Mechanics not on a manifold

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Abstract
The free scalar field is studied on the Y-junction of three semi-infinite axes
which is the simplest example of a non-manifold space. It is shown that the
transition rules for this system uniquely follow from conservation of energy
and charge. A discrete version of the model gives the same result.

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1. Introduction

Hamiltonian mechanics on manifolds now is practically completed [1, 2], but there appeared
a serious need for the formulation of mechanics not on manifolds. The problems arise both
in nanoelectronics and string theory. For example, three quantum wires with a Y junction do
not compose a manifold (the vicinity of the junction is not homeomorphic to some domain in
Euclidean space). Moreover, one can compose a network of strings [3, 4] which also is not a
manifold. It is extremely important to have the Hamiltonian formalism on such structures. In
nanoelectronics: to describe motion of electrons; in string theory: to model space [4].

There is no regular theory of such processes. The best way to find the solution of a
complex problem is to consider the simplest case possessing all its essential features. As the
first step to this end, a 3-tail system may be studied, i.e., the Y junction of three semi-infinite
sets of classical harmonic oscillators related to a theory of a free classical scalar field on such
a 3-ray star.

Usually more serious problems arise when one turns to a quantum description even in the
manifold case. Quantum mechanics (QM) can be deduced from classical mechanics only in
the Euclidean space (this Dirac's recipe was confirmed by experiments). Even curved spaces
cause serious difficulties. There are two points of view in this case.

(1) The curved space is considered as that embedded into the flat space, and one has to
    consider dynamics with constraints.
(2) QM should be deduced from its classical counterpart without using the embedding space.

These are two principally differing approaches, but none of these gives a unique recipe.
In case (1), there are the following recipes:

  (i) the Dirac method (modification of the Poisson brackets) [5];

 (ii) the conversion method [6, 7];

(iii) the thin-layer method [8]; and

(iv) the reduction method [9, 10].

The Dirac recipe is not unambiguous [11]. The result depends even on the way one parameterizes the curved space [12]. In case (ii), the authors increase the number of unphysical variables. Approaches (i) and (ii) give different results [11]. In both cases, it is assumed that in QM the unphysical degrees of freedom cannot influence the physical dynamics. That is correct only in the classical theory. In recipe (iii), one approximates the motion on a surface by motion on a thin layer. This looks reasonable. In method (iv), one excludes the normal to the surface motions demanding

$$\hat{P}_\perp \psi_{\mathrm{ph}} = 0, \tag{1}$$

where $\hat{P}_\perp$ is normal to the surface momentum and ψ_{ph} is a state vector from the physical Hilbert space. Methods (iii) and (iv) give the identical results [13], but the latter allows one to avoid rather cumbersome calculations. As for case (2), QM cannot be deduced unambiguously from classical mechanics, because there are a lot of QM giving $\hbar \to 0$ the same classical limit [14].

Wave scattering in thin tubes and associated theory of quantum graphs were actively studied in the last decade (see [15–19] and especially in the excellent paper [20]). Most publications on this subject are concerned with analytical properties of the corresponding solutions. However, several underlying physical principles were not discussed in full. The present paper is especially devoted to elucidate the role of basic physical principles.

Returning to our problem (the formulation of QM not on a manifold, e.g. on three semi-infinite straight lines having one common point), we note that we do not know any regular investigation of the problem. It turns out that in this case it is reasonable to reverse the standard approach (classical mechanics $\to$ quantum mechanics) and begin with fields (or wavefunctions). Really, formulating new theory one should, from the very beginning, assume some inalienable principles. If one looks for theories conserving energy and charge, then the corresponding conditions should be postulated. It turns out that it is more natural to do this working with fields. In this framework, the conservation laws lead to the translation rules at the junction point, manifesting the fact that the physical space is not a manifold. Therefore, the classical Hamiltonian mechanics not on a manifold follows from QM. Paradoxically, even this reasoning can be reversed if one considers a free relativistic field as a continuous limit of an ordered set of harmonic oscillators. In this framework, one can readily formulate the corresponding Hamiltonian mechanics. Coincidence between the continuous limit of this theory and the primary one confirms the sensibility of our general approach.

We also found that the junction plays the role of a potential (scatterer). The corresponding scattering amplitudes are calculated. Actually, in this context, our problem may be considered from both classical and quantum points of view. Indeed in spaces of this type, the scattering of a complex classical free relativistic field is, in fact, identical to the scattering of a particle in relativistic QM.

Within our model, the scattering amplitudes do not depend on the angles between the rays, because there is no special reason for such dependence. Indeed, the dynamics may be modeled by the sets of harmonic oscillators, vibrating in the direction orthogonal to the plane embedding the 'star' (i.e. it is supposed that all the rays belong to the plane). What about the 'junction oscillator'? It is assumed that its oscillations do not depend on the angles between the rays.

The importance of this problem for strings is self-evident. Gradually, it becomes clear that at the Planck scales, matter manifests itself in the form of strings. Polymers and nanostructures are important for modern technologies. Study of strings is of special interest, also because a 3D network of superstrings can model the physical spacetime at the Planck scales, and one should know how to describe the propagator of excitations over the structure. Besides, it opens the way to the unification of all interactions, including gravitation [4, 10].

It is worth noting that for three waves coming from different rays, the junction point plays the role of a three-particle potential. It is significant that the latter can not be reduced to a sum of two-particle ones. In this sense, the 3-tail problem may be considered as an analog to the three-body scattering problem in QM.

The paper is organized as follows. In section 2, we briefly discuss the model. In section 3, we obtain an exact form of *S*-matrix from the conservation of energy and charge. Section 4 is devoted to the corresponding discrete model.

2. General properties of *S*-matrix

Consider a complex scalar field, φ, defined on three strings with the spatial coordinates $x \in [0, \infty)$, $y \in [0, \infty)$ and $z \in [0, \infty)$. The junction point corresponds to $x = y = z = 0$. On each string, the field φ satisfies the Klein–Fock–Gordon equation (we take $\hbar = 1$, $c = 1$),

$$\frac{\partial^2 \varphi}{\partial t^2} = \frac{\partial^2 \varphi}{\partial q^2} - m^2 \varphi, \qquad q = x, y, z, \quad q > 0. \tag{2}$$

Our purpose is to obtain a global solution defined on the whole structure. Firstly, we demand that it is continuous at the junction point

$$\lim_{x \to 0} \varphi(x) = \lim_{y \to 0} \varphi(y) = \lim_{z \to 0} \varphi(z). \tag{3}$$

This condition was postulated, in particular, also in [21] together with the following one:

$$\partial_x \varphi|_{x=0} + \partial_y \varphi|_{y=0} + \partial_z \varphi|_{z=0} = 0, \tag{4}$$

but its physical meaning (in connection with the problem of the formulation of mechanics not on a manifold) was not investigated. In the present paper, we show that together with (3) condition (4) guarantees both the energy and the charge conservation for our system.

The solutions of equation (2) on strings satisfy the superposition principle. It is natural to begin the investigation with the study of a monochromatic wave propagating from $x = \infty$,

$$\varphi(k, x, t) = e^{-i(\omega t + kx)} + R(k) e^{-i(\omega t - kx)},$$
$$\varphi(k, y, t) = T_y(k) e^{-i(\omega t - ky)}, \qquad \varphi(k, z, t) = T_z(k) e^{-i(\omega t - kz)}. \tag{5}$$

Here, $R(k)$ and $T(k)$ are correspondingly the reflection and transition coefficients, while

$$\omega^2 = k^2 + m^2, \qquad \omega \geqslant m. \tag{6}$$

The incoming particle has momentum $k > 0$.

According to (3), $T_y(k) = T_z(k) = 1 + R(k)$. A *unitarity* condition,

$$|R(k)|^2 + 2|R(k) + 1|^2 = 1, \tag{7}$$

is proved in the following section. According to it, the coefficient $R(k)$ may be parameterized as

$$R(k) = \tfrac{1}{3} e^{i\theta(k)} - \tfrac{2}{3}. \tag{8}$$

3. *S*-matrix and conservation of energy and charge

Equation (2) on a line follows from the Lagrangian

$$\mathcal{L} = \partial_0 \bar{\varphi} \partial_0 \varphi - \partial_1 \bar{\varphi} \partial_1 \varphi - m^2 \bar{\varphi} \varphi, \tag{9}$$

where ∂_0 and ∂_1 denote differentiations with respect to time and spatial coordinate q respectively. The energy–momentum tensor of the field is given by the general formula [22]

$$T^{ij} = \frac{\partial \mathcal{L}}{\partial(\partial_i \varphi)} \partial^j \varphi + \frac{\partial \mathcal{L}}{\partial(\partial_i \bar{\varphi})} \partial^j \bar{\varphi} - g^{ij} \mathcal{L}. \tag{10}$$

Here g^{ij} is the Minkowski tensor $g^{ij} = \mathrm{diag}(1, -1)$ and the derivatives ∂^j are related to ∂_j by $\partial^i = g^{ij} \partial_j$. Using (9), we obtain

$$T^{00} = \partial^0 \bar{\varphi} \partial^0 \varphi - \partial^1 \bar{\varphi} \partial^1 \varphi + m^2 \bar{\varphi} \varphi, \qquad T^{10} = -(\partial^1 \bar{\varphi} \partial^0 \varphi + \partial^0 \bar{\varphi} \partial^1 \varphi). \tag{11}$$

The energy–momentum conservation follows from the equation

$$\partial_i T^{ij} = 0. \tag{12}$$

According to (12), the energy in a segment $q_1 \leqslant q \leqslant q_2$:

$$E(q_1, q_2) = \int_{q_1}^{q_2} T^{00}(q) \, \mathrm{d}q \tag{13}$$

satisfies the relation

$$\frac{\mathrm{d}E(q_1, q_2)}{\mathrm{d}t} = T^{10}(q_1) - T^{10}(q_2). \tag{14}$$

For system (9) on a line with boundary conditions $\varphi(\pm\infty) \to 0$ equation (14) results in the conservation of energy $E(-\infty, \infty) = \mathrm{const}$. Postulating the energy conservation for the system on the Y-junction, we obtain from (14) the following condition:

$$T^{10}(x)|_{x\to 0} + T^{10}(y)|_{y\to 0} + T^{10}(z)|_{z\to 0} = 0, \tag{15}$$

or, according to (11) and (12),

$$\partial_t \bar{\varphi}(\partial_x \varphi + \partial_y \varphi + \partial_z \varphi) + (\partial_x \bar{\varphi} + \partial_y \bar{\varphi} + \partial_z \bar{\varphi})\partial_t \varphi|_{x=y=z=0} = 0. \tag{16}$$

Although this condition is weaker than (4), it puts a strong enough restriction on the function $R(k)$. Substituting into (16) the monochromatic solution (5), we obtain the unitarity condition (7). However, equation (16) must also be true for superposition of several monochromatic waves with different k or, equivalently, for the sum

$$\varphi_{\mathrm{in}}(x, t) = \sum_k a(k) \, \mathrm{e}^{-\mathrm{i}(\omega_k t - kx)}. \tag{17}$$

Then in equation (16), interference terms appear. Since expression (11) for T^{10} is bilinear with respect to φ and $\bar{\varphi}$, the crossing terms originate from *two* monochromatic waves with different frequencies. Therefore, in order to obtain the corresponding restrictions on the function $R(k)$, it is sufficient to study the two-mode solution

$$\varphi(k_1, k_2, x, t) = \mathrm{e}^{-\mathrm{i}(\omega_{k_1} t + k_1 x)} + R(k_1) \, \mathrm{e}^{-\mathrm{i}(\omega_{k_1} t - k_1 x)} + \mathrm{e}^{-\mathrm{i}(\omega_{k_2} t + k_2 x)} + R(k_2) \, \mathrm{e}^{-\mathrm{i}(\omega_{k_2} t - k_2 x)},$$

$$\varphi(k_1, k_2, y, t) = (1 + R(k_1)) \, \mathrm{e}^{-\mathrm{i}(\omega_{k_1} t - k_1 y)} + (1 + R(k_2)) \, \mathrm{e}^{-\mathrm{i}(\omega_{k_2} t - k_2 y)}, \tag{18}$$

$$\varphi(k_1, k_2, z, t) = (1 + R(k_1)) \, \mathrm{e}^{-\mathrm{i}(\omega_{k_1} t - k_1 z)} + (1 + R(k_2)) \, \mathrm{e}^{-\mathrm{i}(\omega_{k_2} t - k_2 z)}.$$

We have assumed here that the wave vectors do not change after the scattering.

Substituting (18) into (16) and extracting the constant terms, we obtain equation (7). However, the terms proportional to $e^{i(\omega_{k_1} - \omega_{k_2})t}$ give the following condition:

$$\omega_{k_1} k_2 (1 + \bar{R}(k_1))(1 + 3R(k_2)) + \omega_{k_2} k_1 (1 + 3\bar{R}(k_1))(1 + R(k_2)) = 0, \tag{19}$$

and its complex conjugate. With equations (6) and (8), these two relations give

$$e^{i\theta(k)} = \frac{k + i\alpha\sqrt{k^2 + m^2}}{k - i\alpha\sqrt{k^2 + m^2}}. \tag{20}$$

Here α is a real constant. Thus, equation (16) admits nontrivial dependence of the transition coefficients on k. It means that the junction point also may be considered as a nontrivial scatterer, and this should be taken as an important feature of the 'space'.

Another important conserved quantity is charge (or particle number) [22] related to the current

$$j^l = i(\bar{\varphi} \partial^l \varphi - \varphi \partial^l \bar{\varphi}), \qquad l = 0, 1. \tag{21}$$

From equation (2), it follows that

$$\partial_0 j_0 - \partial_1 j_1 = 0, \tag{22}$$

and in analogy with equation (15), we obtain the second condition

$$j_1(x)|_{x \to 0} + j_1(y)|_{y \to 0} + j_1(z)|_{z \to 0} = 0, \tag{23}$$

or

$$\bar{\varphi}(\partial_x \varphi + \partial_y \varphi + \partial_z \varphi) - (\bar{\partial}_x \varphi + \partial_y \bar{\varphi} + \partial_z \bar{\varphi})\varphi|_{x=y=z=0} = 0. \tag{24}$$

Like equation (16), this condition also follows from equation (4). Now we substitute solutions (5), (18) into equation (24). The substitution of (5) gives again the unitarity condition (7); however, the substitution of (18) results in

$$k_2(1 + \bar{R}(k_1))(1 + 3R(k_2)) + k_1(1 + 3\bar{R}(k_1))(1 + R(k_2)) = 0, \tag{25}$$

or

$$e^{i\theta(k)} = \frac{k + i\beta}{k - i\beta}, \tag{26}$$

where β is a new real constant.

As we see from (20) and (26), the energy and charge are conserved simultaneously only if

$$\alpha = \beta = 0, \tag{27}$$

or

$$\alpha = \beta = \infty. \tag{28}$$

In the first case,

$$R(k) = -\tfrac{1}{3}, \qquad T(k) = \tfrac{2}{3}. \tag{29}$$

However, in the second case,

$$R(k) = -1, \qquad T(k) = 0. \tag{30}$$

For $T(k) = 0$, the three strings behave as disjoints, and solution (30) is of little physical interest. On the other hand, by substituting (5) into (4), we find that for monochromatic waves condition (4) is equivalent to systems (16) and (24). Since both of these solutions are linear, this equivalence is also true for a general solution (17). An outstanding feature of solution (29) is its universality: it does not depend on k. This is important for modeling of 3D space by a network composed of strings [4, 10].

We conclude that equation (4) represents the only nontrivial condition compatible with the continuity condition (3), superposition principle and the conservation of both the energy and charge.

4. Harmonic oscillators network approximation

It is instructive to approximate our system by a harmonic oscillator network. In fact, it gives an independent approach to the problem. The network is presented by three linear chains of harmonic oscillators, described by variables $\varphi_{q,n}$, where $n = 1, 2, \ldots, q = x, y, z$, and the junction point oscillator described by φ_0. The Lagrangian is given by

$$L = \frac{1}{2} \sum_q \sum_n \left[\dot{\varphi}_{q,n}^2 - \frac{1}{\Delta^2}(\varphi_{q,n+1} - \varphi_{q,n})^2 - m^2 \varphi_{q,n}^2 \right]$$
$$+ \frac{1}{2} \left[\dot{\varphi}_0^2 - \frac{1}{\Delta^2} \sum_q (\varphi_0 - \varphi_{q,1})^2 - m^2 \varphi_0^2 \right], \tag{31}$$

where Δ is the lattice constant.

Two remarks are of principal importance.

1. Lagrangian (31) describes a classical system, so there are no problems with the structure of space.

2. It describes a system with constraints. Indeed, the sites of oscillators on the plane are fixed by coordinates $q_n : x_{n_1} = n_1 \Delta$, $y_{n_2} = n_2 \Delta$, $z_{n_3} = n_3 \Delta$, so that $\varphi_{q,n}(t) = \varphi_{n_q \Delta}(t)$, i.e., they belong to the semi-infinite lines. Thus, the system can be described in the framework of Hamiltonian mechanics with constraints. It justifies the thin-tube approach [15–20] as a version of the thin-layer method [8].

Lagrangian (31) gives the following equations of motion:

$$\ddot{\varphi}_0 = \frac{1}{\Delta^2} \left(\sum_q \varphi_{q,1} - 3\varphi_0 \right) - m^2 \varphi_0, \tag{32}$$

$$\ddot{\varphi}_{q,1} = \frac{1}{\Delta^2}(\varphi_{q,2} + \varphi_0 - 2\varphi_{q,1}) - m^2 \varphi_{q,1}, \tag{33}$$

$$\ddot{\varphi}_{q,n} = \frac{1}{\Delta^2}(\varphi_{q,n+1} + \varphi_{q,n-1} - 2\varphi_{q,n}) - m^2 \varphi_{q,n}, \qquad n > 1. \tag{34}$$

Their solution

$$\varphi_{x,n}(t) = \mathrm{e}^{-\mathrm{i}(\omega_k t + kn\Delta)} + R(k)\,\mathrm{e}^{-\mathrm{i}(\omega_k t - k\Delta n)},$$
$$\varphi_{y,n}(t) = \varphi_{z,n}(t) = (1 + R(k))\,\mathrm{e}^{-\mathrm{i}(\omega_k t - kn\Delta)}, \tag{35}$$
$$\varphi_0(t) = (1 + R(k))\,\mathrm{e}^{-\mathrm{i}\omega_k t}$$

is analogous to (5). The normal frequencies

$$\omega_k^2 = \frac{4}{\Delta^2} \sin^2 \frac{k\Delta}{2} + m^2, \tag{36}$$

coincide with (6) in the limit $\Delta \to 0$.

Substituting (35) into (32) and taking into account the equation

$$\ddot{\varphi}_0 + m^2 \varphi_0 = -\frac{4}{\Delta^2} \sin^2 \frac{k\Delta}{2}(1 + R(k))\,\mathrm{e}^{-\mathrm{i}\omega_k t}, \tag{37}$$

we obtain

$$\left[4\sin^2 \frac{k\Delta}{2} + 3(\mathrm{e}^{\mathrm{i}k\Delta} - 1) \right](R(k) + 1) = 2\mathrm{i}\sin k\Delta. \tag{38}$$

Since $\mathrm{e}^{\mathrm{i}k\Delta} - 1 = 2\mathrm{i}\sin\frac{k\Delta}{2}\cos\frac{k\Delta}{2} - 2\sin^2\frac{k\Delta}{2}$ and $\sin k\Delta = 2\sin\frac{k\Delta}{2}\cos\frac{k\Delta}{2}$, equation (38) becomes

$$\left(3\mathrm{i}\cos\frac{k\Delta}{2} - \sin\frac{k\Delta}{2} \right)(R(k) + 1) = 2\mathrm{i}\cos\frac{k\Delta}{2}, \tag{39}$$

or

$$\mathrm{e}^{\mathrm{i}\theta(k)} = -\frac{\sin\frac{k\Delta}{2} + 3\mathrm{i}\cos\frac{k\Delta}{2}}{\sin\frac{k\Delta}{2} - 3\mathrm{i}\cos\frac{k\Delta}{2}}. \tag{40}$$

Using (8), in the limit $\Delta \to 0$, we obtain for $R(k)$ and $T(k)$ solution (29).

We conclude

1. The junction plays the role of a universal scatterer.

2. It appears that probabilities ($|R|^2 + 2|T|^2 = 1$ equation (7)). Thus, the formulation of CM (in particular, the Hamiltonian mechanics) not on a manifold demands introduction into the formalism of additional assumptions (characteristics of the scatterer) and presumably using the probability theory.

Acknowledgments

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