mathbf{R}_{ij}}\right),$$

$$\mathbf{F}_{ij} \overset{\text{def}}{=} \frac{\partial U_j}{\partial \mathbf{R}_{ji}} - \frac{\partial U_i}{\partial \mathbf{R}_{ij}}. \tag{9}$$

One can see that introduced definition for $\mathbf{F}_{ij}$ satisfies Newton's third law, i.e., $\mathbf{F}_{ij}=-\mathbf{F}_{ji}$. It can be shown that forces $\mathbf{F}_{ij}$ are central in the case of pair potentials and embedded-atom potential. Moreover in these particular cases definitions (5) and (9) exactly coincide. However in general this is not true. Note that the partition of the total energy [Eq. (8)] is not unique. According to formula (9) the partition can, in general, affect the value of the force $\mathbf{F}_{ij}$. However the majority of commonly used potentials are based on partition [Eq. (8)] as well. For example, in the case of the Tersoff potential and the Stillinger-Weber potential the partition is determined by formula (3). The comparison of different partitions will be carried out below for a simple example [see formulas (21) and (23)].

Let us compare definitions (5) and (9) in the case of three-body potentials. Rewriting the expression for potential energy [Eq. (3)] in the form analogous to Eq. (8) one obtains

$$U = \sum_i U_i, \quad U_i = \frac{1}{2}\sum_{k,n\neq k}\tilde{U}_{ikn}(\mathbf{R}_{ik},\mathbf{R}_{in}),$$

$$\tilde{U}_{ikn}(\mathbf{R}_{ik},\mathbf{R}_{in}) = U_{ikn}(R_{ik},R_{in},R_{kn}). \tag{10}$$

One can show that in this case expression (9) for $\mathbf{F}_{ij}$ takes the form

$$\mathbf{F}_{ij} \overset{\text{def}}{=} \frac{1}{2}\sum_{k\neq i,j}\left[\frac{\partial}{\partial \mathbf{R}_{ji}}(\tilde{U}_{jik}+\tilde{U}_{jki}) - \frac{\partial}{\partial \mathbf{R}_{ij}}(\tilde{U}_{ijk}+\tilde{U}_{ikj})\right]. \tag{11}$$

Let us substitute the last formula from Eq. (10) in Eq. (11) and calculate the derivatives. Then $\mathbf{F}_{ij}$ can be expressed in the following form:

$$\mathbf{F}_{ij} \overset{\text{def}}{=} -\frac{1}{2}\sum_{k\neq i,j}\left[\frac{\partial(U_{ijk}+U_{ikj}+U_{jik}+U_{jki})}{\partial R_{ij}}\mathbf{e}_{ij} + \frac{\partial(U_{jik}+U_{jki})}{\partial R_{ik}}\mathbf{e}_{ik} + \frac{\partial(U_{ijk}+U_{ikj})}{\partial R_{kj}}\mathbf{e}_{kj}\right]. \tag{12}$$

One can see that expressions (4) and (12) are different. In particular, from Eq. (4) it follows that forces $\mathbf{F}_{ij}$ are parallel to $\mathbf{R}_{ij}$. According to Eq. (12) this is not true. Further these statements will be explicitly shown for a simple example [see Eqs. (16), (20), and (22)].

III. CALCULATION OF CAUCHY STRESS TENSOR

Let us consider practical consequences of different ways of partition for the total force. It was mentioned above that results of MD simulation are usually compared with predictions of continuum theory. Equivalent continuum quantities, such as Cauchy stress tensor, are calculated for this purpose.

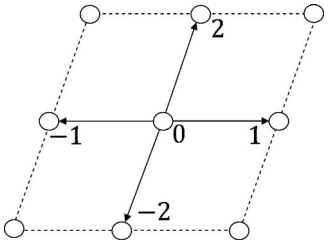

FIG. 1. Particle number 0 and its nearest neighbors.

The stress tensor characterizes external forces acting on the material surface surrounding the volume selected from the continuum media. Therefore the forces should be divided into internal and external in order to calculate stress. The analogous situation occurs if one defines equivalent stress tensor for discrete system. Obviously, it is impossible to express stress tensor in terms of the total forces acting on the particles. Therefore partition [Eq. (2)] is required. It was shown above that the partition is not unique. Thus we obtain the result that stresses in a material can depend on the choice of definition for $\mathbf{F}_{ij}$. Let us consider the simplest example, notably a pure shear of a perfect zero-temperature square lattice. Let particles interact via angular springs connecting two neighboring bonds. Only nearest neighbors are taken into account. Longitudinal springs may also be added but their contribution to forces $\mathbf{F}_{ij}$ is the same for both expressions (5) and (9). Let us consider particle number 0 with radius-vector $\mathbf{R}_0$ and denote its neighbors as in Fig. 1. Note that this numbering takes symmetry into account, for example, $\mathbf{R}_{01}=-\mathbf{R}_{0(-1)}$. Assume that potential energy of the spring connecting bonds $\mathbf{R}_{01}$ and $\mathbf{R}_{02}$ is given by the following expressions:

$$U_{012}=\frac{c}{2}\left(\frac{R_{01}^2+R_{02}^2-R_{12}^2}{2R_{01}R_{02}}\right)^2, \quad \tilde{U}_{012}=\frac{c}{2}(\mathbf{e}_{01}\cdot\mathbf{e}_{02})^2. \tag{13}$$

Note that $U_{012}\equiv\tilde{U}_{012}$. However different representations for the energy are required in order to use definitions (5) and (9). In the case of small deformations formulas (13) correspond to the energy of harmonic angular spring with stiffness c. Let us derive expressions for forces $\mathbf{F}_{01}$, $\mathbf{F}_{02}$, $\mathbf{F}_{12}$, $\mathbf{F}_{1(-2)}$. The remaining forces can be obtained using symmetry or Newton's third law, for example, $\mathbf{F}_{12}=\mathbf{F}_{(-2)(-1)}$, $\mathbf{F}_{01}=-\mathbf{F}_{10}$. First let us use definition (5). For example, let us calculate $\mathbf{F}_{01}$. Form the symmetry reasons the following identity is satisfied:

$$\frac{\partial}{\partial R_{01}}(U_{012}+U_{01(-2)})=\frac{\partial}{\partial R_{0(-1)}}(U_{0(-1)2}+U_{0(-1)(-2)}). \tag{14}$$

One can show using identity (14) and definition (5) that force $\mathbf{F}_{01}$ has form

$$\mathbf{F}_{01}=-\frac{\partial U}{\partial R_{01}}\mathbf{e}_{01}=-2\frac{\partial}{\partial R_{01}}(U_{012}+U_{01(-2)})\mathbf{e}_{01}, \tag{15}$$

The resulting expression for $\mathbf{F}_{01}$ can be obtained substituting the first formula from Eq. (13) into formula (15) and calculating the derivatives. Analogous derivations can be carried out for forces $\mathbf{F}_{02}$, $\mathbf{F}_{12}$, $\mathbf{F}_{1(-2)}$. As a result one obtains

$$\mathbf{F}_{01}=\frac{4c}{R}\sin^2\varphi\mathbf{e}_{01}, \quad \mathbf{F}_{12}=\frac{2\sqrt{2}c}{R}\sin\varphi\sqrt{1-\sin\varphi}\mathbf{e}_{12},$$

$$\mathbf{F}_{02}=\frac{4c}{R}\sin^2\varphi\mathbf{e}_{02}, \quad \mathbf{F}_{1(-2)}=-\frac{2\sqrt{2}c}{R}\sin\varphi\sqrt{1+\sin\varphi}\mathbf{e}_{1(-2)}. \tag{16}$$

where $R=R_{01}=R_{02}$, $\varphi\overset{\text{def}}{=}\arcsin(\mathbf{e}_{01}\cdot\mathbf{e}_{02})$. It is clear that forces [Eq. (16)] are central. Linearizing the expressions in the case of small shear $|\varphi|\ll 1$ and leaving first order terms only one obtains

$$\mathbf{F}_{01}\approx 0, \quad \mathbf{F}_{02}\approx 0,$$

$$\mathbf{F}_{12}\approx\frac{2\sqrt{2}c\varphi}{R}\hat{\mathbf{e}}_{12}, \quad \mathbf{F}_{1(-2)}\approx-\frac{2\sqrt{2}c\varphi}{R}\hat{\mathbf{e}}_{1(-2)}, \tag{17}$$

Here and below $\hat{\mathbf{e}}_{ij}\overset{\text{def}}{=}\mathbf{e}_{ij}|_{\varphi=0}$.

Let us use definition (9). It was mentioned above that representation [Eq. (8)] of the total energy used in formula (9) is not unique. Let us compare two possible ways of the partition for the total energy. In the case under consideration particle number 0 is surrounded by four nearest neighbors and four corresponding spring. First, let us assume that the energy of the springs contribute to energy U_0 of particle number 0 only, i.e.,

$$U_0=\tilde{U}_{012}+\tilde{U}_{01(-2)}+\tilde{U}_{0(-1)2}+\tilde{U}_{0(-1)(-2)}. \tag{18}$$

This way of partition is the simplest one and it is similar to the partition used in the definition for the Tersoff potential and the Stillinger-Weber potential [Eq. (10)]. For example, let us calculate $\mathbf{F}_{01}$ using definition (9).

$$\mathbf{F}_{01}=\frac{\partial U_1}{\partial\mathbf{R}_{10}}-\frac{\partial U_0}{\partial\mathbf{R}_{01}}=-2\frac{\partial U_0}{\partial\mathbf{R}_{01}}=-2\frac{\partial}{\partial\mathbf{R}_{01}}(\tilde{U}_{012}+\tilde{U}_{01(-2)}), \tag{19}$$

The symmetry of the problem was taken into account ($\frac{\partial U_1}{\partial\mathbf{R}_{10}}=-\frac{\partial U_0}{\partial\mathbf{R}_{01}}$). Formulas analogous to Eq. (19) can be derived for forces $\mathbf{F}_{02}$, $\mathbf{F}_{12}$, $\mathbf{F}_{1(-2)}$. Then straightforward calculations lead to the following results:

$$\mathbf{F}_{01}=-\frac{4c}{R}\sin\varphi(\mathbf{e}_{02}-\mathbf{e}_{01}\sin\varphi), \quad \mathbf{F}_{12}=0,$$

$$\mathbf{F}_{02} = -\frac{4c}{R}\sin\varphi(\mathbf{e}_{01} - \mathbf{e}_{02}\sin\varphi), \quad \mathbf{F}_{1(-2)} = 0. \tag{20}$$

Note that in formula (20) forces $\mathbf{F}_{12}$, $\mathbf{F}_{1(-2)}$ are exactly equal to zero. Obviously forces [Eq. (20)] are noncentral and are not equal to the previous result [Eq. (16)]. Linearizing formulas (20) and leaving first order terms only one obtains

$$\mathbf{F}_{01} \approx -\frac{4c\varphi}{R}\hat{\mathbf{e}}_{02}, \quad \mathbf{F}_{02} \approx -\frac{4c\varphi}{R}\hat{\mathbf{e}}_{01}, \quad \mathbf{F}_{12} = \mathbf{F}_{1(-2)} = 0. \tag{21}$$

The second way of partition for the total energy was proposed in the paper [16]. Energy U_{012} of the spring was divided between particles number 0, 1, and 2 in equal portions, i.e., $\frac{1}{3}U_{012}$ contributes to the energy of each particle. In other respects derivations of expressions for the forces are analogous to the development of formulas (20). The results are as follows:

$$\mathbf{F}_{01} = -\frac{8c}{3R}\sin\varphi(\mathbf{e}_{02} - \mathbf{e}_{01}\sin\varphi),$$

$$\mathbf{F}_{02} = -\frac{8c}{3R}\sin\varphi(\mathbf{e}_{01} - \mathbf{e}_{02}\sin\varphi),$$

$$\mathbf{F}_{12} = \frac{2\sqrt{2}c}{3R}\sin\varphi(1+\sin\varphi)\sqrt{1-\sin\varphi}\mathbf{e}_{12},$$

$$\mathbf{F}_{1(-2)} = -\frac{2\sqrt{2}c}{3R}\sin\varphi(1-\sin\varphi)\sqrt{1+\sin\varphi}\mathbf{e}_{1(-2)}. \tag{22}$$

Note that in contrast to formula (20) forces $\mathbf{F}_{12}$, $\mathbf{F}_{1(-2)}$ determined by formula (22) are not equal to zero. Linearized expressions (22) has the following form:

$$\mathbf{F}_{01} \approx -\frac{8c\varphi}{3R}\hat{\mathbf{e}}_{02}, \quad \mathbf{F}_{02} \approx -\frac{8c\varphi}{3R}\hat{\mathbf{e}}_{01},$$

$$\mathbf{F}_{12} \approx \frac{2\sqrt{2}c\varphi}{3R}\hat{\mathbf{e}}_{12}, \quad \mathbf{F}_{1(-2)} \approx -\frac{2\sqrt{2}c\varphi}{3R}\hat{\mathbf{e}}_{1(-2)}. \tag{23}$$

Thus one can see from formulas (16), (20), and (22) that all approaches mentioned above lead to qualitatively different expressions for forces.

Let us calculate stress vector τ acting on crystal's cross-section with normal orthogonal to vector $\mathbf{e}_{02}$. According to classical continuum mechanics definition, the stress vector is equal to the force acting on the cross-section per unit length. Then τ has the following form

$$\tau = \frac{1}{R}(\mathbf{F}_{10} + \mathbf{F}_{12} + \mathbf{F}_{1(-2)}). \tag{24}$$

Substituting formulas (16), (20), and (22) into formula (24) one obtains that in all the cases the stress vector can be expressed as

$$\tau = \frac{4c}{R^2}\sin\varphi(\mathbf{e}_{02} - \mathbf{e}_{01}\sin\varphi). \tag{25}$$

Thus, we are coming to the conclusion that stresses calculated using different expressions for $\mathbf{F}_{ij}$ are equal. Therefore at least in the case under consideration classical continuum mechanics definition of stresses does not depend on the partition for the total force. Linearizing expression (25) for the case of small shear one obtains

$$\tau \approx C_{44}^{*}\varphi\hat{\mathbf{e}}_{02}, \quad C_{44}^{*} \overset{\text{def}}{=} \frac{4c}{R^2}. \tag{26}$$

The second formula from Eq. (26) coincides with the well-known expression for elastic constant C_{44} of the square lattice, obtained, for example, in [17]. Index star is used in order to mark the exact solution.

Application of mentioned above definition for the stress is not very convenient, especially for dynamical problems involving large thermal motion, structural transformations, fracture, etc. Therefore in practice different approaches for calculation of stress are used (see papers [10,11] for detailed reviews). In particular, Hardy's formalism [12] is frequently applied [11,13,16]. In papers [13,16] it was shown that in the framework of Hardy's formalism the potential part of Cauchy stress tensor at spatial point $\mathbf{R}_0$ and time t has the form

$$\sigma_{pot}(\mathbf{R}_0, t) = -\frac{1}{2}\sum_i \sum_{j\neq i} \mathbf{F}_{ij}\mathbf{R}_{ij}\int_0^1 \psi(\lambda\mathbf{R}_{ij} + \mathbf{R}_j - \mathbf{R}_0)d\lambda, \tag{27}$$

where ψ is so-called localization function (see [16] for details). Formula (27) was used in the paper [13] and in the Appendix of the paper [16]. However the quantity $\mathbf{F}_{ij}$ has different meanings in them. Formula (5) was used as a definition for $\mathbf{F}_{ij}$ in the paper [13]. In contrast in the paper [16] quantity $\mathbf{F}_{ij}$ was calculated using formula (9). It was shown above that, in general, forces calculated with the use of Eqs. (5) and (9) are different. Thus corresponding stress tensors are also different. The accurate comparison of the stress tensors will be addressed in a separate paper. In the present work only the simplest example is analyzed.

Consider the example of linear pure shear of the square lattice. Let us calculate Cauchy stress tensor at the point $\mathbf{R}_0$, where particle number 0 is placed. For simplicity the radial step function is used as a localization function. Function ψ is equal to $1/(\pi r_L^2)$ inside the localization volume and zero in the remaining space. Here and below r_L is radius of the localization volume. One can prove substituting formulas (17), (21), and (23) into formula (27) that in all these cases stress tensor is symmetric. Note that, in general, this is not obvious as forces [Eqs. (21) and (23)] are noncentral. Let us show that this is indeed the case. Consider the forces given by formula (21) and assume that $r_L = R$. Then expression (27) for stress tensor takes form

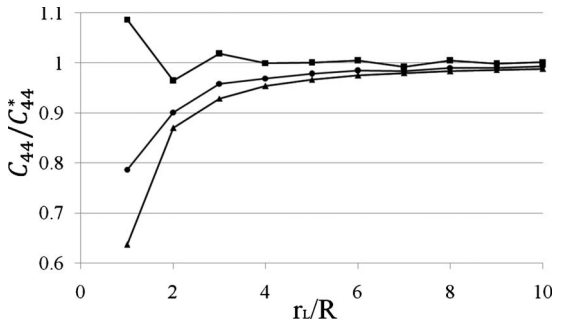

FIG. 2. Calculated elastic constant C_{44} divided by the exact solution C^*_{44}. Squares, triangles and circles correspond to elastic constant calculated using expressions (17), (21), and (23), respectively.

$$\sigma_{pot} = -\frac{1}{\pi R^2}(\mathbf{F}_{01}\mathbf{R}_{01} + \mathbf{F}_{0(-1)}\mathbf{R}_{0(-1)} + \mathbf{F}_{02}\mathbf{R}_{02} + \mathbf{F}_{0(-2)}\mathbf{R}_{0(-2)})$$

$$= -\frac{2}{\pi R^2}(\mathbf{F}_{01}\mathbf{R}_{01} + \mathbf{F}_{02}\mathbf{R}_{02}) = \frac{8c\varphi}{\pi R^2}(\hat{\mathbf{e}}_{02}\hat{\mathbf{e}}_{01} + \hat{\mathbf{e}}_{01}\hat{\mathbf{e}}_{02}), \quad (28)$$

where the following identity was used $\mathbf{F}_{0(-1)} = -\mathbf{F}_{01}$. One can see that tensor [Eq. (28)] is symmetric. Analogous derivations can be carried out for the forces determined by formula (23).

Let us calculate elastic constant C_{44} of the system as it completely determines stresses in the case of linear pure shear. The exact solution of this problem is given by the second formula from Eq. (26). The elastic constant calculated with different values of r_L is shown in Fig. 2. One can see from Fig. 2 that for small r_L/R elastic constants calculated using expressions (5) and (9) for $\mathbf{F}_{ij}$ are different. Furthermore in the second case elastic constant C_{44} depend on the partition for the total energy. However the expressions converge to the same value C^*_{44} with increasing radius of localization function. Note that the elastic constant that corresponds to definition (5) converges to the exact solution more rapidly. The practical consequence of this fact is that the first approach requires a smaller value of r_L than the second one. Therefore the first approach is more efficient from computational point of view.

IV. RESULTS AND DISCUSSION

Let us summarize the results. The problem of the partition for forces acting in the discrete system with multibody interactions into pair contributions is analyzed. Two methods for partition, differing in the way of representation for the potential energy U, are discussed. It is shown that in the framework of both methods the total force $\mathbf{F}_i$ is expressed as a sum of pair contributions $\mathbf{F}_{ij}$. In both cases the definition for $\mathbf{F}_{ij}$ is rather natural as the analog of Newton's third law is satisfied, i.e., $\mathbf{F}_{ij} = -\mathbf{F}_{ji}$. However the definitions coincide only in the case of pair potentials and embedded-atom potential. In particular, according to the approach proposed in papers [13,14] forces $\mathbf{F}_{ij}$ are always central. In the framework of the approach proposed in papers [15,16] forces $\mathbf{F}_{ij}$ are, in general, noncentral. The difference was explicitly shown in the case of three-body potentials [see Eqs. (16), (20), and (22)]. Thus the partition mentioned above is not unique. It depends on the representation of the potential energy. The influence of the partition on the value of stress tensor is analyzed for the simplest example of pure shear of perfect zero-temperature square lattice. Two definitions for the stress are considered. If the stress is calculated as a force acting on the cross section of the crystal per unit length then all expressions for $\mathbf{F}_{ij}$ considered above lead to exactly the same value of stress. In contrast, Hardy's definition (27) gives different values of stress depending on the size of localization volume. The differences depend strongly on the way of force definition. Accurate comparison of different expressions for stress tensor in the case on nonlinear deformation involving thermal motion is addressed in our future work.

Finally let us note that in the case of multibody interactions a common point of view on the definition for the force acting between two particles does not exist. Summarizing the results of the present paper one can formulate several advantages of definition (5). First, it was mentioned that forces defined by formula (5) are central. In this case equation of angular momentum balance is satisfied for any subsystem of the discrete system [18]. It leads, in particular, to unconditional symmetry of corresponding Cauchy stress tensor. Note that in the framework of classical continuum mechanics the symmetry is required [18]. On the other hand, in the paper [16] it was shown that definition (9) is more appropriate for the formulation of equivalent micromorphic continuum theory for discrete systems. The second appealing feature of definition (5) is that, at least in the considered case, corresponding stress tensor converges to the exact solution more rapidly than in the case of definition (9). In the last case it is shown that the convergence rate depends on the way of partition for the total energy.

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