

On certain nonlinear many-body problems on lines and circles

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WE DISCUSS certain essentially nonlinear dynamical models of one-dimensional lattices with internal parameters. These parameters may be interpreted as coupling amplitudes; forces acting between lattice points depend on them in a quadratic way. However, they are not coupling constants in the usual sense; on the contrary, they are dynamical variables subject to equations of motion on the same footing with lattice points positions. Interparticle forces corresponding to this model have certain realistic features of physical intermolecular forces. The models considered are derivable from some highly symmetric Hamiltonian systems on certain manifolds of matrices. This implies that, in principle, they are rigorously solvable. Introducing to them appropriately chosen correction terms and making use of perturbation techniques, we can obtain more realistic and, at the same time, computationally effective models.

Przedmiotem pracy są pewne istotnie nieliniowe modele sieci jednowymiarowych z parametrami wewnętrznymi. Parametry te interpretuje się jako amplitudy sprzężeń; siły działające między punktami sieci zależą od nich w sposób kwadratowy. Amplitudy te nie są jednak stałymi sprzężenia w zwykłym sensie, mają bowiem charakter zmiennych dynamicznych, które wraz ze współrzędnymi punktów sieci spełniają zamknięty układ równań ruchu. Siły międzycząsteczkowe wynikające z tego modelu mają pewne realistyczne cechy siły międzyatomowych i międzymolekularnych znanych z fizyki. Modele przedstawione w pracy są wyprowadzalne z maksymalnie całkowalnych Hamiltonowskich układów dynamicznych na pewnych rozmaitościach macierzowych. Wynika stąd między innymi, że równania ruchu można w zasadzie uważać za ściśle rozwiązywalne w funkcjach elementarnych, bądź w typowych funkcjach specjalnych znanych z fizyki matematycznej. Wprowadzając do naszych modeli odpowiednio dobrane człony korekcyjne i korzystając ze znanych metod perturbacyjnych (jak np. metoda małego parametru), można otrzymać modele bardziej realistyczne, a jednocześnie efektywne pod względem rachunkowym.

Предметом работы являются некоторые существенно нелинейные модели одномерных решеток с внутренними параметрами. Эти параметры интерпретируются как амплитуды сопряжений; силы действующие между точками решетки зависят от них квадратным способом. Эти амплитуды не являются однако постоянными сопряжения в обычном смысле, ибо имеют характер динамических переменных, которые совместно с координатами точек решетки удовлетворяют системе уравнений движения. Межмолекулярные силы, вытекающие из этой модели, имеют некоторые реалистические свойства межтомных и межмолекулярных сил известных из физики. Модели, представленные в работе, выводимы из максимально интегрируемых гамильтоновых динамических систем на некоторых матричных многообразиях. Оттуда следует, между прочим, что уравнения движения можно в принципе считать точно решаемыми в элементарных функциях, или в типичных специальных функциях известных из математической физики. Вводя в наши модели соответственно подобранные коррекционные члены и используя известные пертурбационные методы (как, например, метод малого параметра), можно получить более реалистические модели и одновременно эффективные в расчетном отношении.

1. General motivation

A SIGNIFICANT part of the theory of condensed matter is based on nonrelativistic and potential models of many-body systems, i.e., on Lagrangians of the form

$$(1.1) \quad L = T - V = \frac{1}{2} \sum_{A=1}^n m_A v_A^T v_A - V(x_1 \dots x_n),$$

or, equivalently, on Hamiltonians

$$(1.2) \quad H = T + V = \sum_{A=1}^n \frac{1}{2m_A} p_A^T p_A + V(x_1 \dots x_n),$$

where m_A , x_A , v_A , p_A denote, respectively, the mass, radius-vector, velocity and linear momentum of the A -th particle, thus, $v_A = \frac{d}{dt} x_A$, $p_A = m_A v_A$. All spatial vectors in our formulas are represented by 3×1 matrices.

It is convenient to represent the potential energy V as a series of multiparticle interactions (clusters),

$$(1.3) \quad V = V^1 + V^2 + V^3 + \dots,$$

where

$$(1.4) \quad \begin{aligned} V^1(x_1 \dots x_n) &= \sum_{A=1}^n V_A^1(x_A), \quad V^2(x_1 \dots x_n) = \frac{1}{2} \sum_{A,B=1}^n V_{AB}^2(x_A, x_B), \\ V^3(x_1 \dots x_n) &= \sum_{A,B,C=1}^n V_{ABC}^3(x_A, x_B, x_C) \dots, \quad \text{etc.} \end{aligned}$$

The one-body term V^1 describes the resulting effect of external fields acting separately on all constituents of the system. Higher-order terms V^k , $k > 1$, describe mutual interactions of constituents, with a possible admixture of external influences. Usually the binary model is sufficient for realistic estimations, for example, in ionic and molecular crystals the contribution of non-binary internal interactions does not exceed 10% [2].

If the system is translationally-invariant, then V depends on x_A only through mutual positions $x_{AB} = x_B - x_A$, thus, for example, $V_{AB}^2(x_A, x_B) = W_{AB}^2(x_A - x_B)$, and $V_A^1 = 0$. If translationally-invariant interactions are also rotation-invariant, then V depends on the relative positions $x_B - x_A$ only through their moduli $r_{AB} = |x_B - x_A| = \sqrt{x_{BA}^T x_{BA}}$, thus, e.g., $W_{AB}^2(x_A - x_B) = U_{AB}^2(r_{AB})$.

If all constituents are identical, then U_{AB}^2 , U_{ABC}^3 , etc., do not depend on the indices AB , ABC , etc. Thus, for homogeneous and isotropic binary models of systems of identical particles we have

$$(1.5) \quad V(x_1 \dots x_n) = \frac{1}{2} \sum_{AB} U(|x_A - x_B|), \dagger$$

From now on we concentrate on binary models. Quite often binary interactions W_{AB} split naturally into well-defined attractive and repulsive parts,

$$(1.6) \quad W_{AB} = W_{AB}^{\text{att}} + W_{AB}^{\text{rep}}.$$

It is also typical that the expressions W^{att} , W^{rep} factorize into internal parameters characterizing the strength of interaction, and purely geometric shape functions,

$$(1.7) \quad U_{KL}^{\text{att}} = A_{KL} \alpha(r_{KL}), \quad U_{KL}^{\text{rep}} = R_{KL} \varrho(r_{KL}).$$

One often uses phenomenological models of the form

$$(1.8) \quad \alpha(r) = r^\nu, \quad \varrho(r) = r^\mu.$$



FIG. 1.

Roughly speaking, U_{KL}^{att} may be interpreted as an extended string put between particles K , L and tending to pull them together. U_{KL}^{rep} , on the contrary, is a compressed spring, which pushes the particles away. Typical examples:

(i) gravitational attraction, $A_{KL} = -km_K m_L$, k being gravitational constant and m_K , m_L — masses of particles, $\nu = -1$;

(ii) electrostatic repulsion, $R_{KL} = Q_K Q_L$, $\mu = -1$, Q_K , Q_L denoting electric charges of particles; we assume $Q_K Q_L > 0$.

Repulsive forces between atoms or molecules arise due to the electrostatic interactions between positively charged ionic cores and the exchange interaction between clouds of internal electrons from filled shells. There are various mechanisms of attraction. One kind of attractive force is universal, common to all atoms and molecules. Those are Van der Waals forces (dispersion forces) arising as a result of electrostatic interaction between spontaneously induced electric dipole moments. They are very weak and their effect is often obscured by other mechanisms of attraction. Molecular crystals provide an exception; their cohesion is based exclusively on dispersion forces. In ionic crystals the main part of attraction is due to the very strong electrostatic interactions between oppositely charged ions. Attractive forces in valence crystals are carried by collective valence electrons. As a consequence of the exchange mechanism, a negatively charged cloud of those electrons is sucked into the region between positively charged ionic cores, and attracting them leads to the effective attraction of cores themselves [2, 6, 7, 8, 9].

For interatomic and intermolecular interactions, U^{rep} prevails at small distances, whereas at large distances U^{att} becomes dominant. A typical situation is:

$$(1.9) \quad U^{\text{att}} = Ar^\nu, \quad U^{\text{rep}} = Rr^\mu,$$

where $A < 0$, $R > 0$, $\mu < \nu < 0$. Usually one takes $\mu = -10$; for Van der Waals forces $\nu = -6$ [2, 6, 7, 8, 9].

This relationship between U^{att} and U^{rep} implies that the total potential $U = U^{\text{att}} + U^{\text{rep}}$ has the shape qualitatively pictured in Fig. 2.

There exists stable equilibrium corresponding to the distance r_0 at which $U'(r_0) = 0$. The characteristic asymmetry of the diagram of U is responsible for the thermal expansion of bodies.

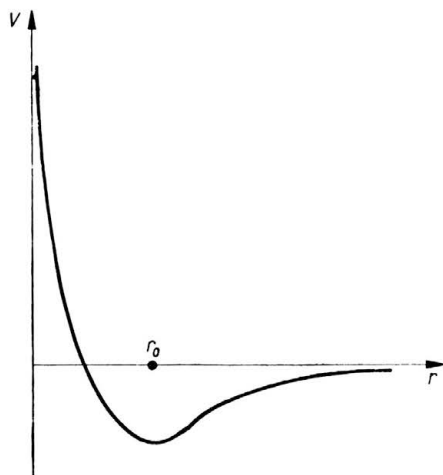


FIG. 2.

It is clear even from the above elementary remarks concerning the mechanism of intermolecular forces that the factorization of U into products of coupling constants and geometric functions describing the dependence of forces on the distance is rather rough. Indeed, forces acting on the centres of mass of molecules depend on internal properties of molecules (electric charge distribution in the examples mentioned) and conversely, those internal parameters are influenced by translational motion. This seems to suggest the following modification: Coupling "constants" (elastic constants of "springs" mentioned above) should not be any longer constant, rather, they will be functions of internal structure parameters. Those parameters, together with coordinates of particles should satisfy a certain closed system of differential equations of motion. Let us recall in this connection that the idea of interpreting coupling constants as additional state variables is rather old; it was introduced to mechanics by Hertz, and, in a slightly different context, by Kaluza and Klein in their 5-dimensional electrodynamics. According to Hertz, coupling constants are canonical momenta conjugate to certain auxiliary cyclic coordinates [5] (in the 5-dimensional electrodynamics by Kaluza and Klein, electric charge is interpreted as a momentum conjugate to the 5-th dimension). The cyclic character of additional coordinates implies that such coupling constants are actually constant. However, if we once decide to interpret coupling parameters as additional state variables, we intuitively feel that it is rather natural to admit them to oscillate. If they happen to perform quick vibrations about some background, then this background, i.e., their average values, can be interpreted as phenomenological coupling constants observed on the macroscopic level.

It is not easy to give up canonical Hamiltonian methods. However, in view of the mentioned Hertz–Kaluza–Klein interpretation of coupling parameters, it would be rather artificial to identify them with new generalized coordinates — they seem to have more to do with canonical momenta. Therefore, we suggest an approach based on Poisson structures. Namely, besides the coordinates x_K , $K = 1, \dots, n$, and their conjugate momenta p_K , we introduce auxiliary internal variables N_{KL} , M_{KL} responsible for the binary interac-

tion, respectively attraction and repulsion, between the K -th and L -th particle. The manifold of the variables

$$(\dots z^a \dots) = (\dots x_A \dots, \dots p_A \dots; \dots N_{KL} \dots; \dots M_{KL} \dots)$$

will be an extended phase space of our problem. It will be endowed with a Poisson structure, i.e., with a binary operation attributing to any pair of smooth functions $F(z), G(z)$, a new function denoted by $\{F, G\}$ and referred to as the Poisson bracket of F, G . This operation is assumed to satisfy the following conditions [4]:

$$\begin{aligned} (i) \quad & \{F, G\} = -\{G, F\}, \\ (1.10) \quad (ii) \quad & \{h(F_1 \dots F_k), G\} = \sum_{p=1}^k h_{,p}(F_1 \dots F_k) \{F_p, G\}, \\ (iii) \quad & \{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0. \end{aligned}$$

These conditions imply, in particular, that the Poisson bracket $\{F, G\}$ is bilinear in F, G and satisfies the Leibnitz rule,

$$(1.11) \quad \{FH, G\} = F\{H, G\} + \{F, G\}H.$$

The condition (1.10) implies also that

$$(1.12) \quad \{F, G\} = \sum_{a,b} \frac{\partial F}{\partial z^a} \frac{\partial G}{\partial z^b} \{z^a, z^b\}.$$

The Poisson brackets for the coordinates,

$$(1.13) \quad \{z^a, z^b\} = C^{ab}(z),$$

define uniquely $\{F, G\}$ for any functions F, G . The conditions (1.10) impose certain restrictions on the functional shape of C^{ab} [4]. The particular choice of structure functions C^{ab} belongs to the definition of the model. It is obvious that always

$$(1.14) \quad \{x_A^i, p_B^j\} = \delta^{ij} \delta_{AB}, \quad \{x_A^i, x_B^j\} = \{p_A^i, p_B^j\} = 0.$$

Other brackets should be defined separately. Since N_{AB}, M_{AB} are parameters logically independent of x and p , it is reasonable to assume that their Poisson brackets with (x, p) -variables vanish. The definition of Poisson brackets for N_{AB}, M_{AB} is one of the constitutive properties of the model.

Dynamics is defined by a choice of the Hamilton function (energy) H depending on state variables $z = (x, p, N, M)$. Equations of motion have the form

$$(1.15) \quad \frac{dz^a}{dt} = \{z^a, H\} = C^{ab}(z) \frac{\partial H}{\partial z^b}.$$

Antisymmetry of C implies conservation of energy,

$$\frac{dH}{dt} = \frac{\partial H}{\partial z^a} \frac{dz^a}{dt} = C^{ab} \frac{\partial H}{\partial z^a} \frac{\partial H}{\partial z^b} = 0.$$

Let us notice that our coupling parameters have a binary character — they are not attributed to single particles, but to their pairs; they are really “springs” in the sense of Fig. 1. They need not factorize into products of one-particle “charges”. Besides, they need not coincide with interaction strengths A_{KL} , R_{KL} defined in Eqs. (1.7) and (1.6). Rather, the classical formulas $-km_k m_L$, $Q_K Q_L$ and certain general ideas of the quantum theory of intermolecular forces suggest the conjecture about the quadratic dependence of A , R on N , M .

In this paper we restrict ourselves to one-dimensional problems, i.e. to multiparticle systems on a line (e.g., onedimensional crystals with internal variables). We aim at constructing certain intuitive, qualitatively acceptable, and at the same time — rigorously solvable dynamical models. Those models are still rather academic, nevertheless, they constitute the first step towards the construction of realistic and analytically solvable models.

Let us describe briefly the general motivation of the undertaken effort.

It is known that mechanical problems solvable in terms of elementary functions or typical special functions are rather exceptional. As a rule, realistic dynamical models are treatable only with the help of qualitative, numerical or approximate methods. This is characteristic, first of all, of systems with a large number of degrees of freedom and of essentially nonlinear models. Microscopic theories of crystals and other solids provide the best example. The modern computational and numerical methods are very effective; nevertheless, the knowledge of rigorous solutions is always very desirable. It gives us a better understanding of the problem and facilitates the very use of approximate and numerical methods. “Realistic” equations usually fail to be integrable in terms of elementary functions or simple special functions. This motivates the following trick: “rigorous”, but nonintegrable equations are replaced by a simplified, thus less rigorous, however, integrable model. Obviously this methodology is effective if we are in a position to construct an integrable model which, although “academic”, gives an account of all those qualitative features of a “realistic” model which are relevant for the investigated phenomena. In this way, approximation inventiveness is carried over from the field of solutions to the field of equations. If a constructed “academic” model is structurally stable, then its rigorous analytical solutions provide a reliable description of the considered phenomena. Besides, they can be used as a tool for constructing effective and quickly convergent numerical procedures for “rigorous” models.

This methodology is commonly used in the theory of condensed matter. A wide class of phenomena in solids, fluids and gases (including phase transitions) can be described in a satisfactory way with the use of phenomenological and rather academic models of binary intermolecular potentials. Quite often, theoretical predictions of those models are rather weakly dependent on the functional form of the potential curve pictured in Fig. 2. What matters is only a general qualitative shape of this curve and a few quantitative characteristics, e.g., the depth of its minimum. Nevertheless, to be able to calculate anything, we must assume some particular shape. Thus the most reasonable choices within the class symbolized by Fig. 2 are those “integrable”, i.e., computationally effective.

The theory of rigorously solvable dynamical systems has been recently the subject of very intensive research. New methods of solution have been invented, much more effective

than the classical separation of variable technique (e.g., the Lax pair method). One of the fundamental tasks of applied mechanics consists in formulating phenomenological models based on rigorously solvable equations. Particularly effective are Hamiltonian systems whose configuration spaces are Lie groups, and kinetic energies correspond to left-invariant or right-invariant metric tensors.

2. One-dimensional n-body problems and mechanical models on manifolds of $n \times n$ matrices

Nonlinear one-dimensional many-body problems have been the subject of intensive investigations for some forty years. Nowadays they have become a theoretical laboratory for studying integrable systems.

One considers one-dimensional lattices on a straight-line [3] and on a circle. The second model may be used, e.g., for describing a finite one-dimensional crystal on a straight line. The motion of its constituents is confined by some collective self-consistent part of internal interactions to a fixed compact segment of the line; the ends of the segment are identified (periodic boundary conditions).

Instead of the original coordinate x running over the range $[0, a]$ (a denoting the length of the crystal), one uses the angularly normalized coordinate $q = \frac{2\pi}{a}x$, taking

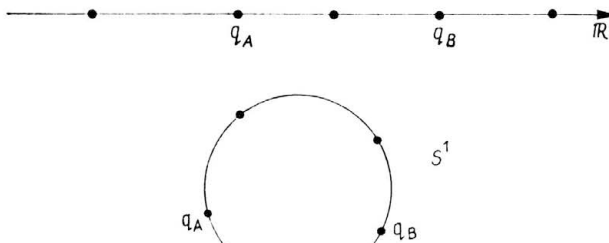


FIG. 3.

values in $[0, 2\pi]$ or $[-\pi, \pi]$ (Fig. 3). As an example, let us quote the Hamiltonians $H = T + V$ of a few most known completely integrable lattices.

(i) Toda lattice on \mathbb{R} ,

$$(2.1) \quad H_T = \frac{1}{2} \sum_{A=1}^n p_A^2 + \sum_{A=1}^{n-1} \exp(q_A - q_{A+1}),$$

(ii) Calogero–Moser lattice on \mathbb{R} ,

$$(2.2) \quad H_{CM} = \frac{1}{2} \sum_{A=1}^n p_A^2 + \frac{1}{2} \sum_{A \neq B} \frac{1}{(Q_A - Q_B)^2},$$

(iii) Hyperbolic-Sutherland lattice on \mathbb{R} ,

$$(2.3) \quad H_{Sh} = \frac{1}{2} \sum_{A=1}^n p_A^2 + \frac{1}{2} \sum_{A \neq B} \frac{1}{\operatorname{sh}^2 \frac{q_A - q_B}{2}},$$

(iv) Sutherland lattice on S^1 ,

$$(2.4) \quad H_S = \frac{1}{2} \sum_{A=1}^n p_A^2 + \frac{1}{2} \sum_{A \neq B} \frac{1}{\sin^2 \frac{q_A - q_B}{2}}.$$

The models (iii) and (iv) are related to each other through the substitution $q_A \rightarrow iq_A$, $p_A \rightarrow -ip_A$, and the reversal of the Hamiltonian sign.

All lattices above consist of identical particles with unit masses. In the Toda lattice there are only nearest neighbour interactions. The remaining Hamiltonians ((2.2), (2.3), (2.4)) contain, in a completely symmetric way, all possible binary interactions; they are invariant under permutations of particles. Coupling constants are actually constant and identical for all pairs of constituents. If they were not equal, the systems would not be integrable.

Unfortunately, internal interactions described by Hamiltonians ((2.1), (2.2), (2.3), (2.4)) are repulsive, and without extra introduced periodic boundary conditions, lattices ((2.1), (2.2), (2.3)) decay; then one has to do with purely scattering situations. Thus, without artificial confinement based on an auxiliary collective interaction, Hamiltonians ((2.1), (2.2), (2.3)) are useless as models of one-dimensional condensed matter. Interactions in the Sutherland lattice on S^1 , (2.4), are also purely repulsive; however, in a consequence of the compactness of S^1 , the Hamiltonians (2.4) predict the existence of stable equilibria (modulo rigid uniform rotations of the lattice, $q_A = q_A^0 + wt$, $w = \text{const}$). Nevertheless, the lack of attractive binary forces in Eq. (2.4) is a non-physical feature of the model, at least from the point of view of the condensed matter theory.

In the models ((2.2), (2.3), (2.4)) the particles are impenetrable — coincidences are prevented by positive singularities of the potentials.

All models ((2.1), (2.2), (2.3), (2.4)) are in principle rigorously solvable; moreover, they are completely integrable in the sense that there exist n (as many as degrees of freedom) functionally independent constants of motion with pairwise vanishing Poisson brackets. In literature, the complete integrability of the models ((2.1), (2.2), (2.3), (2.4)) is usually established by reducing the Hamilton equations of motion to the Lax form,

$$(2.5) \quad \frac{dL}{dt} = [L, A],$$

L , A being certain matrices depending on the positions and velocities of the lattice points. There is also another, more intuitive, method, developed by Kazhdan, Kostant and Sternberg [10]. They construct auxiliary, higher-dimensional Hamiltonian systems with certain Lie groups or Lie algebras of $n \times n$ matrices as configuration spaces. As Hamiltonians, simple geometric objects are used, e.g., second-order Casimir invariants of Lie algebras.

The corresponding Hamiltonian systems are highly symmetric. Restricting them to value-surfaces of certain constants of motion and performing the reduction process, we obtain new, secondary, Hamiltonian systems with fewer degrees of freedom. They are completely integrable in a consequence of properties of the original model. Nevertheless, without connection with this model, their integrability is not self-evident. Kazhdan, Kostant and Sternberg showed that Calogero–Moser and Sutherland n -element lattices can be obtained in this way. Configuration spaces of the corresponding Hamiltonian systems are respectively $u(n)$, i.e., Lie algebra of anti-Hermitian matrices (for the Calogero–Moser lattice) and $U(n)$, i.e., Lie group of unitary matrices (for the Sutherland lattice). In both cases, the Hamiltonian equals the second Casimir invariant. The coordinates and momenta of lattice points have to do with certain diagonal matrices appearing in the reduction process. In a similar way, the hyperbolic–Sutherland model (2.3) can be obtained from a Hamiltonian system with $GL(n, \mathbb{R})$, the group of real $n \times n$ matrices, as a configuration space.

The KKS-approach [10] suggests us some hints concerning the construction of rigorously solvable dynamical models of one-dimensional lattices with internal variables. In the models we construct, “coupling constants” are no longer constant; in accordance with the ideas presented in Sect. 1, they are internal parameters which, together with the positions of particles, satisfy a closed system of Hamiltonian–Poisson equations of motion. Our models are qualitatively compatible with general properties of intermolecular forces. They are also similar to the lattices ((2.2), (2.3), (2.4)) and are obtained from them by elastization of coupling constants. However, in contrast to purely repulsive lattices ((2.2), (2.3), (2.4)), our structured lattices admit attractive, condensed situations. At the same time they are rigorously solvable. Just as in the KKS-approach, we shall use auxiliary Hamiltonian systems with n^2 degrees of freedom. The configuration space is either $GL^+(n, \mathbb{R})$, i.e., the group of real $n \times n$ matrices with positive determinants, or $U(n)$ — the group of complex unitary matrices in n dimensions. We shall use the common symbol G for both models; G will be specified to $GL^+(n, \mathbb{R})$ or $U(n)$ only when necessary. It is not accidental that we use $GL^+(n, \mathbb{R})$ and $U(n)$ as alternative models; they are different (and mutually opposite) real forms of the same complex Lie group $GL(n, \mathbb{C})$. As usual, Lie algebra of $GL^+(n, \mathbb{R})$ will be identified with $L(n, \mathbb{R})$ — the space of all real $n \times n$ matrices; similarly, Lie algebra of $U(n)$ is identified with $u(n)$ — the space of all $n \times n$ complex anti-Hermitian matrices. We use the common symbol g for Lie algebras $L(n, \mathbb{R})$, $u(n)$.

By analogy to the KKS-approach, the coordinates of lattice points will have to do with certain diagonal matrices. The correspondence between Hamiltonian systems on $GL^+(n, \mathbb{R})$ and Poisson–Hamiltonian dynamical models of lattices with internal parameters is based on the two-polar decomposition of $GL^+(n, \mathbb{R})$

$$(2.6) \quad X = LDR^T,$$

where $L, R \in SO(n, \mathbb{R})$ are $n \times n$ orthogonal matrices with positive determinants, and D is a diagonal matrix with positive diagonal elements. These diagonal elements are deformation invariants of X in \mathbb{R}^n , i.e., square roots of eigenvalues of the Green deformation matrix $X^T X$. The diagonal elements of D will be denoted by Q_A , $A = 1, \dots, n$; $D = \text{diag}(Q_1, \dots, Q_n)$. We shall also use the quantities

$$(2.7) \quad q_A = \ln Q_A;$$

their range coincides with the total real axis \mathbb{R} . The two-polar splitting resembles polar coordinates: D is a system of n “radial” coordinates, and L, R are “angular” variables. Representation (2.6) is singular at configurations X with degenerate spectra of $X^T X$, i.e., with repeated elements on the diagonal of D . For X with non-degenerate spectra of $X^T X$, the splitting

$$(2.8) \quad GL^+(n, \mathbb{R}) \mapsto \mathbb{R}^{+n} \times SO(n) \times SO(n)$$

described by the representation (2.6) is unique up to discrete transformations

$$(2.9) \quad (D, L, R) \mapsto (U_P^{-1} D U_P, L U_P, R U_P),$$

where $P \mapsto U_P$ is an orthogonal representation of the permutation group, such that

$$(2.10) \quad U_P^{-1} \text{Diag}(Q_1, \dots, Q_n) U_P = \text{Diag}(Q_{P(1)}, \dots, Q_n).$$

By analogy to the representation (2.6), unitary matrices will be represented as

$$(2.11) \quad X = L D R^T,$$

where again L, R are elements of $SO(n, \mathbb{R})$, but D is a diagonal unitary matrix. In calculations we shall represent it as

$$(2.12) \quad D = \text{diag}(\exp(iq_1) \dots \exp(iq_n));$$

q_A run over the range $(0, 2\pi)$. The expressions (2.6), (2.11) can be obtained from each other by substitution: $q_A \mapsto iq_A$. Obviously, the representation (2.11) is also non-unique, in a similar sense as the expression (2.6).

Formally, the splitting (2.6) (or (2.11)) turns the original G -system into a new mechanical system consisting of two n -dimensional rigid bodies with configurations L, R and an n -tuple of indistinguishable material points on the straight-line R (respectively on the circle S^1) with the coordinates (q_1, \dots, q_n) .

The motions of the system are described by the curves $R \ni t \mapsto X(t) \in G$. The corresponding vectors of generalized velocities will be denoted by $\dot{X} = dX/dt$. The algebraic structure of G distinguishes two natural quasi-velocities (linear functions of generalized velocities, with configuration-dependent coefficients),

$$(2.13) \quad E(X, \dot{X}) := \dot{X} X^{-1}, \quad E'(X, \dot{X}) := X^{-1} \dot{X}.$$

They are related to each other through the formula

$$E(X, \dot{X}) = X E'(X, \dot{X}) X^{-1}.$$

The range of matrices E, E' coincides with the Lie algebra of G , i.e., with $L(n, \mathbb{R})$ if $G = GL^+(n, \mathbb{R})$ and $u(n)$ if $G = U(n)$. In the latter case we have $E^+ = -E, E'^+ = -E'$.

The quasi-velocities E, E' are Lie-algebraic objects characteristic of all mechanical systems whose configuration spaces can be identified with Lie groups. Obviously, G is non-Abelian, thus E, E' are non-holonomic (fail to be time-derivatives of any generalized coordinates). If we restrict G to the subgroup of matrices with determinants equal to unity, then E, E' become traceless. If G is restricted to $SO(n, \mathbb{R})$ (n -dimensional rigid body), then E, E' become skew-symmetric matrices of angular velocity, respectively, in spatial and co-moving representation. When constructing Lagrangians and Hamiltonians, we shall use the Casimir invariants $C(k), k = 1, \dots, n$; they are given by

$$(2.14) \quad C(k) := \text{Tr}(E^k) = \text{Tr}(E'^k).$$

The peculiarity and defining property of these quantities is that they are functions of (X, \dot{X}) invariant under all transformations of the form

$$(2.15) \quad X \mapsto AXB, \quad A, B \in G.$$

We shall consider geodesic Hamiltonian models on G ; their Lagrangians are “kinetic energy” forms, i.e., functions of (X, \dot{X}) , quadratic in \dot{X} . As usual in mathematical physics, it is reasonable to expect that particularly useful (or, at least, mathematically interesting) should be highly symmetric models, invariant under “large” transformation groups. Our configuration space is a Lie group, thus, maximally-symmetric Lagrangians are those invariant under the left and right regular translations (2.15). All functions of (X, \dot{X}) invariant under the translations (2.15) have the form

$$(2.16) \quad F(X, \dot{X}) = f(C(1) \dots C(n)).$$

If F is to be quadratic in derivatives, then the only possibility is a linear combination of $C(2)$ and $C(1)^2$. Thus we consider kinetic Lagrangians of the form

$$(2.17) \quad L = T = \frac{A}{2} \text{Tr}(E^2) + \frac{B}{2} (\text{Tr} E)^2 = \frac{A}{2} \text{Tr}(E'^2) + \frac{B}{2} \text{Tr}(E')^2,$$

A, B being constant. $C(2) = \text{Tr}(E^2)$ is the main term of Eq. (2.17); it is always nonsingular as a quadratic form of X . On the contrary, $C(1)^2$ is strongly degenerate (it equals the squared dilatational velocity in R^n), thus, it is merely a correction term.

The kinetic energies obtained by specifying Eq. (2.17) to $G = GL^+(n, R)$ or $G = U(n)$ have different definiteness properties. Namely, $U(n)$ is compact and $\text{Tr}(E^2) = -\text{Tr}(E^+E)$ is negatively definite on $u(n)$, thus, the main term of Eq. (2.17) is positively definite on $u(n)$ iff $A < 0$. $GL^+(n, R)$ is non-compact and Eq. (2.17) is never definite on $L(n, R)$.

Indeed, the quadratic form $\text{Tr}(E^2)$ has the signature $\left(\frac{1}{2}n(n-1) -, \frac{1}{2}n(n+1+)\right)$; the minus and plus signs correspond, respectively, to compact and non-compact generators of $GL^+(n, R)$,

$$\text{Tr}(E^2) = \text{Tr}(w^2) + \text{Tr}(l^2) = -\text{Tr}(w^T w) + \text{Tr}(l^T l),$$

where $E = w + l$, $w^T = -w$, $l^T = l$.

One is intuitively reluctant to kinetic energies with hyperbolic signatures; genuine kinetic energies faced with in analytical mechanics are positive. However, our Hamiltonian system on $GL^+(n, R)$ is introduced only as a tool for investigation of one-dimensional n -particle systems. The reduced Hamiltonian system has no pathological properties; moreover, it turns out that negative contributions to T describe attractive forces acting between particles moving along a line. Besides, it turns out that Eq. (2.17) may be made positive by adding certain constants of motion which have vanishing Poisson brackets with all quantities relevant for the reduced dynamics. This correction does not modify forces acting between lattice points. The metric element corresponding to Eq. (2.17) has the form

$$(2.18) \quad ds^2 = A \text{Tr}(dXX^{-1}dXX^{-1}) + B(\text{Tr}(dXX^{-1}))^2.$$

The resulting pseudo-Riemannian structure is curved and invariant under the transformations (2.15).

The second term of Eq. (2.17) has no essential influence on the qualitative properties of L . Thus, from now on we shall omit it and consider kinetic Lagrangians of the form

$$(2.19) \quad L = T = \frac{m}{2} \text{Tr}(E^2), \quad m > 0, \quad \text{if } G = GL^+(n, R),$$

$$L = T = -\frac{m}{2} \text{Tr}(E^2) = \frac{m}{2} \text{Tr}(E^+ E), \quad m > 0, \quad \text{if } G = U(n).$$

From the point of view of G , the Lagrangians (2.19) describe geodetic, i.e., purely geometric, motion. However, from the point of view of one-dimensional lattices (reduced dynamics), the Hamiltonians corresponding to the forms (2.19) consist of two parts: kinetic energy of the one-dimensional n -particle system, and the effective potential of interparticle interactions. These interactions are qualitatively compatible with what we know about intermolecular forces; at the same time they have a geometric origin because we derive them from doubly-invariant geodetic problems on G . This geometric character implies that in principle the resulting equations of motion are rigorously solvable. Nevertheless, in some problems it may be convenient to introduce "by hands" certain auxiliary potentials of non-geometric origin, i.e., to use the Lagrangians $L = T - V$. One assumes that V depends only on the D -term in the splitting (2.6) i.e., it is invariant under the transformations (2.15) with $A, B \in SO(n, R)$. This restriction is necessary if the L -dynamics is to be reducible to the one-dimensional n -particle system with internal variables. Such models are effective only if the functional shape of V is somehow suited to T .

For certain reasons, it will be instructive to consider also kinetic Lagrangians of the form

$$(2.20) \quad L = \frac{m}{2} \text{Tr}(\dot{X}^T \dot{X});$$

they correspond to the metric elements

$$(2.21) \quad ds^2 = m \text{Tr}(dX^T dX).$$

The peculiarity and defining property of Eq. (2.20) is that it is invariant under the transformations $X \mapsto AXB + C$, $C \in L(n, R)$, $A, B \in SO(n, R)$. For dynamical models based on Eq. (2.20), it is more natural to use $L(n, R)$ as a configuration space; $GL^+(n, R)$ would be too restrictive. As we shall see, without extra introduced non-geometric potentials, or periodic boundary conditions, the lattice systems based on Eq. (2.20) decay to infinity; there are no "condensed matter" solutions.

Let us now express L ((2.19), (2.20)) and the resulting Hamiltonians through the (L, D, R) -variables. To achieve this, we have to introduce non-holonomic velocities and momenta corresponding to the splittings ((2.6), (2.11)). Instead of E or E' , we shall use the non-holonomic velocities

$$(2.22) \quad (\dot{D}, l, r) = (\dot{D}, L^{-1}\dot{L}, R^{-1}\dot{R}).$$

The matrices (l, r) are skew-symmetric. The matrix elements of l are co-moving components of the angular velocity of the fictitious L -rigid-body. Similarly, r is the co-moving angular

velocity of the R -top. We shall also use non-holonomic canonical momentum (P, J, K) conjugate to (D, l, r) . The matrix P is diagonal, $P = \text{diag}(P_1, \dots, P_n)$, and J, K are skew-symmetric $n \times n$ matrices representing in co-moving terms canonical angular momenta of fictitious (L, R) -tops. We use here the following duality convention:

$$\begin{aligned}
 (2.23) \quad \langle (P, J, K), (\dot{D}, l, r) \rangle &= \text{Tr}(P\dot{D}) + \frac{1}{2} \text{Tr}(Jl) + \frac{1}{2} \text{Tr}(Kr) \\
 &= \sum_A P_A \dot{Q}_A - \frac{1}{2} \sum_{A,B} J_{AB} l_{AB} - \frac{1}{2} \sum_{A,B} K_{AB} r_{AB} = \sum_A P_A \dot{q}_A - \frac{1}{2} \sum_{A,B} J_{AB} l_{AB} \\
 &\qquad\qquad\qquad - \frac{1}{2} \sum_{A,B} K_{AB} r_{AB},
 \end{aligned}$$

where

$$\begin{aligned}
 (2.24) \quad Q_A &= \exp(q_A) \quad \text{if } G = GL^+(n, R), \\
 Q_A &= \exp(iq_A) \quad \text{if } G = U(n);
 \end{aligned}$$

q_A and their conjugate momenta p_A are always real.

Non-holonomic quantities introduced above establish a local identification of mechanical state spaces TG, T^*G with the manifold $C \times M$, where

$$\begin{aligned}
 (2.25) \quad C &:= SO(n) \times SO(n), \\
 M &:= \begin{cases} R^n \times R^n \times so(n) \times so(n) & \text{if } G = GL^+(n, R), \\ T^n \times R^n \times so(n) \times so(n) & \text{if } G = U(n); \end{cases}
 \end{aligned}$$

$T^n = (S^1)^n$ denotes the n -dimensional torus (configuration space of the n -particle system in S^1), and $so(n)$ is the space of skew-symmetric $n \times n$ real matrices (Lie algebra of $SO(n, R)$).

Configuration-velocity states (X, \dot{X}) are represented by objects (L, R, D, \dot{D}, l, r) . Hamiltonian states (X, Y) are represented by objects (L, R, D, P, J, K) ; here Y denotes the canonical momentum conjugate to X in the sense of pairing $\langle Y, X \rangle = \text{Tr}(YX) = \sum_{AB} Y_{AB} X_{BA}$.

The M -quantities $(Q_A, \dot{Q}_A, l_{AB}, r_{AB})$ and $(Q_A, P_A, J_{AB}, K_{AB})$ are unique up to simultaneous permutations of indices.

The space of smooth functions depending only on canonical M -variables (Q, P, J, K) is closed under Poisson-bracket-operation. The basic Poisson brackets have the form

$$\begin{aligned}
 (2.26) \quad \{Q_A, P_B\} &= \{q_A, p_B\} = \delta_{AB}, \\
 \{J_{AB}, J_{CD}\} &= J_{AD} \delta_{CB} - J_{CB} \delta_{AD} + J_{DB} \delta_{CA} - J_{AC} \delta_{DB}, \\
 \{K_{AB}, K_{CD}\} &= K_{AD} \delta_{CB} - K_{CB} \delta_{AD} + K_{DB} \delta_{CA} - K_{AC} \delta_{DB}.
 \end{aligned}$$

All remaining Poisson brackets of the basic quantities (Q, P, J, K) vanish. Equations (2.26)_{2,3} express the fact that (J, K) are, respectively, Hamiltonian generators of transformation groups $L \mapsto LU, R \mapsto RU, U \in SO(n, R)$. Together with the general equations (1.10), (1.12), the formulas (2.26) turn the manifold M into singular Poisson manifold. Its centre is generated by Casimir invariants of $SO(n) \times SO(n)$

$$(2.27) \quad C(k, J) := \text{Tr}(J^k), \quad C(k, K) := \text{Tr}(K^k).$$

It is obvious that $C(k, J)$, $C(k, K)$ really have vanishing Poisson brackets with all M -quantities.

When expressed through $C(M)$ -variables, the kinetic energies ((2.19), (2.20)) have the form

$$(2.28) \quad T = \pm \frac{m}{2} \text{Tr}[D^{-2}\dot{D}^2 + l^2 + r^2 - 2D^{-1}lDr], \quad m > 0,$$

the plus and minus signs correspond, respectively, to $GL^+(n, R)$, $U(n)$. For the model (2.20) we obtain

$$(2.29) \quad T = \frac{m}{2} \text{Tr}[\dot{D}^2 - D^2l^2 - D^2r^2 + 2DlDr].$$

All Lagrangians invariant under $X \mapsto AXB$, $A, B \in SO(n, R)$, in particular kinetic energies ((2.28), (2.29)), and Lagrangians obtained from them by subtracting auxiliary potentials $V(D)$, have the following properties:

(i) They depend only on M -arguments (D, \dot{D}, l, r) . This means that from the point of view of non-holonomic description, (L, R) are cyclic variables.

(ii) T does not contain terms linear in \dot{D} and in (l, r) ; roughly speaking, (L, R) -variables are orthogonal to D -variables.

(iii) Hamiltonians H depend only on M -arguments, thus, they belong to the Poisson-Lie algebra generated by Eqs. (2.26) and (1.12).

(iv) Quantities

$$(2.30) \quad \bar{J} := LJL^{-1}, \quad \bar{K} := RKR^{-1}$$

are constants of motion because they are Hamiltonian generators of transformation groups $L \mapsto UL$, $R \mapsto UR$, $U \in SO(n, R)$ (i.e., equivalently, $X \mapsto UX$, $X \mapsto XU^T$). Thus we have

$$\{\bar{J}_{AB}, H\} = \{\bar{K}_{AB}, H\} = 0.$$

There are also obvious constants of motion independent of (L, R) , thus useful on the level of the M -space, namely, $C(k, J) = C(k, \bar{J})$, $C(k, K) = C(k, \bar{K})$.

The properties (i, ii, iii) imply that the equations of motion following from L are reducible to M . Namely, to solve them we should perform subsequently the following operations:

(i) Solution of the reduced equations

$$(2.31) \quad \frac{dQ_A}{dt} = \{Q_A, H\} = \frac{\partial H}{\partial P_A}, \quad \frac{dq_A}{dt} = \{q_A, H\} = \frac{\partial H}{\partial p_A}$$

or, equivalently,

$$(2.31') \quad \frac{dP_A}{dt} = \{P_A, H\} = -\frac{\partial H}{\partial Q_A}, \quad \frac{dp_A}{dt} = \{p_A, H\} = -\frac{\partial H}{\partial q_A},$$

$$(2.31'') \quad \frac{dJ_{AB}}{dt} = \{J_{AB}, H\} = \frac{\partial H}{\partial J_{CD}} \{J_{AB}, J_{CD}\},$$

$$(2.31''') \quad \frac{dK_{AB}}{dt} = \{K_{AB}, H\} = \frac{\partial H}{\partial K_{CD}} \{K_{AB}, K_{CD}\};$$

the Poisson brackets of J and K to be substituted from the form (2.26). This step gives us the evolution of M -parameters, $Q_A(t)$, $P_A(t)$, $q_A(t)$, $p_A(t)$, $J_{AB}(t)$, $K_{AB}(t)$.

(ii) Determination of the time evolution of quantities l , r . This is achieved with the help of the inverse Legendre transformation,

$$(2.32) \quad \dot{Q}_A = \frac{\partial H}{\partial P_A}, \quad l_{AB} = \frac{\partial H}{\partial J_{AB}}, \quad r_{AB} = \frac{\partial H}{\partial K_{AB}}.$$

Substituting to the transformation (2.32) the quantities $Q(t)$, $P(t)$, $J(t)$, $K(t)$ determined in (i), we obtain $l(t)$, $r(t)$.

(iii) Determination of the time evolution of cyclic variables (L , R). To do this, we solve time-dependent dynamical systems on the orthogonal group $SO(n, R)$,

$$(2.33) \quad \frac{dL}{dt} = Ll, \quad \frac{dR}{dt} = Rr$$

Substituting here $l(t)$, $r(t)$ from (ii), we obtain $L(t)$, $R(t)$.

(iv) From (i) and (iii) we obtain the final solutions

$$(2.34) \quad X(t) = L(t)D(t)R^T(t).$$

For applications to one-dimensional lattices with internal parameters, we need only the step (i). The (L, R) -variables are "hidden parameters"; they have no direct influence on forces acting between lattice points.

3. Discussion of one-dimensional lattice models implied by Hamiltonian systems on matrix manifolds

Performing the Legendre transformation

$$(3.1) \quad P_A = \frac{\partial L}{\partial \dot{Q}_A}, \quad \text{i.e.,} \quad p_A = \frac{\partial L}{\partial \dot{q}_A}; \quad J_{AB} = \frac{\partial L}{\partial l_{AB}}, \quad K_{AB} = \frac{\partial L}{\partial r_{AB}},$$

inverting it, i.e., expressing \dot{q}_A , l_{AB} , r_{AB} as functions of p_A , J_{AB} , K_{AB} , and substituting these functions to the formulas (2.28) and (2.29) for kinetic energies, we obtain geodetic Hamiltonians, $H = T(p, J, K)$. These Hamiltonians contain interference terms in (J, K) -variables. To diagonalize them, we introduce auxiliary quantities:

$$(3.2) \quad N_{AB} = J_{AB} - K_{AB}, \quad M_{AB} = -J_{AB} - K_{AB}.$$

The centre of mass (arithmetic mean value) of q^i will be denoted by

$$(3.3) \quad q = \frac{1}{n} \sum_A q_A = \frac{1}{n} \ln \det X.$$

The total linear momentum of q -particles is denoted by

$$(3.4) \quad p = \sum_A p_A.$$

Obviously,

$$\{q, p\} = 1, \quad \{q_A - q_B, p\} = 0.$$

The basic system of Poisson brackets (2.26) in the M -space will be written as

$$(3.5) \quad \begin{aligned} \{q_A, p_B\} &= \{Q_A, P_B\} = \delta_{AB}, \\ \{M_{IJ}, M_{AB}\} &= \{N_{IJ}, N_{AB}\} = -M_{IB} \delta_{JA} + M_{AJ} \delta_{IB} - M_{BJ} \delta_{AI} + M_{IA} \delta_{BJ}, \\ \{M_{IJ}, N_{AB}\} &= -N_{IB} \delta_{AJ} + N_{AJ} \delta_{IB} - N_{BJ} \delta_{AI} + N_{IA} \delta_{BJ}, \end{aligned}$$

all other coordinate brackets vanish.

Geodetic Hamiltonians corresponding to the Lagrangians (2.28) and (2.29) have the form

$$(3.6) \quad H = T^l(\dots p_A \dots) + U^l(\dots q_A, M_{AB}, N_{AB} \dots),$$

where T^l, U^l are, respectively, kinetic and interaction energy of the resulting n -element lattice.

Explicitly,

$$(3.7) \quad H = \frac{1}{2m} \sum_A p_A^2 + \frac{1}{32m} \sum_{AB} \frac{M_{AB}^2}{\operatorname{sh}^2 \frac{q_A - q_B}{2}} - \frac{1}{32m} \sum_{AB} \frac{N_{AB}^2}{\operatorname{ch}^2 \frac{q_A - q_B}{2}}$$

for $G = GL^+(n, R)$, and

$$(3.8) \quad H = \frac{1}{2m} \sum_A p_A^2 + \frac{1}{32m} \sum_{AB} \frac{M_{AB}^2}{\sin^2 \frac{q_A - q_B}{2}} + \frac{1}{32m} \sum_{AB} \frac{N_{AB}^2}{\cos^2 \frac{q_A - q_B}{2}}$$

for $G = U(n)$.

For the model (2.29), defined on $L(n, R)$, we obtain

$$(3.9) \quad H = \frac{1}{2m} \sum_A p_A^2 + \frac{1}{8m} \sum_{AB} \frac{M_{AB}^2}{(Q_A - Q_B)^2} + \frac{1}{8m} \sum_{AB} \frac{N_{AB}^2}{(Q_A + Q_B)^2}.$$

Let us notice that the only change introduced by the correction term $\frac{b}{2} (\operatorname{Tr} E)^2$ in the form (2.17) would consist in modifying the expressions (3.7), (3.8) by the additional term $p^2/2b$ (correction to the kinetic energy of the centre of mass).

The structure of the Hamiltonians ((3.7), (3.8), (3.9)) is very clear and convincing. It is obvious that they may be used as models of one-dimensional lattices with internal parameters. The quantities q_A (resp. Q_A) are interpreted as positions of lattice points on a straight line (3.7), (3.9) or on a circle (3.8); p_A are canonical momenta of translational motion. M_{AB}, N_{AB} are internal variables responsible for the strength of interparticle interactions; they are amplitudes of mutual repulsive and attractive forces.

As Hamiltonians of systems on matrix spaces, the models (3.7), (3.8), (3.9) are purely kinetic, i.e., geodetic. However, when interpreted as Hamiltonians of structured lattices on straight lines or circles, they split into n -particle kinetic energy terms and dynamical terms $U^l(q, M, N)$ describing interparticle forces. In the models (3.7), (3.8) the quantities M_{AB}, N_{AB} are responsible, respectively, for repulsion and attraction. Expression (3.8) is posi-

tively definite, whereas the range of Eq. (3.7) is identical with the whole real line. In the model (3.9) there are only scattering-repulsive interactions, thus without periodic boundary conditions on R , or without extra introduced non-geometric potentials $V(Q_1, \dots, Q_n)$, the model (3.9) is useless as a model of condensed matter.

Similarity of the expressions (3.7), (3.8), (3.9) to integrable lattices (2.3), (2.4), (2.2) is obvious. There are also very important differences. Namely, the coupling parameters in Eqs. (3.7), (3.8), (3.9) are no longer degenerate; moreover, they are no longer constant; instead, they are internal state variables subject to equations of motion. Besides, the Hamiltonians (3.7), (3.8) contain the N -terms, interpretable as interparticle attraction. Thus we can try to apply them as an academic model of one-dimensional condensed matter.

Just as in Eqs. (2.3), (2.4), (2.2), all models are rigorously solvable because they are derived from rigorously solvable Hamiltonian systems on matrix spaces.

The lattices (3.7), (3.8), (3.9) are ruled by dynamical systems (2.31) in the M -space, i.e., in the manifold of the variables q, p, M, N . Thus Eqs. (3.5) and (1.12) imply that

$$(3.10) \quad \begin{aligned} \frac{dq_A}{dt} &= \frac{1}{m} p_A, \\ \frac{dp_A}{dt} &= m \frac{d^2 q_A}{dt^2} = - \frac{\partial U}{\partial q_A}, \\ \frac{dM_{IJ}}{dt} &= \{M_{IJ}, M_{AB}\} \frac{\partial U^I}{\partial M_{AB}} + \{M_{IJ}, N_{AB}\} \frac{\partial U^I}{\partial N_{AB}}, \\ \frac{dN_{IJ}}{dt} &= \{N_{IJ}, M_{AB}\} \frac{\partial U^I}{\partial M_{AB}} + \{N_{IJ}, N_{AB}\} \frac{\partial U^I}{\partial N_{AB}}, \end{aligned}$$

where the Poisson brackets of M and N are to be substituted from the form (3.5).

It is seen from Eqs. (3.7), (3.8), (3.9) that particles are impenetrable; coincidences are forbidden by singularities of the repulsive terms. In the model (3.7) situations with $\det X = Q_1 \dots Q_n = 0$ are unapproachable in a finite time; motion in the matrix space is restricted to the connected group $GL^+(n, R)$. On the contrary, without an auxiliary potential $V(Q_1, \dots, Q_n)$, the scattering Hamiltonian (3.9) admits the sign changes of $\det X$; motion in the matrix space $L(n, R)$ is no longer restricted to $GL^+(n, R)$. It is interesting to note that in model (3.9) there exists not only the usual repulsion between the lattice points, but also the repulsion between lattice points and their mirror images with respect to the fixed origin of one-dimensional space.

All Hamiltonians (3.7), (3.8), (3.9) have binary structure,

$$(3.11) \quad H = \sum_{AB} h(q_A, q_B; p_A, p_B; M_{AB}, N_{AB}),$$

what makes them realistic as models of physical lattices. The models (3.7), (3.8) are also translationally-invariant (dilatational invariance on matrix groups). This binary structure is very peculiar, namely, our Hamiltonians are superpositions of $\frac{1}{2}n(n-1)$ clusters corresponding to 2-dimensional situations, i.e., to groups $GL(2, R)$, $U(2)$. Thus the two-body problems on R or S^1 , i.e., the Hamiltonians (3.7), (3.8), (3.9) corresponding to $n = 2$,

are crucial for understanding the character of intermolecular forces predicted by Eqs. (2.28), (2.29). Let us discuss briefly the 2-dimensional problems.

If $n = 2$, then $\bar{J}_{AB} = J_{AB} = J\varepsilon_{AB}$, $\bar{K}_{AB} = K_{AB} = K\varepsilon_{AB}$, where $\varepsilon_{AB} = -\varepsilon_{BA}$, $\varepsilon_{12} = 1$. This is a consequence of the Abelian character of $SO(2)$. We have seen that J, K are constants of motion, thus, for $n = 2$, the quantities J, K are also constants of motion. Just as in Eq. (3.2), we define

$$(3.12) \quad N := J - K, \quad M := -J - K.$$

The Hamiltonian systems on $GL(2, R)$ and $U(2)$ can be effectively reduced to Hamiltonian systems on the Cartan groups of diagonal matrices (maximal Abelian subgroups of $GL(2, R)$ and $U(2)$) i.e., to autonomous Hamiltonian equations involving only variables $q_A, p_A, A = 1, 2$. This is just due to the fact that for $n = 2$, M and N are constants of motion (coupling "constants" are actually constant).

1. For the model (3.7), the effective reduced Hamiltonian corresponding to fixed values of constants of motion M, N has the form

$$(3.13) \quad H_{MN}^{\text{eff}} = \frac{1}{2m} (p_1^2 + p_2^2) + \frac{M^2}{16msh^2 \frac{q_1 - q_2}{2}} - \frac{N^2}{16mch^2 \frac{q_1 - q_2}{2}} = T^l + U_{MN}^{\text{eff}}.$$

Introducing an auxiliary potential $V(D)$, we merely modify the term U_{MN}^{eff} .

M, N are, respectively, repulsive and attractive coupling constants. Exactly as in the approach to mechanics suggested by Hertz, they are canonical momenta conjugate to cyclic variables.

The repulsive part of Eq. (3.31) is a monotonically decreasing function of the interparticle distance $|q_1 - q_2|$, positively singular for a coincidence of particles (nonpenetrability) and vanishing at infinity. The attractive term is a negative, monotonically increasing function of the distance; it is finite all over the half-axis of distances (including a coincidence situation) and vanishes at infinity. Thus, for small distances the repulsive mechanism prevails if $M \neq 0$. The vanishing value of M is an exceptional situation: there is no repulsion, particles are penetrable (coincidences admissible) and we obtain a nonlinear oscillator with attractive forces vanishing at infinity. The behaviour of U^{eff} at large distances depends on the relationship between M and N . If $|M| > |N|$, i.e., $JK > 0$, then U_{MN}^{eff} is repulsive and we deal with a scattering situation. If $|N| > |M|$, i.e., $JK < 0$, then at large distances attraction prevails, the shape of U^{eff} is qualitatively given by Fig. 2, and there exist bounded situations (Fig. 4). The sharper inequality $|N| > |M|$, the deeper the potential well. Translational invariance of the two-body problem (dilatational invariance in $GL(2, R)$) implies that the relative motion and the centre of mass motion are independent (From the viewpoint of $GL(2, R)$, H is a direct sum of the dilatational term and the $SL(2, R)$ term),

$$(3.14) \quad H = \frac{1}{m} p_-^2 + \frac{M^2}{16msh^2 \frac{q_-}{2}} - \frac{N^2}{16mch^2 \frac{q_-}{2}} + \frac{1}{m} p_+^2,$$

where $q_{\pm} = q_1 \pm q_2$, and p_{\pm} are conjugate momenta of q_{\pm} . The centre of mass moves uniformly. Separable auxiliary potentials of the form $V = V_+(q_+) + V_-(q_-)$ do not violate this splitting. If V_+ is nontrivial, the centre of mass motion is non-uniform.

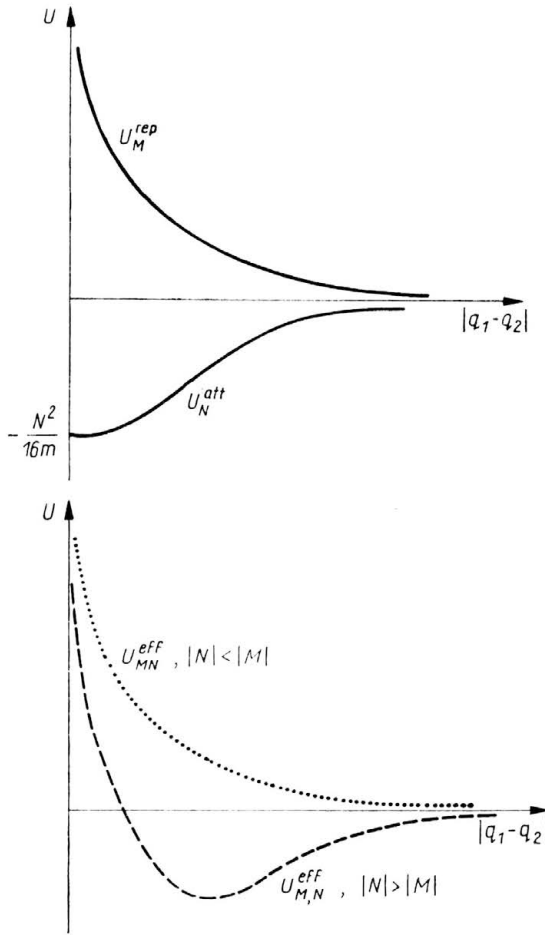


FIG. 4.

2. For the S^1 -model (3.8) we obtain

$$(3.15) \quad H_{MN}^{eff} \neq \frac{1}{2m} (p_1^2 + p_2^2) + \frac{M^2}{16m \sin^2 \frac{q_1 - q_2}{2}} + \frac{N^2}{16m \cos^2 \frac{q_1 - q_2}{2}}.$$

Both repulsive and attractive terms are positive (if their “coupling constants” M, N do not vanish). If $M \neq 0$, the particles are non-penetrable; the repulsive term is positively singular for coincidences and decreases with $|q_1 - q_2|$. For $|q_1 - q_2| = \pi$, i.e., for antipodal configurations it attains its minimal value $M^2/16m$. Thus, antipodal configurations are stable equilibria (modulo uniform rigid rotations $q_1 = q_1^0 + wt, q_2 = q_2^0 + wt$) for the repulsive term U_{MN}^{eff} (Fig. 5). The existence of such equilibria for purely repulsive potentials is a consequence of the compactness of S^1 . The attractive part of H has an absolute minimum at $(q_1 - q_2) = 0$, where it equals $N^2/16m$, and is positively singular at $|q_1 - q_2| = \pi$; thus, if $N \neq 0$, antipodal configurations are forbidden. If both M, N

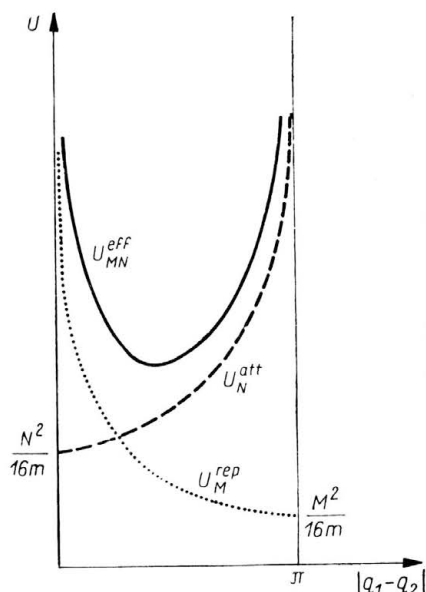


FIG. 5.

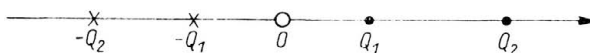


FIG. 6.

do not vanish, then U_{MN}^{eff} has exactly two stable equilibria (modulo uniform rigid rotation), namely

$$|q_1 - q_2| = \pm 2 \arcsin \sqrt{\frac{|M|^2}{|M|^2 + |N|^2}}.$$

In contrast to what we were faced with in Eq. (3.13), the attractive part resembles a harmonic oscillator in that it has no upper bound.

By analogy to Eq. (3.14), we have the following splitting of H into relative motion and the centre of mass motion, i.e., into the $SU(2)$ -part and unitary-dilatational part:

$$(3.16) \quad H = \frac{1}{m} p_-^2 + \frac{M^2}{16m \sin^2 \frac{q_-}{2}} + \frac{N^2}{16m \cos^2 \frac{q_-}{2}} + \frac{1}{m} p_+^2$$

with the same as previously meaning of symbols q_{\pm}, p_{\pm} .

3. For the $L(n, R)$ -kinetic energy we obtain

$$(3.17) \quad H_{MN}^{\text{eff}} = \frac{1}{2m} (P_1^2 + P_2^2) + \frac{M^2}{4m(Q_1 - Q_2)^2} + \frac{N^2}{4m(Q_1 + Q_2)^2}.$$

Without an auxiliary potential $V(D)$ the Hamiltonian (3.17) is purely scattering, thus inapplicable as a model of intermolecular forces. Particles are non-penetrable if $M \neq 0$; moreover, if $N \neq 0$, they cannot approach positions corresponding to mirror-reflections of other particles with respect to the origin of R .

If there is no auxiliary potential $V(D)$, then nothing prevents the sign changes of Q , thus the representation $Q_A = \exp q_A$ is no longer possible. The model (3.17) is never translationally-invariant in R : Q_1, Q_2 are coupled not only through their distance $|Q_1 - Q_2|$, but also, when $N \neq 0$, through their centre of mass $\frac{1}{2}(Q_1 + Q_2)$ (Fig. 6).

The above analysis of two-dimensional models provides a satisfactory understanding of the structure of binary interactions for general n -particle lattices with internal parameters. The general character of interparticle forces based on the balance between M -repulsive and N -attractive terms is essentially the same for the n -body problem and the two-body problem. Nevertheless, the dynamics of general n -particle lattices is much more complicated and has many qualitatively new features. If $n > 2$, the quantities M, K fail to be constants of motion. Coupling parameters are oscillating, just as instantaneous dipole moments spontaneously induced in particles of molecular crystals. Geodetic dynamics on G is not any longer reducible to an effective autonomous dynamics (with frozen values of internal parameters) on Abelian groups of diagonal matrices (parametrized by the coordinates q_1, \dots, q_n). This means that there is a nontrivial mutual interaction between lattice points and their internal parameters.

It is obvious that for any n , the models (3.7), (3.8) are translationally-invariant on R or S^1 . The Hamiltonians (3.7), (3.8) are direct sums of terms describing the relative motion of lattice points, and dilatational terms corresponding to the non-interesting uniform motion of the centre of mass. The relative motion terms correspond to doubly-invariant-geodetic models on $SL(n, R)$ or $SU(n)$. They split into superpositions of $\frac{1}{2}n(n-1)$ terms corresponding to all possible binary relative motions. These binary terms are identical with $SL(2, R)$ and $SU(2)$ expressions (3.14), (3.16). Thus we have

$$(3.18) \quad H = \frac{1}{4m} \sum_{IJ} \left[\frac{1}{n} (p_I - p_J)^2 + \frac{1}{8} M_{IJ}^2 \varrho \left(\frac{q_I - q_J}{2} \right) + \frac{1}{8} N_{IJ}^2 \alpha \left(\frac{q_I - q_J}{2} \right) \right] + \frac{p^2}{2an},$$

where the meaning of the functions α, ϱ is as follows:

$$(3.19) \quad \begin{aligned} \alpha(x) &= -\operatorname{ch}^{-2}x, & \varrho(x) &= \operatorname{sh}^{-2}x & \text{if } G &= GL^+(n, R), \\ \alpha(x) &= \cos^{-2}x, & \varrho(x) &= \sin^{-2}x & \text{if } G &= U(n). \end{aligned}$$

Equations of motion of nonlinear lattices described by the Hamiltonians (3.18) can be written down in the following common form:

$$(3.20) \quad m \frac{d^2 q_I}{dt^2} = \frac{1}{16m} \sum_J M_{IJ}^2 C \left(\frac{q_I - q_J}{2} \right) S^{-3} \left(\frac{q_I - q_J}{2} \right) - \sum_J N_{IJ}^2 C^{-3} \left(\frac{q_I - q_J}{2} \right) S \left(\frac{q_I - q_J}{2} \right),$$

$$\frac{d}{dt} (M+N) = [M+N, \bar{M} + \bar{N}], \quad \frac{d}{dt} (M-N) = [M-N, \bar{M} - \bar{N}],$$

where the meaning of the symbols \bar{M}, \bar{N}, S, C is as follows:

$$\bar{M}_{IJ} := \frac{1}{8m} M_{IJ} S^{-2} \left(\frac{q_I - q_J}{2} \right), \quad \bar{N}_{IJ} := \frac{1}{8m} N_{IJ} C^{-2} \left(\frac{q_I - q_J}{2} \right),$$

$$\begin{aligned} S(x) &= \operatorname{sh} x, & C(x) &= \operatorname{ch} x & \text{if } G &= GL^+(n, R), \\ S(x) &= \sin x, & C(x) &= \cos x & \text{if } G &= U(n). \end{aligned}$$

The symbol $[A, B]$ denotes the matrix commutator, $[A, B] := AB - BA$.

These equations are strongly nonlinear. Nevertheless, they are, in principle, rigorously solvable because they are equivalent to evidently integrable Hamiltonian systems on G . On the level of the group space G , the general solution is given by the system of all possible one-parameter subgroups and their cosets,

$$(3.21) \quad X(t) = \exp(Et)A = A \exp(A^{-1}Et),$$

where A is an arbitrary element of G , and E is an arbitrary element of the Lie algebra $\mathfrak{g}(L(n, R))$ if $G = GL^+(n, R)$, $\mathfrak{u}(n)$ if $G = U(n)$.

Obviously, it is a rather complicated task, especially when the system is large (large n), to obtain from the system (3.21) the explicit values of the lattice parameters $q(t)$, $M(t)$, $N(t)$. Nevertheless, one can do this without essential difficulties with the help of approximate or numerical methods, the more so, due to the explicit formula (3.21), we need not use any numerical algorithm for differential problems. The explicit, algebraic knowledge of the solutions (3.21) facilitates the choice of an effective and quickly converging procedure. The formula (3.21) facilitates also the use of analytical qualitative methods.

Let us finish with some comments concerning the problem of multiparticle interactions. Geodetic Hamiltonians (3.7), (3.8), (3.9) on groups lead to binary problems which as mentioned, are up to 90% satisfactory in crystal dynamics at least for some kind of crystals. Nevertheless, within essentially the same framework, we can take multiparticle interactions into account. They are described by Lagrangians constructed in a polynomial way from Casimir invariants.

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