MATHEMATICAL QUANTIZATION OF
HAMILTONIAN FIELD THEORIES

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ABSTRACT. We define the renormalized evolution operator of the Schrödinger equation in the infinite dimensional Weyl–Moyal algebra during a time interval for a wide class of Hamiltonians depending on time. This leads to a mathematical definition of quantum field theory $S$-matrix and Green functions. We show that for renormalizable field theories, our theory yields the renormalized perturbation series of perturbative quantum field theory. All the results are based on the Feynman graph series technique.

INTRODUCTION

The purpose of this paper is to construct mathematical quantization of Hamiltonian field theories. The main new feature of the theory is that instead of the algebra of operators in the Fock space, we use the Weyl–Moyal algebra corresponding to the infinite dimensional Schwartz symplectic phase space. This allows one to avoid using perturbation theory in the defining constructions of the theory. The use of the Weyl–Moyal algebra has many conceptual and computational advantages, the physical output for the renormalizable case being the same as that of perturbative QFT. For example, it allows quantization on curved (space-like) surfaces and action of the group of diffeomorphisms of space-time, thus giving a natural background for great unification with general relativity. Note that in the framework of the Fock space, quantization on curved surfaces is impossible even for free scalar field for the space-time of dimension greater than two [5].

The starting points of this work were the author’s paper [1] and Connes–Kreimer’s paper [2]. With [2] it became clear that the problem posed in [1] should be corrected. It became clear that Connes–Kreimer’s construction leads to a non-perturbative treatment of the Feynman diagram series. In the present paper, we define, using the graph technique from [2], the renormalized evolution operator for the Schrödinger equation in the Weyl–Moyal algebra with almost arbitrary Hamiltonian during a time interval. This renormalized evolution operator is defined non-uniquely, it depends on regularization of the theory.
We also consider mathematical interaction representation which leads to a definition of mathematical quantum field theory $S$-matrix and Green functions. It is almost obvious that in the framework of perturbation theory, our theory yields the usual renormalized perturbation series of perturbative quantum field theory.

The paper is organized as follows. In §1 we study the evolution operator of the Schrödinger equation in the Weyl–Moyal algebra with a regularized Hamiltonian, and decompose it into a sum over Feynman graphs. In §2 we extend the summands of this sum for disjoint unions of tree graphs to certain class of non-regular Hamiltonians. In §3 we perform the renormalization procedure, essentially following [2], and define the renormalized evolution operator for non-regular Hamiltonians. In §4 we study the classical limit of this construction and show that it coincides with the classical Hamiltonian field theory. In §5 we study the mathematical interaction representation, and define a mathematical quantum field theory $S$-matrix and Green functions. We show that we obtain the renormalized perturbation series of perturbative QFT. Finally, §6 contains concluding remarks.

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1. THE WEYL–MOYAL ALGEBRA AND THE SchröDINGER EQUATION

Let $\mathcal{S}$ be the Schwartz topological vector space of real smooth functions $\varphi = \varphi(x)$, $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$, rapidly decreasing at infinity, and let $V = \mathcal{S} \times \mathcal{S}$ be the phase space with the standard symplectic form

$$\omega : V \otimes V \to \mathbb{R},$$

$$\omega((\varphi_1, \pi_1), (\varphi_2, \pi_2)) = \int (\pi_1(x)\varphi_2(x) - \varphi_1(x)\pi_2(x))dx.$$  

(In fact, one can start with an arbitrary symplectic real nuclear space, but we choose the space $V$ for concreteness.) The form (1) yields an inclusion of $V$ into the dual space $V''$ of distributions as a dense subspace. By a (polynomial) Hamiltonian we mean a polynomial continuous functional $H = H(\varphi, \pi)$ on the phase space $V$. The Hamiltonians form a commutative algebra, the topological symmetric algebra of the space $V'$, denoted by

$$SV' = \bigoplus_{n=0}^{\infty} S^n V'.$$
where $S^nV'$ is the $n$-th topological symmetric power of $V'$ (the space of Hamiltonians of degree $n$). The coefficient functions of a Hamiltonian of degree $n$ are symmetric distributions of several sets of variables $x_1, \ldots, x_n$. If all these distributions are smooth rapidly decreasing functions, then the Hamiltonian is called regular (or non-local). Regular Hamiltonians form the topological symmetric algebra of the space $V$, denoted by

$$SV = \bigoplus_{n=0}^{\infty} S^nV.$$ 

There are natural inclusions

$$S^nV \hookrightarrow S^nV', \quad SV \hookrightarrow SV'$$

as dense subspaces. These inclusions are induced by the form (1), as usual in polylinear algebra.

The space $SV$ of regular Hamiltonians has a structure of the Weyl–Moyal associative algebra which we now recall. To each classical regular Hamiltonian $H$ we assign an element $\hat{H}$ of the Weyl–Moyal algebra, which coincides with $SV$ as a vector space but with another product, the Moyal product, given by the formula

$$H_1 \ast H_2(\varphi, \pi) = \exp \frac{i\hbar}{2} \int \left( \frac{\delta}{\delta \varphi_1(x)} \frac{\delta}{\delta \varphi_2(x)} - \frac{\delta}{\delta \pi_1(x)} \frac{\delta}{\delta \pi_2(x)} \right) d\mathbf{x} \ H_1(\varphi_1, \pi_1)H_2(\varphi_2, \pi_2)|_{\varphi_1 = \varphi_2 = \varphi, \pi_1 = \pi_2 = \pi}.$$

A Hamiltonian field theory is given by a classical Hamiltonian $H(t)$ depending on time $t$. Assume first that $H(t)$ is regular. Consider the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}(t)\Psi,$$

where $\Psi = \Psi(t)$ is an element of an arbitrary vector space on which the Weyl–Moyal algebra acts (the concrete choice of this space is inessential here, for example, one can take as this space the Weyl–Moyal algebra itself). We are interested in the formula for the evolution operator $U = U(T_0, T_1)$ of the Schrödinger equation from the (fixed) time $t = T_0$ to the (fixed) time $t = T_1$. This evolution operator is given by the well known time ordered exponent

$$U = T \exp \int_{T_0}^{T_1} \frac{1}{i\hbar} \hat{H}(t) \, dt$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!(i\hbar)^k} \int_{T_0 \leq t_1 \leq \cdots \leq t_k \leq T_1} T \hat{H}(t_1) \ast \cdots \ast \hat{H}(t_k) dt_1 \ldots dt_k.$$
Here $T \hat{H}(t_1) \ast \ldots \ast \hat{H}(t_k)$ denotes the chronologically ordered product, i. e., the product of $\hat{H}(t_i)$ in the decreasing order of time moments $t_i$.

Let us decompose this formula in terms of the homogeneous components of the Hamiltonians $H(t)$. It is easy to see that this formula is a sum over the Feynman graphs of certain integrals. We consider graphs $\Gamma$ with several vertices, joined by edges. An edge can join two vertices (internal edge) or go from outside to a vertex (external edge). Multiple edges between two vertices (or from outside to a vertex) are allowed. To each such graph with $k$ vertices one assigns a summand in the sum (5) as follows. We mark the vertices of the graph by numbers $1, \ldots, k$ (the corresponding summand of the sum (5) will not depend on this numeration). Further, to a vertex $i$ we assign the homogeneous component $\hat{H}_{n_i}(t_i) \in S_{n_i}V$, where $n_i$ is the number of edges (internal and external) going to the $i$-th vertex. We obtain a tensor in $S^{n_1}V \otimes \ldots \otimes S^{n_k}V$. To each internal line joining the vertices $i$ and $j$ we assign a contraction of tensors $\hat{H}_{n_i}(t_i)$ and $\hat{H}_{n_j}(t_j)$ using the form (1), the first tensor being the one with the greater time, and the second tensor being the one with the lower time. Finally, we multiply all the obtained tensors in the symmetric algebra $SV$, integrate them over $t_1, \ldots, t_k$, and assign certain coefficient to this integral, responsible for the combinatorics of the graph and for the power of $ih$. We obtain a summand, denoted by $U(\Gamma) \in SV$, in the sum (5), so that

$$U = \sum_{\Gamma} U(\Gamma). \tag{6}$$

2. THE FADDEEV–TAKHTAJAN ALGEBRA

In the usual classical field theories, the Hamiltonian $H(t)$ is non-regular, $H(t) \in SV'$. The question is how to extend the definition of the evolution operator $U$ to this case. The direct extension of the procedure above fails, since the integrals in the product formula for the Weyl–Moyal algebra are not defined for irregular Hamiltonians. Equivalently, the integrals in the graph series are not defined since they contain pairings of distributions.

To overcome this difficulty, we first solve this problem for forest graphs, i. e. graphs without loops, or, in other words, disjoint unions of tree graphs. To this end, let us first specify the class of classical Hamiltonians considered. This class of Hamiltonians in $SV'$ was discovered by Faddeev and Takhtajan [3] and rediscovered by the author [1], and they form a Poisson algebra extending the Poisson algebra of
regular Hamiltonians $SV$ with the Poisson bracket

\[
\{H_1, H_2\} = \int \left( \frac{\delta H_1}{\delta \pi(x)} \frac{\delta H_2}{\delta \varphi(x)} - \frac{\delta H_1}{\delta \varphi(x)} \frac{\delta H_2}{\delta \pi(x)} \right) dx.
\]

We call this extended Poisson algebra by the *Faddeev–Takhtajan algebra* and denote it by $\mathcal{FT}$. Let us describe it.

By definition, a Hamiltonian $H = H(\varphi, \pi) \in SV'$ belongs to $\mathcal{FT}$ if and only if it generates a well defined analytical Hamiltonian flow on the phase space $V = S \times S$. This means that the functional derivatives $(\delta H/\delta \varphi(x), \delta H/\delta \pi(x))$ belong to $S \times S \subset V'$ for any $(\varphi, \pi) \in V$, and, moreover, the map

\[
V \to V, \ (\varphi, \pi) \mapsto (\delta H(\varphi, \pi)/\delta \varphi(x), \delta H(\varphi, \pi)/\delta \pi(x))
\]

is analytic. In the language of homogeneous components $H_n \in S^n V'$, this means that

\[
H_n \in S^n V' \cap \text{Hom}(V \otimes \ldots \otimes V, V).
\]

It is easy to check that the usual Hamiltonians of field theory, namely, integrals over $x$ of densities smoothly depending on $x$ and polynomially depending on $\varphi(x), \pi(x)$ and their derivatives, belong to $\mathcal{FT}$.

It is also easy to check that $\mathcal{FT}$ is closed under the usual multiplication and under the Poisson bracket (7). Moreover, for any forest graph $\Gamma$ and for the Hamiltonian $H(t) \in \mathcal{FT}$, the corresponding element $U(\Gamma) \in \mathcal{FT}$ is well defined by continuity.

From now on we assume that our Hamiltonians $H(t)$ belong to $\mathcal{FT}$.

3. Renormalization and the Hopf algebra of graphs

Let us pass to the problem for general graphs $\Gamma$. Let us regularize the Hamiltonian $H(t)$, i.e., replace it by a regular Hamiltonian $H_\varepsilon(t) \in SV$ where $\varepsilon$ is the regularization parameter, $\varepsilon > 0$, so that $H_\varepsilon(t) \to H(t)$ as $\varepsilon \to 0$. The corresponding element $U_\varepsilon$ is well defined for nonzero $\varepsilon$, but diverges as $\varepsilon \to 0$. The main assumption on the Hamiltonian and the regularization that we make is that for any graph $\Gamma$ the divergent part $T(U_\varepsilon(\Gamma))$ of $U_\varepsilon(\Gamma)$ is a polynomial in $\varepsilon^{-1}$ and $\log \varepsilon$ without constant term. This is a usual situation for not very pathological Hamiltonians and regularizations. Thus, $U_\varepsilon(\Gamma)$ belongs to the algebra $SV \otimes \mathcal{A}$, where $\mathcal{A} = \mathbb{C}[[\varepsilon, \varepsilon^{-1}, \log \varepsilon]]$. This algebra decomposes into the direct sum of two subalgebras $\mathcal{A} = \mathcal{A}_+ \oplus \mathcal{A}_-$, where $\mathcal{A}_+ = \mathbb{C}[[\varepsilon]]$ and $\mathcal{A}_- = \varepsilon^{-1}\mathbb{C}[\varepsilon^{-1}, \log \varepsilon] + \log \varepsilon \mathbb{C}[\varepsilon^{-1}, \log \varepsilon]$. Denote by $T : \mathcal{A} \to \mathcal{A}_-$ the projector map with the kernel $\mathcal{A}_+$ (the singular part of a series).
Now we apply the usual renormalization procedure of extracting finite values to $U_\varepsilon(\Gamma)$ as in [2].

Denote by $\mathcal{H}$ the complex vector space with the basis consisting of all graphs $\Gamma$. The space $\mathcal{H}$ has a commutative multiplication defined by disjoint union of graphs,

$$\Gamma \Gamma' = \Gamma \cup \Gamma'.$$

It also has a less obvious coproduct $\Delta : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$ defined as

$$\Delta(\Gamma) = \sum_{\gamma \subset \Gamma} \tilde{\gamma} \otimes \Gamma/\tilde{\gamma}.$$

Here the notation is as follows. $\gamma \subset \Gamma$ is a full subgraph of $\Gamma$ (possibly empty, $\gamma = \Gamma_\emptyset = 1$, or full, $\gamma = \Gamma$), i.e. the vertices of $\gamma$ are a subset of the set of vertices of $\Gamma$, and the edges of $\gamma$ are the external or internal edges of $\Gamma$ which meet at least one vertex of $\gamma$. This subgraph $\gamma$ can be uniquely decomposed into a forest graph whose “vertices” are either one-vertex graphs or one-particle irreducible (1PI) full subgraphs (i.e. connected graphs with more than one vertex which remain connected after removing any one edge). Then $\tilde{\gamma}$ is defined as the disjoint union of these 1PI full subgraphs. Further, $\Gamma/\tilde{\gamma}$ is defined as the quotient graph of $\Gamma$ by $\tilde{\gamma}$, i.e. each connected component of $\tilde{\gamma}$ is contracted in $\Gamma/\tilde{\gamma}$ to the subgraph with a single vertex whose edges are identified with the external edges of this connected component of $\tilde{\gamma}$.

A bialgebra very close to our bialgebra $\mathcal{H}$ appears in [2] under the name $\mathcal{H}_c$. In loc. cit. it is proven that $\mathcal{H}_c$ is actually a Hopf algebra. This proof transfers without difficulties to our bialgebra $\mathcal{H}$, so it is also a bigraded Hopf algebra. Details concerning the Hopf algebra $\mathcal{H}_c$, in particular the bigrading, the recursive formula for antipode, and examples of coproducts, see in loc. cit.

Now, exactly as in [2], we define the counterterms $C(\Gamma)$ and the Bogoliubov–Parasiuk–Hepp $R$-operation $R(\Gamma)$ by the following recursive formulas. We denote by $U : \mathcal{H} \to SV \otimes \mathcal{A}$ the linear map given by $U(\Gamma) = U_\varepsilon(\Gamma)$. It is easy to check that $U$ is a homomorphism of algebras. Further, for forest graphs $\Gamma$, put $C(\Gamma) = 0$, $R(\Gamma) = U(\Gamma)$. For 1PI graphs $\Gamma$ without proper 1PI subgraphs, we put

$$C(\Gamma) = -T(U(\Gamma))$$

and

$$R(\Gamma) = U(\Gamma) + C(\Gamma).$$

For general graphs $\Gamma$ we put

$$C(\Gamma) = -T(\overline{R}(\Gamma)).$$
\( R(\Gamma) = \overline{R}(\Gamma) - T(\overline{R}(\Gamma)) \)

where the \( \overline{R} \)-operation is defined by the recursive formula
\[
\overline{R}(\Gamma) = U(\Gamma) + \sum_{\gamma \subset \Gamma, \gamma \neq \Gamma} C(\tilde{\gamma}) U(\Gamma/\tilde{\gamma})
\]
in the notation (11).

Exactly as in [2], one shows that the counterterm operation \( C(\Gamma) \) and the \( R \)-operation \( R(\Gamma) \) can be extended to homomorphisms of algebras (characters)
\[
C : \mathcal{H} \to SV' \otimes A_-, \quad R : \mathcal{H} \to SV' \otimes A_+;
\]
here \( \mathcal{H} = \text{Ker} \varpi \) is the augmentation ideal in \( \mathcal{H} \), where \( \varpi(\Gamma_0) = 1 \), \( \varpi(\Gamma) = 0 \) for \( \Gamma \neq \Gamma_0 \). Moreover, these maps satisfy the relation
\[
R(X) = (C \star U)(X),
\]
where
\[
(C \star U)(X) = \langle C \otimes U, \Delta(X) \rangle
\]
is the multiplication in the Lie group of characters of \( \mathcal{H} \), whose universal enveloping algebra is the dual to the Hopf algebra \( \mathcal{H} \), by the Milnor–Moore theorem.

**Definition.** The element
\[
\hat{U} = \sum_{\Gamma} R(\Gamma)|_{\varepsilon=0}
\]
is called the renormalized evolution operator corresponding to the interval \([T_0, T_1]\) of time.

Note that all the constructions of this paper are \( \text{Sp}(V) \)-invariant, where \( \text{Sp}(V) \) is the symplectic group of the space \( V \) corresponding to the form (1).

### 4. The classical limit

To study the classical limit \( \hbar \to 0 \), let us first assume that the Hamiltonian \( H(t) \) is regular. Consider the Heisenberg equation for an element \( \hat{F}(t) \in SV' \),
\[
\hbar \frac{\partial \hat{F}}{\partial t} = [\hat{H}(t), \hat{F}] \overset{\text{def}}{=} \hat{H}(t) \ast \hat{F} - \hat{F} \ast \hat{H}(t).
\]
The evolution operator of this equation from the time \( T_0 \) to the time \( T_1 \) is an automorphism of the Weyl–Moyal algebra given by conjugation
by $U$, where $U \in SV$ is the element (5). By formula (3) for the Moyal product, the classical limit of equation (21) is the Hamilton equation

\[ \frac{\partial F}{\partial t} = \{ H(t), F \}. \]

One checks that the evolution operator of this equation is an automorphism of Poisson algebras $SV \rightarrow SV$, which corresponds to certain sum over forest graphs. One checks that renormalization does not affect this result.

By continuity, all these results on the classical limit hold with $SV$ replaced by $FT$, since the corresponding notions for $FT$ make sense, according to the results on $FT$ in §2. Hence, for $H(t) \in FT$, the classical limit is the theory of equation (22) equivalent to the canonical Hamilton equations, i.e. the classical Hamiltonian field theory, as required.

5. The interaction representation and the $S$-matrix

In this Section we consider standard field theory Hamiltonians of a real scalar field

\[ H(t, \varphi, \pi) = H_0(t, \varphi, \pi) + H_1(t, \varphi, \pi), \]

where $H_0$ is a quadratic Hamiltonian from $FT$, namely,

\[ H_0 = \int \frac{1}{2} \left( \pi(x)^2 + \sum_{i=1}^{d} \left( \frac{\partial \varphi}{\partial x_i} \right)^2 + m^2 \varphi(x)^2 \right) dx, \]

and

\[ H_1(t, \varphi, \pi) = \int V(t, x, \varphi(x)) dx \in FT \]

is the interaction potential. It is easy to see that the quadratic Hamiltonians from $FT$ form the Lie algebra of the symplectic group $Sp(V)$, and generate (in both the classical and the quantum case) the action of this group on $SV'$. In particular, the evolution operator for the Hamiltonian $H_0$ from $t = T_0$ to $t = T_1$ yields the action of the symplectic transformation which takes the Cauchy data $(\varphi(x), \pi(x) = \partial \varphi/\partial t)$ of the Klein–Gordon equation

\[ \frac{\partial^2 \varphi}{\partial t^2} - \sum_{i=1}^{d} \frac{\partial^2 \varphi}{\partial x_i^2} + m^2 \varphi = 0 \]

for a function $\varphi(t, x)$ at the time $t = T_0$ to the Cauchy data at $t = T_1$.

Since all the constructions of the preceding Sections are $Sp(V)$-invariant, it is now natural to go to the interaction representation,
i. e. replace the symplectic vector space $V = S \times S$ by the isomorphic symplectic vector space $W$ of smooth solutions $\varphi = \varphi(t, x)$ of the Klein–Gordon equation (26) rapidly decreasing at infinity in the space directions. The isomorphism between $V$ and $W$ is given by taking the Cauchy data at an arbitrary moment of time.

Under this isomorphism, the Hamiltonian (23) goes to the interaction Hamiltonian

$$\tilde{H}_1(t, \varphi) = \int V(t, x, \varphi(t, x)) dx \in SW'.$$

It is also useful to make Fourier transform and to pass to the symplectic space $\tilde{W}$ of functions $\tilde{\varphi}(p)$, $p = (p_0, \ldots, p_d)$ on mass shell

$$p^2 \equiv p_0^2 - \sum_{i=1}^{d} p_i^2 = m^2$$

in the space of momenta $p \in \mathbb{R}^{1+d}$.

The corresponding renormalized evolution operator

$$\tilde{U} = \tilde{U}(-\infty, \infty) \in S\tilde{W}'$$

from $T_0 = -\infty$ to $T_1 = \infty$, defined according to §3, is called the mathematical $S$-matrix. The constant term $Z$ of $\tilde{U}$ is called the statistical sum of the theory, or the generating functional of Green functions, if the Hamiltonian (27) contains the summand

$$\int j(t, x) \varphi(t, x) dx$$

and $Z = Z(j)$ is decomposed into the power series with respect to the function $j$. The coefficient functions of this power series are called the Green functions of the theory.

It is almost obvious that these quantities, decomposed into perturbation series in powers of the Hamiltonian (27), coincide with the renormalized perturbation series for the $S$-matrix and Green functions of perturbative quantum field theory. Indeed, the Weyl–Moyal algebra $SW$ naturally acts on the Fock space. A non-regular Hamiltonian (27) differs from the normally ordered Hamiltonian in the Fock space by a sum of normally ordered terms of lower degree with divergent coefficients. Thus, in order to obtain the perturbative $S$-matrix and Green functions in the Fock space, it suffices to make an additional renormalization involving these counterterms.
6. Concluding remarks

1) **Fermions.** The constructions of the paper are literally generalized to the case of fermionic fields. Instead of a symplectic nuclear vector space $V$, one considers a nuclear space with a symmetric non-degenerate bilinear form, and instead of the symmetric algebra $S V$, one considers the exterior algebra $\Lambda V$. Instead of the symplectic group $\text{Sp}(V)$, one considers the orthogonal group $O(V)$. The rest is essentially the same.

2) **Inner symmetries.** The constructions are compatible with symmetries from affine symplectic (resp. orthogonal) group.

3) **Quantization on curved surfaces and general relativistic invariance.** Our constructions also yield what is called quantization on curved surfaces. The generally covariant Hamiltonian formalism for curved surfaces corresponding to a field theory given by a variational principle, is contained in [1,4]. According to this formalism, the space $V$ is identified with the phase space of classical field theory on a parameterized curved (space-like) surface in space-time. The evolution of parameterized curved surface yields a Hamiltonian flow on the phase spaces of surfaces. This Hamiltonian flow is integrable, i.e., the result of evolution does not depend on the evolution itself but only on the initial and final surfaces. The question is whether the corresponding renormalized quantum evolution operator is integrable. This directly leads to the problem of mathematical unification of quantum field theory with general relativity.

4) **Some open questions.** First of all, it is unclear how strongly the mathematical renormalized $S$-matrix depends on a regularization (at least for renormalizable theories). Secondly, one would like to state general principles (like Bogoliubov or Wightman axioms) that this construction satisfies. These two problems are closely related. One more problem is the behavior of the mathematical $S$-matrix (or Green functions) under diffeomorphisms of space-time and other possible transformations, like gauge symmetries (local affine symplectic transformations depending on time). Finally, a general problem is to take into account locality of the Hamiltonians in space-time, and to state the main principles of the theory in a local form in space-time.

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