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PARTICLES WITH INTERNAL DEGREES OF FREEDOM

Kostyantyn M. Kulyk[1*], **Maryna A. Ratner**[1], **Volodymyr V. Yanovsky**[1,2]
[1]*Institute for Single Crystals, NAS Ukraine, 60 Nauky Ave., Kharkov, 61072, Ukraine*
[2]*V. N. Karazin Kharkiv National University, 4 Svobody Sq., Kharkiv, 61022, Ukraine*
[*]*Corresponding Author e-mail: koskul@isc.kharkov.ua*
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A development of a structurally complex particle concept to the case of general interaction potentials between its components is proposed. A structurally complex particle is defined by the restricted problem of N+1 bodies of different masses, which is reduced to the N body problem. Based on the Lagrangian description, a Hamiltonian formalism is formulated and the resulting first integrals of motion are discussed. The absence of equipartition among the degrees of freedom is demonstrated. Using the virial theorem, it is proved that the energy of internal degrees of freedom does not exceed a certain fraction of the initial energy, depending on the ratio of the masses of internal particles to the mass of the shell. An exactly integrable case of a one-dimensional particle with two internal degrees of freedom is considered. The oscillation frequencies of such a structurally complex particle are determined by their masses and the mass of the shell. The energy distribution over them is not uniform. Universal relations are obtained for the distribution of the kinetic and potential energies of internal particles, which are independent of the choice of initial conditions. These relations provide more detailed information about the energy distribution than the virial relations.

Keywords: *Structurally complex particle; Internal degrees of freedom; Equations of motion; Virial relations*

1. INTRODUCTION

Small particles are often thought of as structureless point particles. This is one of the abstractions widely used in physics. It would seem that such a representation remains fairly reliable if one studies particle properties on scales significantly exceeding its size. In fact, in many cases this is not true. The presence of internal degrees of freedom manifests itself even on observation scales significantly exceeding the particle size. For example, when a structurally complex particle is reflected from a perfectly elastic barrier, a "violation" of the energy conservation law occurs for a supposedly point particle. The reason for this is related to the possibility of transferring the energy of internal degrees of freedom to a translation motion of a structurally complex particle, which can lead to an increase in the particle's velocity after reflection [1]. Naturally, if the internal degrees of freedom are taken into account, the conservation laws for energy and momentum are satisfied in this case. Moreover, in a number of cases, the properties of particles that depend on their internal structure and size are of interest. Such particles can no longer be considered as point ones, and their structure, i.e. internal degrees of freedom can affect virtually all relevant processes m and lead to unusual behavior. Of particular interest are particles with a small number of internal degrees of freedom, when partucle's properties depend essentially on this number. Such cases are interesting because thermodynamic laws are not applicable there. It should be emphasized that systems with a finite number of internal degrees of freedom demonstrate both pecularities of dynamic behavior [1,3], and clear manifestations of statistical anomalies [2]. Nanopeapods [5–8] and rotaxanes [9, 10] (see Fig.1) can be cited as real objects that fully correspond to one-dimensional structurally complex particles. In principle, the nature of such objects has a deeper meaning. If we consider a small particle of a medium, it typically contains quasiparticles of certain types. It's easy to see that the motion of quasiparticles in such a particle is accompanied by their reflection from the boundary of the medium. This leads to the transfer of momentum and energy to the particle itself and its surface, which corresponds to the model of a structurally complex particle. This provides a more general example of structurally complex particles.

Another type of an object with internal degrees of freedom was proposed quite a long time ago [15] and led to one of the popular models of polymer physics. Such a complex particle consists of beads connected in series by harmonic interaction in a chain. In the model, the beads experience strong friction and inertial forces in this case are insignificant. Examples of the implementation of this simple model in polymer physics are quite numerous [11–13]. The main method used for such systems consists in the use of Langevin equations (see, for example, [14]).

Another popular model of polymer molecules corresponds to a chain of rigid links connected by hinges [16]. The mechanical response of an individual polymer chain can be obtained by measuring the end-to-end length as a function of the applied force. Idealized models of individual chains, such as the freely jointed chain model, allow one to quantify these physical phenomena. It is important to note that experiments on stretching individual molecules of arbitrary length required the study of the statistical mechanics of small systems. In these cases, the thermodynamic limit is not satisfied; different macroscopic boundary conditions, corresponding to different ensembles of statistical mechanics, yield different force-displacement curves. A more comprehensive approach to approximating the mechanical response of individual chains with free joints required taking into account link extensions [17]. Among these models, exactly solvable ones

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have been discovered that correspond to special cases of harmonic bond potentials [18, 19]. In a certain sense, this is the opposite case to the structurally complex particles under consideration. Inertnal forces play a primary role in the behavior of structurally complex particles.

Nanodevices inevitably require internal degrees of freedom to function, which enable the device to perform certain actions. Examples of such nanodevices are currently quite numerous (see, for example, [20–23]) and are closely linked to the rapidly developing field of active particle physics [24]. Therefore, the development of the theory of structurally complex particles holds promise for the creation of new nanodevices.

Most results for particles with internal degrees of freedom have been obtained within the framework of the generalized billiard formalism [1]. This formalism considres perfectly elastic collisions between any components of a structurally complex particle. A model of a structurally complex particle can be represented as a shell of mass M within which N particles of different masses and possibly sizes move. In a certain sense, this reduces to the restricted problem of $N + 1$-bodies. The billiard formalism is useful for describing kinematic and dynamic properties of structurally complex particles with a small number of internal degrees of freedom. As the number of degrees of freedom increases, their properties of such particles can be studied using computer simulation. However, in some cases, such an idealization may not be realized. Therefore, this paper proposes a more general formalism that will allow us to consider the general case of potential interactions between the components of a structurally complex particle. In the proposed simple model of a particle with internal degrees of freedom, the interaction potential of the particles with the shell and with each other can be chosen in any suitable form. The most general kinematic and dynamic properties of such a particle are studied. It is shown that this problem of $N + 1$ bodies can be reduced to the problem of N bodies or to the behavior of only internal particles. The behavior of a structurally complex particle or shell is determined by the sum of the displacements of its internal particles. Lagrangian and Hamiltonian equations of motion for internal particles are derived, and the emergence of additional conservation laws is demonstrated. An analysis of the general equations of motion reveals the absence of equipartition among internal degrees of freedom for different particle masses. Using a modification of virial relations, it is shown that the energy of internal degrees of freedom cannot exceed a certain fraction of the initial energy, which depends on the ratio of the masses of the internal particles to the mass of the shell. These results indicate the emergence of unusual statistical properties of internal particles in their statistical description. As an example, a simple integrable case of a shell with two internal particles is considered. Exact solutions were obtained and universal patterns of energy distribution among individual components of a structurally complex particle were established.

2. DYNAMICS OF PARTICLES WITH INTERNAL DEGREES OF FREEDOM

Let us consider the Lagrangian description of a particle with N internal degrees of freedom. The model of such a system consists of a spherical shell with mass M with internal particles of various masses m_α. We will number internal particles with Greek indices $\alpha = 1, ..., N$. Let the internal particles interact with the shell and with each other. The potential energy of the interaction of the internal degrees of freedom with the shell is denoted by U, and between themselves by V. Let us denote the shell center position as $\vec{R}$, and the coordinates of the internal particles as $\vec{x}_\alpha$. Latin indices are reserved for the numbering of vector coordinates. Then the Lagrangian of such a system takes the form

$$\mathcal{L} = \frac{M\dot{\vec{R}}^2}{2} + \sum_{\alpha=1}^{N} \frac{m_\alpha \dot{\vec{x}}_\alpha^2}{2} - \sum_{\alpha=1}^{N} U(\vec{R} - \vec{x}_\alpha) - \sum_{\alpha,\beta}^{N} V(\vec{x}_\alpha - \vec{x}_\beta) \tag{1}$$

Here vector $\vec{R}$ plays the role composite particle's coordinate, i.e. the position of the spherical shell center, while $\dot{\vec{R}}$ is the composite particle's velocity. The role of the potential energy of the interaction of the internal degrees of freedom with each other, $V(\vec{x}_\alpha - \vec{x}_\beta)$, actually boils down to the appearance of chaos and the redistribution of energy between them. In a certain sense, the role of this interaction is not very significant. The same processes are carried out due to the interaction of internal particles with the shell. The choice of potential energy V can be dictated by the physics of the system and the simplicity of the calculation. Let's dwell on the potential energy $U(\vec{R} - \vec{x}_\alpha)$ of the interaction of internal particles with the shell. The simplest choice of such a potential corresponds to local interactions or absolutely elastic collisions of internal particles and the shell. Such a potential is determined by an unlimited barrier of circular shape, $U(\vec{R} - \vec{x}_\alpha) = U_0\delta(R_0^2 - |\vec{R} - \vec{x}_\alpha|^2)$, where R_0 the radius of the spherical shell or the size of the particle. In fact, such a potential corresponds to a cylindrical potential well (see Fig.2). In general, the potential can be more complicated, but preserving its symmetry, we will preserve its dependence on coordinates $|\vec{R} - \vec{x}_\alpha|^2$. The transition to coordinates $\vec{Q} = \sqrt{M}\vec{R}, \vec{y}_\alpha = \sqrt{m_\alpha}\vec{x}_\alpha$ transforms the Lagrangian (1) into the form

$$\mathcal{L} = \frac{\dot{\vec{Q}}^2}{2} + \sum_{\alpha=1}^{N} \frac{\dot{\vec{y}}_\alpha^2}{2} - U\left(\frac{\vec{Q}}{\sqrt{M}} - \frac{\vec{y}_1}{\sqrt{m_1}}, ..., \frac{\vec{Q}}{\sqrt{M}} - \frac{\vec{y}_M}{\sqrt{m_N}}\right) -$$

$$- \sum_{\alpha,\beta}^{N} V\left(\frac{\vec{y}_\alpha}{\sqrt{m_\alpha}} - \frac{\vec{y}_\beta}{\sqrt{m_\beta}}\right) \tag{2}$$

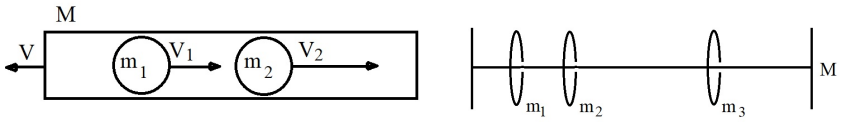

Figure 1. Type of one-dimensional particle with internal degrees of freedom. On the right, there is shown the equivalent model in the form of a chemical compound with topological bonds — rotaxanes.

Where $U\left(\frac{\vec{Q}}{\sqrt{M}} - \frac{\vec{y}_1}{\sqrt{m_1}}, ..., \frac{\vec{Q}}{\sqrt{M}} - \frac{\vec{y}_M}{\sqrt{m_N}}\right) = \sum_{\alpha=1}^{N} U(\frac{\vec{Q}}{\sqrt{M}} - \frac{\vec{y}_\alpha}{\sqrt{m_\alpha}})$.

It is easy see that, via introducing $3(N+1)$-dimensional configurational space, this Lagrangian can be considered as the Lagrangian of one particle of unit mass moving in a potential well in $3(N+1)$-dimensional space. In a certain sense, it can be considered as a generalization of the billiard formalism for the case of arbitrary interaction potentials.

Returning to the Lagrangian (1) we note that the limit $M \to \infty$ corresponds to a classical gas of a finite number of particles in a spherical vessel. Even this classical case demonstrates unusual statistical properties [2], which differ from the known ones associated with Boltzmann distributions. Of course, the potential $U(\vec{R}-\vec{x}_\alpha)$ may also have other dependences on the coordinates in general case. The Lagrangian (1) completely determines the general dynamics of a particle with internal degrees of freedom. The equations of motion of all $N+1$ components of the particle arise as Lagrange equations from the variational principle of the least action.

Naturally, the total energy, angular momentum, and total momentum of such a closed system are preserved. Taking into account the conservation of momentum, it is convenient to switch to a frame of reference associated with the center of mass.

$$M\vec{R} + \sum_{\alpha=1}^{N} m_\alpha \vec{x}_\alpha = 0 \tag{3}$$

In this reference system, the position of the particle is determined by the internal degrees of freedom coordinates as

$$\vec{R} = -\frac{\sum_\alpha^N m_\alpha \vec{x}_\alpha}{M} \tag{4}$$

Let's move on to the new coordinates of the internal particles, which correspond to their positions relative to the center of the shell

$$\vec{q}_\alpha = \vec{R} - \vec{x}_\alpha \tag{5}$$

In the new coordinates, the position of the particle is determined as

$$\vec{R} = \frac{\sum_\alpha^N m_\alpha \vec{q}_\alpha}{M_s} \tag{6}$$

Where $M_s = M + \sum_\alpha^N m_\alpha$ is the total mass of the particle. In a certain sense, the shell's position is determined by the sum of the "trajectories" of the internal degrees of freedom at each moment of time. The statistical properties of this sum differ from the statistical properties of the trajectories of a Brownian particle due to the shell's constraints on the quantities that make up the sum. Using this relation, we exclude the collective coordinate $\vec{R}$ from the Lagrangian (1) and obtain

$$\mathcal{L} = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2} - \frac{1}{2M_s}\left(\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha\right)^2 - \\ - \sum_{\alpha=1}^{N} U(\vec{q}_\alpha) - \sum_{\alpha,\beta}^{N} V(\vec{q}_\alpha - \vec{q}_\beta) \tag{7}$$

First of all, it is important to note that now a complete description of a particle with internal degrees of freedom is achieved by a system of a smaller number of objects of different masses. In other words, the problem of $N+1$ bodies is reduced to the problem of N bodies. The shell coordinate is determined according to the equation (6). The explicit form of the equations of motion can be obtained from the variational principle as Lagrange's equations

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_{\alpha i}} - \frac{\partial \mathcal{L}}{\partial q_{\alpha i}} = 0 \tag{8}$$

Using Lagrangian (7), we obtain a system of equations of motion for internal degrees of freedom

$$m_\alpha \ddot{q}_{\alpha i} - \frac{m_\alpha}{M_s}\sum_{\beta}^{N} m_\beta \ddot{q}_{\beta i} = -\frac{\partial U(\vec{q}_\alpha)}{\partial q_{\alpha i}} - \sum_{\beta} \frac{\partial V(\vec{q}_\alpha - \vec{q}_\beta)}{\partial q_{\alpha i}} \tag{9}$$

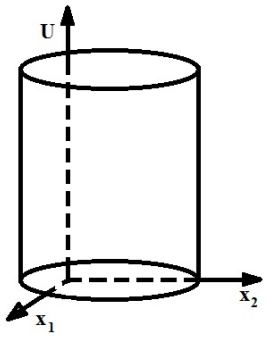

Figure 2. The form of a cylindrical potential well in two dimensional case; in three dimensional case, the cylinder's base is sphere S^3.

This system of equations fully describes the dynamic properties of a particle with internal degrees of freedom. It is easy to notice some differences from the usual equations of particles in a potential well. Already from these equations it is possible to understand the presence of two limiting cases in the system: $\frac{m_\alpha}{M} \gg 1$ and $\frac{m_\alpha}{M} \ll 1$. In the second limiting case, the system is close to the system of a finite number of particles in a potential well. In fact, the value of the second contribution in the left part of Eq.(9) is a measure of difference from this canonical physical case. Each of the Eq. (9) includes accelerations of all internal particles. They can be reduced to Newton's equations, via solving this linear equation system (9) with respect to accelerations

$$m_\alpha \ddot{\vec{q}}_{\alpha i} = \vec{F}_\alpha + \frac{m_\alpha}{M} \sum_{\beta=1}^{N} \vec{F}_\beta \tag{10}$$

Here we use the notation $\vec{F}_\alpha = -\frac{\partial U(\vec{q}_\alpha)}{\partial \vec{q}_\alpha} - \sum_{\beta=1}^{N} \frac{\partial V(\vec{q}_\alpha - \vec{q}_\beta)}{\partial \vec{q}_{\alpha i}}$ to reduce the cumbersomeness of notation. In this form, the dynamic equations correspond to the motion of interacting particles in a more complex potential well. It is important to note that the position of this potential well is independent of time. Returning to the behavior of a structurally complex particle, we note that relation (6) resembles the formation of a Brownian trajectory by summing successive jumps. However, the nature of this relation is different and is related to the sum of instantaneous jumps. In other words, the first distintion lies in the execution of not one, but multiple steps per unit time. The number of steps is determined by the number of internal degrees of freedom. The change in the shell's position over time can be estimated

$$\vec{R}(t + \Delta t) \approx \frac{\sum_\alpha^N m_\alpha \vec{q}_\alpha(t)}{M_s} + \frac{\sum_\alpha^N m_\alpha \dot{\vec{q}}_\alpha(t)}{M_s} \Delta t \tag{11}$$

Thus, the jump in the particle's position over time Δt is determined by the sum of $m_\alpha \dot{\vec{q}}_\alpha$ internal particles and effectively determines the Brownian jump of the entire particle. However, the magnitude of the possible changes in the particle's position is limited by the inequalities

$$\frac{\min \left| \sum_\alpha^N m_\alpha \vec{q}_\alpha \right|}{M_s} \leq \left| \vec{R} \right| \leq \frac{\max \left| \sum_\alpha^N m_\alpha \vec{q}_\alpha \right|}{M_s}$$

Here the length of the vector is indicated by straight brackets |...|. The minimum and maximum values of these amounts are easy to estimate. The minimum is reached when all internal particles are located in the center of the shell and the relative deviations $\vec{q}_\alpha = 0$, and the maximum is reached when they are all close to an arbitrary point on the shell boundary, with a radius R_0. From this we obtain $0 \leq \left| \vec{R} \right| \leq \frac{R_0 \sum_\alpha^N m_\alpha}{M_s}$. This leads to the second distinction from Brownian motion. This is the presence of an a priori limitation on deviations from the particle's initial position. Some other features of the dynamic equations (10) will be discussed in the following sections.

3. HAMILTONIAN EQUATIONS OF MOTION

We now turn to the Hamiltonian formalism, which has a number of advantages. In addition to its clarity and exceptional geometric representations, these include advantage of finding exact solutions. It simplifies the transition to quantum mechanics and is useful in the statistical description of physical systems. The transition from the Lagrangian to the Hamiltonian formalism is achieved by performing a Legendre transformation [25, 26]. To do this, we define the generalized momenta according to

$$\vec{p}_\alpha = \frac{\partial L}{\partial \dot{\vec{q}}_\alpha} \tag{12}$$

Using the form of the Lagrangian (7) we obtain the relation

$$\vec{p}_\alpha = m_\alpha \dot{\vec{q}}_\alpha - \frac{m_\alpha \sum_{\beta=1}^{N} m_\beta \dot{\vec{q}}_\beta}{M_s} \tag{13}$$

Using this equation we obtain the dependence of velocities on momenta

$$m_\alpha \dot{\vec{q}}_\alpha = \vec{p}_\alpha + \frac{m_\alpha}{M} \sum_{\beta=1}^{N} \vec{p}_\beta \tag{14}$$

Now we perform the Legendre transformation of the Lagrange function with respect to velocities. Using the dependence (14) we define the Hamilton function as

$$H = \left(\sum \vec{p}_\alpha \dot{\vec{q}}_\alpha - L \right) \Big|_{\dot{\vec{q}}_\alpha = \frac{\vec{p}_\alpha}{m_\alpha} + \frac{1}{M} \sum_\beta \vec{p}_\beta} \tag{15}$$

After simple transformations we obtain the Hamiltonian in the form

$$H = \frac{1}{2} \sum_{\alpha}^{N} \frac{\vec{p}_\alpha^{\,2}}{m_\alpha} + \frac{(\sum_\alpha \vec{p}_\alpha)^2}{2M} + \sum_{\alpha}^{N} U(\vec{q}_\alpha) + \sum_{\alpha<\beta}^{N} V(\vec{q}_\alpha - \vec{q}_\beta) \tag{16}$$

The equations of motion in the Hamiltonian formalism have the form

$$\begin{aligned} \frac{d\vec{p}_\alpha}{dt} &= -\frac{\partial H}{\partial \vec{q}_\alpha} \\ \frac{d\vec{q}_\alpha}{dt} &= \frac{\partial H}{\partial \vec{p}_\alpha} \end{aligned} \tag{17}$$

Using the resulting Hamiltonian, we obtain the equation of motion.

$$\begin{aligned} \frac{d}{dt}\vec{p}_\alpha(t) &= -\frac{\partial}{\partial \vec{q}_\alpha} U(\vec{q}_\alpha) - \frac{\partial}{\partial \vec{q}_\alpha} \sum_\beta V(\vec{q}_\alpha - \vec{q}_\beta) \\ \frac{d}{dt}\vec{q}_\alpha(t) &= \frac{p_\alpha}{m_\alpha} + \frac{\sum_\beta p_\beta}{M} \end{aligned} \tag{18}$$

This system of $6N$ first-order equations determines the dynamics of internal degrees of freedom in the Hamiltonian approach. The first equation for the change in momentum coincides with the equation for interacting particles in a potential well. The distinction in the second equation, as expected, disappears in the limiting case of an infinitely heavy shell $M \to \infty$. This leads us to the classical system of a gas of a finite number of particles in a spherical potential.

Returning to the form of Hamiltonian (16) we note the absence of time dependence. In this case H is the first integral of Hamiltonian equations (18). It is interesting to note that this conservation law differs from the conservation law of energy for a particle with internal degrees of freedom. Thus, for a particle with internal degrees of freedom, an additional conservation law arises. The presence of an additional conservation law is of great importance not only for dynamic properties but also it introduces significant changes to statistical theory. Thus, when obtaining a microcanonical distribution, a homogeneous distribution will be achieved not on the surface of constant energy, but at its intersection with the surface of constancy of an additional invariant. This radically affects the type of equilibrium distribution functions (see, for example [2]).

4. A SPECIAL CASE OF COLLISIONLESS INTERNAL DEGREES OF FREEDOM

Let us consider in more detail a simple case of interaction between internal particles and the shell in the absence of interactions of particles with each other. In this case, Lagrangian (7) is simplified and takes the form

$$\mathcal{L} = \frac{1}{2} \sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2} - \frac{1}{2M_s} \left(\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha \right)^2 - \sum_{\alpha=1}^{N} U(\vec{q}_\alpha) \tag{19}$$

It's easy to notice the presence of cyclic coordinates and, consequently, additional conservation laws. Thus, cyclic coordinates are the angular variables of rotation relative to the center of the potential $U(\vec{q}_\alpha)$ This is due to its symmetry and dependence only on the lengths of the vectors $|\vec{q}_\alpha|$. Moving on to spherical coordinates, we obtain

$$\mathcal{L} = \frac{1}{2} \sum_{\alpha=1}^{N} m_\alpha (\dot{q}_\alpha^{\,2} + q_\alpha^2 \dot{\theta}_\alpha^2 + q_\alpha^2 \sin(\theta_\alpha)^2 \dot{\varphi}_\alpha^2) -$$

$$-\frac{1}{2M_s}\left(\sum_{\alpha=1}^{N} m_\alpha(\dot{q}_\alpha\vec{r}_0 + q_\alpha\dot{\theta}_\alpha\vec{\theta}_0 + q_\alpha\sin(\theta_\alpha)\dot{\varphi}_\alpha\vec{\varphi}_0)\right)^2 - \tag{20}$$

$$-\sum_{\alpha=1}^{N} U(q_\alpha)$$

Where $\vec{q}_0, \vec{\theta}_0, \vec{\varphi}_0$ are the corresponding unit vectors. The cyclicity of coordinates φ_α results in the conservation of the following quantities:

$$I_\alpha = m_\alpha q_\alpha^2 \sin^2(\theta_\alpha)\dot{\varphi}_\alpha -$$

$$-\frac{1}{M_s} m_\alpha q_\alpha \sin(\theta_\alpha)\left(\sum_{\beta=1}^{N} m_\beta q_\beta \sin(\theta_\beta)\dot{\varphi}_\beta\right) \tag{21}$$

Naturally, their sum is also conserved. Note that from these relations one can explicitly find the velocities of cyclic variables in the form $\dot{\varphi}_\alpha = f_\alpha(q_\alpha, \sin(\theta_\alpha), I_\alpha)$ for given values of the conserved quantities. Using the Routh method (see, for example, [27])]), one can eliminate cyclic coordinates and their velocities by introducing the Routh function.

$$R(q_1, ..., q_N; \theta_1, ..., \theta_N; \dot{q}_1, ..., \dot{q}_N; \dot{\theta}_1, ..., \dot{\theta}_N; I) =$$

$$= \mathcal{L} - \sum_{\alpha=1}^{N} I_\alpha\dot{\varphi}_\alpha|_{\dot{\varphi}_\alpha = f_\alpha(q_\alpha, \sin(\theta_\alpha), I_\alpha)} \tag{22}$$

As a result, we obtain a reduced Lagrangian system, the Lagrangian R, of which depends on $2N$ coordinates (and their velocities) for fixed values of the invariants. It should be noted that the Routh function in our case is found explicitly and is not presented only due to the cumbersome nature of its notation. Thus, the number of equations of motion is reduced to $2N$. It is expected that other conservation laws are also satisfied due to the initial symmetry of the potential energy. Their search is significantly more difficult. However, one additional invariant can be easily found. To do this, it suffices to note that the Lagrangian of the reduced system (22) does not depend explicitly on time. This means that the energy of the reduced system is conserved and provides another additional invariant, using which we can again reduce the number of dynamic equations. In this way, we can achieve a significant reduction in the number of dynamic equations for describing the internal degrees of freedom of a structurally complex particle.

5. ENERGY DISTRIBUTION

Let's return to Lagrangian (19) and consider the general properties of the internal degrees of freedom. We will be interested in the distribution of kinetic and potential energy between the components of the system. Lagrangian (19) contains two contributions. One is a quadratic function of the velocities, which we denote by T. This function has a degree of homogeneity of 2 with respect to velocities. It should be noted that this contribution does not coincide with the kinetic energy. The second contribution is the sum of potential energies that depend only on the coordinates. The potential energies transform in a specific way under coordinate transformations. Indeed, it is easy to verify that, when changing coordinates $\vec{q}_\alpha \to \lambda\vec{q}_\alpha$ the potential energy $U(\vec{q}_\alpha) = U_0\theta(|\vec{q}_\alpha|^2 - R_0^2)$ transforms, taking into account $R_0 \to \lambda R_0$ as $U(\vec{q}_\alpha) = U_0\theta(\lambda(|\vec{q}_\alpha|^2 - R_0{}^2)) = U(\vec{q}_\alpha)$ for $\lambda > 0$. In a more general case, as noted earlier, other potentials can be used, for example, those with a different degree of homogeneity κ. (Let the potential energy transform under rescaling as $U(\lambda\vec{q}_\alpha) = \lambda^\kappa U(\vec{q}_\alpha)$.Then it is a homogeneous function of the coordinates of degree κ. In these cases, Clausius, quite long ago, derived general relations between kinetic and potential energy, which are known as the virial theorem. Using the properties of homogeneity, we obtain for the part depending on the speed according to Euler's theorem on homogeneous functions

$$2T = \sum_{\alpha=1}^{N} \dot{\vec{q}}_\alpha \frac{\partial T}{\partial \dot{\vec{q}}_\alpha} \tag{23}$$

The right side of this equality, using the definition of generalized momentum (see (12), (13)) can be written as

$$2T = \frac{d}{dt}\sum_{\alpha=1}^{N} \vec{p}_\alpha\vec{q}_\alpha - \sum_{\alpha=1}^{N} \vec{q}_\alpha\dot{\vec{p}}_\alpha \equiv \frac{d}{dt}\sum_{\alpha=1}^{N} \vec{p}_\alpha\vec{q}_\alpha + \sum_{\alpha=1}^{N} \vec{q}_\alpha\frac{\partial U}{\vec{q}_\alpha} \tag{24}$$

It should be emphasized that, due to energy conservation and the restriction of coordinates of particles in a potential well, momenta and coordinates are bounded functions of time. To obtain virial relations, we use time averaging, which is denoted by angle brackets. $\langle ... \rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^T ...dt$. Averaging the previous ratio over time, we obtain

$$2\langle T\rangle = \left\langle \sum_{\alpha=1}^{N} \vec{q}_\alpha\frac{\partial U}{\vec{q}_\alpha} \right\rangle \tag{25}$$

Taking into account Euler's theorem for homogeneous functions, we obtain the virial theorem

$$2\langle T\rangle = \kappa\langle U\rangle \tag{26}$$

For the case under consideration, this relationship can be written as,

$$2\left\langle \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2}\right\rangle - 2\left\langle \frac{1}{2M_s}\left(\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha\right)^2\right\rangle = \kappa\langle U\rangle \tag{27}$$

The first term on the left coincides with the kinetic energy of the particles, while the second one is more complex. Now, using conservation of energy, we find what fraction of the initial energy is concentrated in potential energy.

$$\left\langle \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2}\right\rangle - \frac{1}{2M_s}\left\langle\left(\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha\right)^2\right\rangle + \langle U\rangle = E_0 \tag{28}$$

By excluding the average of the square of the sum from the relation (26) we obtain

$$\langle U\rangle = \frac{2E_0}{2+\kappa} \tag{29}$$

which exactly coincides with the initial energy fraction in a conventional system of particles in a potential well. However, estimating the fraction of the kinetic energy of the particles is difficult due to the presence of an additional contribution. Eliminating the potential energy from relation (27) we obtain

$$\left\langle \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2}\right\rangle - \left\langle \frac{1}{2M_s}\left(\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha\right)^2\right\rangle = \frac{\kappa E_0}{2+\kappa} \tag{30}$$

Then, to determine the proportion of the initial energy that goes to kinetic energy, we use an estimate of the second contribution in terms of kinetic energy. For this, we use the Cauchy-Bunyakovsky inequality $(\sum_{\alpha=1}^{N} a_\alpha b_\alpha)^2 \le \sum_{\alpha=1}^{N} a_\alpha^2 \sum_{\alpha=1}^{N} b_\alpha^2$. Let us write down the following relation

$$\left(\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha\right)^2 \equiv \left(\sum_{\alpha=1}^{N} \sqrt{m_\alpha}\sqrt{m_\alpha}\dot{\vec{q}}_\alpha\right)^2 \le$$

$$\le \sum_{\alpha=1}^{N} m_\alpha \cdot \sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2} \tag{31}$$

Denoting the mass of internal degrees of freedom as $M_{in} = \sum_{\alpha=1}^{N} m_\alpha$ we obtain

$$\left(\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha\right)^2 \le M_{in}\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2} \tag{32}$$

This relation sets a limit to the kinetic energy fraction for the internal degrees of freedom in the total energy E_0

$$\left\langle \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\vec{q}}_\alpha^{\,2}\right\rangle \le \frac{\kappa E_0 M_s}{(2+\kappa)M} \tag{33}$$

The distinction from the usual case is that the fraction of kinetic energy depends on the ratio of the shell mass to the total mass of the particles. Thus, the kinetic energy of the internal particles cannot exceed a certain fraction of the total energy, which is determined by the ratio of the mass of the entire particle to the shell mass.

6. TWO INTERNAL DEGREES OF FREEDOM

We present an exact solution of the Lagrangian equations for the internal degrees of freedom, obtained using Lagrangian (19) for the one-dimensional case with two internal particles. For simplicity, we choose the potential of particle interaction with the shell as $U(q) = \frac{k}{2}q^2$. The exact solution to this system of equations can be found easily:

$$q_1(t) = \cos\left(\frac{\omega_1 t}{2}\right)c_1 - \sin\left(\frac{\omega_1 t}{2}\right)c_2 +$$

$$+\cos\left(\frac{\omega_2 t}{2}\right)c_3 - \sin\left(\frac{\omega_2 t}{2}\right)c_4 \tag{34}$$

$$q_2(t) = \frac{M(m_1-m_2)+\eta}{2m_1m_2}\left\{\cos\left(\frac{\omega_1 t}{2}\right)c_1 - \sin\left(\frac{\omega_1 t}{2}\right)c_2\right\} +$$
$$+\frac{M(m_1-m_2)-\eta}{2m_1m_2}\left\{\cos\left(\frac{\omega_2 t}{2}\right)c_3 - \sin\left(\frac{\omega_2 t}{2}\right)c_4\right\} + \tag{35}$$

Where the vibration frequencies are determined by the masses of the internal particles and the shell

$$\omega_1 = \frac{\sqrt{(m_1M + m_2M + 2m_1m_2 + \eta)k}}{\sqrt{m_1m_2M}}$$

$$\omega_2 = \frac{\sqrt{(m_1M + m_2M + 2m_1m_2 - \eta)k}}{\sqrt{m_1m_2M}}$$

$$\eta = \sqrt{M^2m_1^2 - 2M^2m_1m_2 + M^2m_2^2 + 4m_1^2m_2^2}$$

Let's pay attention to the complex dependence of frequencies on the masses of the shell and internal particles. According to relation (6), these frequencies should manifest themselves in the behavior of the shell and, consequently, the structurally complex particle. Thus, it becomes possible to determine the properties of the internal particles and, consequently, its internal structure based on observed particle behavior. Direct observation of the internal structure of such a particle can usually be complicated by both technical reasons and the appearance of additional external influences that alter its behavior.

All other constants are determined by the initial conditions and the masses of the components of the structurally complex particle. Thus, the constants included in solution (34), (35) have the following form.

$$c_1 = q_1(0)\frac{\eta + M(m_2-m_1)}{2\eta} + q_2(0)\frac{m_1m_2}{\eta}$$

$$c_2 = -\dot{q}_1(0)\frac{\eta + M(m_2-m_1)}{2\omega_1\eta} - \dot{q}_2(0)\frac{m_1m_2}{\omega_1\eta}$$

$$c_3 = q_1(0)\frac{\eta + M(m_1-m_2)}{2\eta} - q_2(0)\frac{m_1m_2}{\eta}$$

$$c_4 = -\dot{q}_1(0)\frac{(\eta + M(m_1-m_2))}{\omega_2\eta} + \dot{q}_2(0)\frac{m_1m_2}{\omega_2\eta}$$

The existence of exact solutions makes it possible to directly calculate the energy distribution even among the components of internal degrees of freedom without appealing to virial relations. Moreover, the relations for the energies of individual components cannot be derived from virial relations.

We present the average values of potential and kinetic energies for each internal particle, obtained by directly averaging the corresponding exact quantities over time.

$$\langle U_1\rangle = \frac{1}{2}(c_1^2 + c_2^2 + c_3^2 + c_4^2)$$

$$\langle U_2\rangle = \frac{1}{2(2m_1m_2)^2}((c_1^2 + c_2^2 + c_3^2 + c_4^2)(\eta^2 + M^2(m_1-m_2)^2)+$$
$$+(c_1^2 + c_2^2 - c_3^2 - c_4^2)2M(m_1-m_2)\eta)$$

$$\langle E_1\rangle = (c_1^2 + c_2^2 + c_3^2 + c_4^2)\frac{M(m_1+m_2)+2m_1m_2}{4Mm_2}+$$
$$+(c_1^2 + c_2^2 - c_3^2 - c_4^2)\frac{\eta}{4Mm_2}$$

$$\langle E_2\rangle = \frac{1}{4m_1^2m_2^2M}\left\{(c_1^2 + c_2^2 + c_3^2 + c_4^2)(M^2(M+m_2)(m_1-m_2)+\right.$$
$$+Mm_1m_2^2(3m_1-m_2) + 2m_1^2m_2^3) +$$
$$\left.+ (c_1^2 + c_2^2 - c_3^2 - c_4^2)\eta(M(m_1-m_2)(M+m_2) + m_1m_2^2)\right\}$$

The first two equations allow us to express the initial data $(c_1^2 + c_2^2 + c_3^2 + c_4^2)$ and $(c_1^2 + c_2^2 - c_3^2 - c_4^2)$ the potential energies of the internal particles, and after substituting them into the equations for E_1, E_2 we obtain

$$\langle E_1 \rangle = \langle U_1 \rangle \frac{1}{2Mm_2} \left(M(m_1 + m_2) + \right.$$
$$\left. + 2m_1 m_2 - \frac{\eta^2 M^2 (m_1 - m_2)^2}{2M(m_1 - m_2)} \right) + \langle U_2 \rangle \frac{8m_1^2 m_2}{4M^2(m_1 - m_2)}$$
$$\langle E_2 \rangle = \langle U_1 \rangle B_1 + \langle U_2 \rangle B_2 \tag{36}$$

Where coefficients B_1 and B_2 depend on the masses only as

$$B_1 = \frac{(2 + m_2 - m_1)(m_1 - m_2)^2 M^4}{4m_1^2 m_2^2 M^2 (m_1 - m_2)} +$$
$$+ \frac{m_2 (2 + m_2 - m_1)(m_1 - m_2)^2 M^3}{4m_1^2 m_2^2 M^2 (m_1 - m_2)} +$$
$$+ \frac{\left(5m_1^2 m_2^2 - m_2^3 m_1 - \eta^2\right)(m_1 - m_2) M^2}{4m_1^2 m_2^2 M^2 (m_1 - m_2)} +$$
$$+ \frac{\left(4m_1^3 m_2^3 - 4m_1^2 m_2^4 - \eta^2 m_1 m_2 + \eta^2 m_2^2\right) M - m_1 m_2^2 \eta^2}{4m_1^2 m_2^2 M^2 (m_1 - m_2)}$$
$$B_2 = \frac{(m_1 - M) m_2^2 + (m_1 - M) M m_2 + M^2 m_1}{M^2 (m_I - m_2)}$$

When deriving these relations (36) it was assumed that $m_1 \neq m_2$. In the special case of equality of these masses, all relations are significantly simplified. Thus, the kinetic energy of an internal particle is composed of certain fractions of the potential energies of the components. Let us note, that these relations are independent of the initial conditions and, in this sense, are universal. The existence of these relations can be understood by considering the exchange of energies between internal particles through their interaction with the shell. Such relations cannot be derived from virial relations. In fact, this means that the distribution over the degrees of freedom is non-uniform and is determined by the masses of the internal particles.

7. DISCUSSION AND CONCLUSIONS

A generalization of the structurally complex particle is proposed for interaction potentials more general than perfectly elastic collisions. It is shown that the structurally complex particle is defined by a restricted problem of bodies of different masses. This system can be described as a system of bodies in certain coordinates. For this system of bodies, a Hamiltonian formalism is formulated, and the resulting first integrals of motion are discussed. The achieved advantage, in addition to reducing the number of variables, is that the system moves in a potential well that is at rest. This circumstance significantly simplifies the numerical solution of such systems,as well as, for the case of a small number of internal degrees of freedom, the search for exact analytical solutions. An analysis of the general properties leads to proof of the absence of equipartition among the degrees of freedom and, consequently, to an anomalous energy distribution among them. Using the virial theorem, it is proven that the energy of the internal degrees of freedom does not exceed a certain fraction of the initial energy, which depends on the ratio of the masses of the internal particles to the mass of the shell. This circumstance allows us to expect unusual energy distributions of such particles in statistical theory. This should be expected given the occurrence of additional integrals of motion and the finite number of particles. An exactly integrable case of a one-dimensional particle with two internal degrees of freedom is considered. The oscillation frequencies of the internal particles are determined by their masses and the mass of the shell. The energy distribution among them is non-uniform. Universal relations for the distribution of the kinetic and potential energies of internal particles are obtained, independent of the choice of initial conditions. These relations provide more detailed information about the energy distribution than virial relations. In the following research, it is planned to consider the effect of increasing the number of internal particles on the behavior of structurally complex particles.

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ORCID

Kostyantyn M. Kulyk, https://orcid.org/0000-0007-0283-0584; **Maryna A. Ratner**, https://orcid.org/0000-0002-7755-017X; **Volodymyr V. Yanovsky**, https://orcid.org/0000-0003-0461-749X

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ЧАСТИНКИ З ВНУТРІШНІМИ СТУПЕНЯМИ СВОБОДИ

К.М. Кулик[1], **М.А. Ратнер**[2], **В.В. Яновський**[1,2]

[1]*Інститут монокристалів, Національна Академія Наук України пр. Науки 60, 61072 Харків, Україна*

[2]*Харківський національний університет імені В.Н. Каразіна майдан Свободи, 4, 61022, Харків, Україна*

Запропоновано узагальнену концепції структурно складної частинки на випадок загальних потенціалів взаємодії між її компонентами. Структурно складна частинка визначається обмеженою задачею N+1 тіл різної маси, яка зводиться до задачі N тіл. На основі лагранжіанського опису формулюється гамільтонів формалізм та обговорюються отримані перші інтеграли руху. Демонструється відсутність рівномірного розподілу між ступенями свободи. Використовуючи теорему віріала, доведено, що енергія внутрішніх ступенів свободи не перевищує певної частки початкової енергії, яка залежить від відношення мас внутрішніх частинок до маси оболонки. Розглянуто точно інтегрований випадок одновимірної частинки з двома внутрішніми ступенями свободи. Частоти коливань такої структурно складної частинки визначаються її масами та масою оболонки. Розподіл енергії по них не є рівномірним. Отримано універсальні співвідношення для розподілу кінетичної та потенційної енергій внутрішніх частинок, які не залежать від вибору початкових умов. Ці співвідношення надають детальнішу інформацію про розподіл енергії, ніж віріальні співвідношення.

Ключові слова: *структурно складна частинка; внутрішні ступені свободи; рівняння руху; віріальні співвідношення*