Covariant canonical quantization

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Received: 7 April 2006 / Published online: 27 June 2006 – © Springer-Verlag / Società Italiana di Fisica 2006

Abstract. We present a manifestly covariant quantization procedure based on the de Donder–Weyl Hamiltonian formulation of classical field theory. This procedure agrees with conventional canonical quantization only if the parameter space is d = 1 dimensional time. In d > 1 quantization requires a fundamental length scale, and any bosonic field generates a spinorial wave function, leading to the purely quantum-theoretical emergence of spinors as a byproduct. We provide a probabilistic interpretation of the wave functions for the fields, and we apply the formalism to a number of simple examples. These show that covariant canonical quantization produces both the Klein–Gordon and the Dirac equation, while also predicting the existence of discrete towers of identically charged fermions with different masses. Covariant canonical quantization can thus be understood as a "first" or pre-quantization within the framework of conventional QFT.

PACS. 04.62.+v; 11.10.Ef; 12.10.Kt

1 Introduction

The apparent incompatibility between general relativity and quantum mechanics has long been a topic of concern and interest in the theoretical physics community. Diffeomorphism invariance has to be satisfied on the side of a general relativistic theory, in particular denying any fundamental distinction between the notions of space and time; but it is less clear how to achieve this requirement in, or properly translate it to, a quantum theory. This particularly applies to the canonical formulation of quantum mechanics and quantum field theory based on a Hamiltonian treatment. A neat way around this problem may be seen in path integral quantization which explains why the predictions of the quantized theory still possess the relativistic symmetries of the classical theory; but from the Hamiltonian point of view with its explicit space-time split this is not a special merit of the quantization procedure. This motivates the question whether there is a covariant extension of Hamiltonian methods which also allows for a manifestly covariant quantization procedure.

On the level of classical field theory there is indeed a Hamiltonian formulation that does not rely on singling out a time coordinate but treats all spacetime coordinates equally throughout. This theory was presented already in the nineteen-thirties by de Donder [1] and Weyl [2]. Full covariance is maintained through the use of multi-momenta, where one momentum is associated to each partial deriva-

tive of the fields. While providing a fully covariant equivalent to the standard Hamiltonian formulation of field theory (in the sense of providing the same solutions), the de Donder-Weyl formulation of classical dynamics has not received too much attention. Only recently have there been several attempts to quantize field theories on its basis. An early attempt by Good [3, 4] has been shown to disagree with ordinary quantum mechanics and to give incorrect predictions for the hydrogen spectrum [5]. Subsequently, a quantum equation based on de Donder-Weyl theory has been conjectured by Kanatchikov [6] and Navarro [7]. There have also been attempts to obtain a path integral formulation [8–10] and a version of Bohmian mechanics [11, 12] based on de Donder–Weyl dynamics. Other recent applications of the de Donder-Weyl formulation of field theory include a derivation of the Ashtekar-Wheeler-DeWitt equation of canonical quantum gravity [13].

In this paper, after a brief review of some of the elements of the classical de Donder–Weyl theory in Sect. 2, we will formulate a covariant Poisson bracket. In Sect. 3 we will then proceed to apply the Dirac quantization postulate to the latter. If supplemented with a second, geometrically motivated, quantization postulate, this leads to the same quantum evolution equation that had previously been conjectured on the basis of analogies [7, 14]. Our approach for the first time presents a derivation of this equation, which unifies both the Schrödinger and the Dirac equation, from first principles. We go on to develop the quantum theory in the covariant Schrödinger picture; in particular, we will discuss the representation of operators, the consequences of an indefinite scalar product on the Hilbert

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space which immediately follows from the requirements of covariance, and the probability interpretation of the wave functions. We apply the theory to a number of basic problems in Sect. 4, with sometimes surprising results.

Among them are a new derivation of the Klein–Gordon equation that makes no use of the relativistic energymomentum relation, the emergence of spinors from the quantization of scalar theories, and in particular the emergence of the Dirac equation from the quantization of any scalar field action. This means that the quantization procedure here presented does not replace quantum field theory; instead, it is found to provide a supplementary "first quantization." A result of potential phenomenological interest is the prediction of towers of identically charged fermions that differ only by their masses, providing a qualitative explanation for the generations in the standard model.

2 Covariant Hamiltonians in classical field theory

This section reviews the covariant Hamiltonian treatment of classical field theories, discussed first by de Donder and Weyl [1, 2], which is based on the introduction of multimomenta associated to the partial derivatives of the fields. We then define a new covariant Poisson bracket to rewrite the general phase space evolution equations in an equivalent form suitable for quantization.

2.1 Field theory in the multi-symplectic formalism

Consider a geometrically well-defined field theory which is diffeomorphism invariant on a *d*-dimensional Lorentzian background manifold Σ . We will call this background manifold the parameter space of the theory, coordinatized by parameters $\{\sigma^a\}$ with corresponding partial derivatives $\partial_a = \partial/\partial \sigma^a$. Classical fields q^i are functions on this manifold, i.e.,

$$q^i: \Sigma \to \mathbb{R} \,. \tag{1}$$

In some theories it is convenient to consider a set of n fields $\{q^i\}$ as coordinates of a second, n-dimensional, target space manifold M; in this case, requiring the theory to be geometrically well-defined means it should obey the further diffeomorphism invariance on M. The notion of a target space manifold is, however, secondary. We define the theory on Σ by its action, which is obtained from the integration over Σ of a scalar Lagrangian as follows:

$$S = \int_{\Sigma} \mathrm{d}^d \sigma \sqrt{-g} \, L\left(q^i, \nabla_a q^j\right) \,. \tag{2}$$

Note that the standard quadratic kinetic term in the Lagrangian depends on $\nabla_a q^i$. Forming a scalar from these (covariant) derivatives necessitates the existence of a nondegenerate, and hence invertible, metric g on Σ , the signature of which we take to be $(-, +, \ldots, +)$. The determinant of this metric appears in the integration measure. An explicit dependence of L on the coordinates of Σ is excluded by the requirement of diffeomorphism invariance.

The equations of motion of the theory (2) are the Euler– Lagrange equations derived by variation of the action with respect to the fields,

$$\nabla_a \frac{\partial L}{\partial \nabla_a q^i} - \frac{\partial L}{\partial q^i} = 0, \qquad (3)$$

where the covariant derivative involves the unique torsion free and metric compatible Levi–Civita connection of g. The necessary boundary condition requires a vanishing integral,

$$\int_{\partial \Sigma} \mathrm{d}S^a \frac{\partial L}{\partial \nabla_a q^i} \delta q^i = 0.$$
⁽⁴⁾

The above equations of motion are partial differential equations of second order, for first order Lagrangians. To reduce the order, the standard Hamiltonian treatment introduces canonical momenta $p_i = \partial L/\partial \partial_0 q^i$. Clearly, these momenta are non-covariant quantities, as their definition explicitly depends on the choice of time and hence on the choice of coordinate system on Σ . It follows that the usual Hamiltonian function, depending on the non-covariant canonical momenta, cannot be a scalar.

To remedy this apparent difficulty, we introduce the manifestly covariant multi-momenta associated to each partial derivative of the fields,

$$p_i^a = \frac{\partial L}{\partial \nabla_a q^i} \,, \tag{5}$$

which transform as the components of a vector in the parameter space tangent bundle $T\Sigma$ (and as those of a differential form in T^*M , if the fields form coordinates of a target space manifold). We assume Lagrangians such that the multi-momenta as functions of the fields and their partial derivatives may be solved for these derivatives to yield $\nabla_a q^i \left(q^j, p_k^b\right)$. In terms of the new covariant momenta, we may then also define the covariant Hamiltonian

$$H = p_i^a \nabla_a q^i - L \,, \tag{6}$$

which is a function of the new independent variables q^i and p_i^a and transforms as a diffeomorphism scalar on the parameter space Σ .

The Euler–Lagrange equations imply the covariant Hamiltonian equations

$$\frac{\partial H}{\partial q^i} = -\nabla_a \ p_i^a \,, \tag{7a}$$

$$\frac{\partial H}{\partial p_i^a} = \nabla_a \ q^i \,. \tag{7b}$$

Conversely, given a covariant Hamiltonian $H(q^i, p_j^a)$, we may define a Lagrangian $L(q^i, \nabla_a q^j)$ via (6). Then the covariant Hamiltonian equations imply the Euler-Lagrange equations. Diffeomorphism invariance again implies that the Hamiltonian cannot depend explicitly on the coordinates of Σ . Below we will see that the covariant Hamiltonian formalism nicely reduces to conventional Hamiltonian mechanics if the parameter space Σ is one-dimensional.

2.2 The classical Dirac field as an example

As an example for the powerful finite-dimensional phase space formalism of de Donder and Weyl, we take a brief look at the massive Dirac field. The Lagrangian in its symmetrical form is given by

$$L = \frac{1}{2}\bar{\psi}\gamma^a \nabla_a \psi - \frac{1}{2}\nabla_a \bar{\psi}\gamma^a \psi - M\bar{\psi}\psi, \qquad (8)$$

where we have introduced the Dirac matrices γ^a of the (curved) background, on which we will comment in more detail below. We treat ψ and $\bar{\psi}$ as independent, so that the conjugate covariant momenta follow by definition as

$$\pi^a_{\psi} = \frac{1}{2}\bar{\psi}\gamma^a \,, \qquad \pi^a_{\bar{\psi}} = -\frac{1}{2}\gamma^a\psi \,. \tag{9}$$

These relations are, in fact, primary constraints, relating the spinors and their conjugate momenta. Although these momenta are not invertible to obtain $\nabla_a \psi(\psi, \bar{\psi}, \pi_{\psi}^b, \pi_{\bar{\psi}}^c)$, and similarly $\nabla_a \bar{\psi}$, we can define the covariant Hamiltonian as

$$H = M\bar{\psi}\psi + \left(\pi_{\psi}^{a} - \bar{\psi}\gamma^{a}/2\right)\lambda_{a} + \bar{\lambda}_{a}\left(\pi_{\bar{\psi}}^{a} + \gamma^{a}\psi/2\right), \quad (10)$$

where the constraints have been added with the help of spinorial Lagrange multipliers λ_a and $\bar{\lambda}_a$. The Dirac equation and its conjugate now follow immediately from the covariant Hamiltonian equations (7) above, utilizing the constraint equations.

2.3 Definition of a covariant Poisson bracket

With the aim of facilitating an easier transition to a quantum theory, we consider Poisson brackets in the new formalism. A covariant extension of the standard Poisson bracket is given by the definition

$$\{f,g\}_a = \frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p^a_i} - \frac{\partial f}{\partial p^a_i} \frac{\partial g}{\partial q^i} \tag{11}$$

for any two phase space functions f and g depending on the Hamiltonian variables q^i and p_i^a . This bracket carries a further index, thus mapping two functions of the canonical variables to a differential form in $T^*\Sigma$. In general, it changes the number of indices and with it the tensor structure defined by its arguments. This obstructs the usefulness of this bracket definition, as valuable properties of the Poisson bracket are lost. This applies in particular to the important Jacobi identity, which provides the algebra of phase space functions with the structure of a Lie algebra. Here the Jacobi identity is valid only for equal subscripts, i.e., for expressions of the form $\{\{f,g\}_a,h\}_a$, but these are not allowed as tensors on Σ . Hence we are led to amending the bracket definition and consider brackets of the form

$$\{f,g\} = \{f,g\}_a t^a , \qquad (12)$$

where we introduce an arbitrary vector field in $T\Sigma$ with components t^a , the origin of which we will discuss in the following section on quantization. The only classical requirement that we will make on this field concerns its normalization $N(d) = g_{ab}t^at^b$ which may depend on the dimension of the parameter spacetime Σ . It should be such that N(1) = -1 so that the usual Poisson bracket may emerge when d = 1 with $g_{\sigma\sigma} = -1$. It turns out that the bracket so defined satisfies the formal algebraic properties of the Poisson bracket, which we state for phase space functions f and g and real numbers c (for other definitions of Poisson brackets within the de Donder–Weyl formalism, compare [15–17]).

The Poisson bracket is antisymmetric and annihilates constants,

$$\{f, g\} = -\{g, f\},$$
(13a)

$$\{f, c\} = 0;$$
 (13b)

it is \mathbb{R} -linear in f and g (where linearity in the second argument follows by antisymmetry),

$$\{f_1 + f_2, g\} = \{f_1, g\} + \{f_2, g\}, \qquad (14a)$$

$$\{cf, g\} = c\{f, g\};$$
 (14b)

the Poisson bracket further satisfies a product rule and, importantly, the Jacobi identity:

$$\{f_1 f_2, g\} = \{f_1, g\} f_2 + f_1 \{f_2, g\},$$
(15a)

$$\{\{f,g\},h\} + \{\{g,h\},f\} + \{\{h,f\},g\} = 0.$$
 (15b)

The introduction of the vector field t^a provides another advantage, again with a view towards quantization: it allows us to achieve a one to one correspondence between the fields q^i and the contracted multi-momenta $p_i = -t_a p_i^a$. We find the covariant Poisson brackets

$$\left\{q^{i}, q^{j}\right\} = 0, \qquad (16a)$$

$$\{p_i, p_j\} = 0,$$
 (16b)

$$\left\{q^{i}, p_{i}\right\} = -N(d)\delta^{i}_{i}.$$
(16c)

Brackets including the covariant Hamiltonian generate the following expressions, similar to those appearing in the covariant Hamiltonian equations of motion (7); the fact that there is no precise agreement is due to the appearance of the vector field t^a :

$$\left\{q^i, H\right\} = t^a \nabla_a q^i \,, \tag{17a}$$

$$\{p_i, H\} = -N(d)\nabla_a p_i^a \,. \tag{17b}$$

These brackets are useful in evaluating the evolution equation for phase space functions with respect to the parameters given by the coordinates of Σ . We calculate

$$\{f,H\} = \frac{\partial f}{\partial q^i} t^a \nabla_a q^i + \frac{\partial f}{\partial p^a_i} t^a \nabla_b p^b_i, \qquad (18)$$

which may be rewritten as

$$t^{a}\nabla_{a}f - \{f, H\} - t^{a}\nabla_{a}^{0}f = \frac{\partial f}{\partial p_{i}^{b}} \left(t^{a}\nabla_{a}p_{i}^{b} - \{p_{i}^{b}, H\}\right) .$$

$$(19)$$

This is the form of the general evolution equation which we will use as an important ingredient of the quantization procedure. Note that the parameter space derivatives of the phase space function f are evaluated along the integral curves of the vector field t^a . The derivative operator ∇_a^0 acts only on the σ^a -dependence of f not coming in through the coordinates and momenta. A closer inspection of the equation also reveals that it is trivially satisfied for any phase space function linear in the momenta, e.g., for p_i^a or $t_a p_i^a$. This means we have to supplement it with (17b).

2.4 Hamiltonian mechanics on one-dimensional Σ

The results and constructions above are in complete analogy to the standard Hamiltonian treatment of classical mechanics which is, however, restricted to a one-dimensional parameter space Σ , with time coordinate σ , if diffeomorphism invariance is required.

The Hamiltonian formalism of de Donder and Weyl reduces to the standard one for d = 1. To see this more explicitly, note that the $T\Sigma$ index a of the multi-momentum p_i^a can merely take a single value in this case corresponding to the single coordinate σ on Σ , which may be suppressed. The manifold, its tangent and cotangent spaces are all locally isomorphic to the real numbers. The normalization requirement for the single-component vector field enforces $t^{\sigma} = 1$ because of our signature convention $g_{\sigma\sigma} = -1$. Thus we obtain agreement between our covariant Poisson bracket and the standard one. The equations (16) reduce to the canonical Poisson brackets, and (17) become equivalent to the Hamiltonian equations. The right hand side of the phase space evolution equation (19) cancels; what remains is the well-known time evolution formula

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}f - \{f, H\} - \frac{\partial}{\partial\sigma}f = 0.$$
(20)

3 Covariant canonical quantization

Following Dirac, the quantization of a system in classical mechanics takes as its starting point the Hamiltonian formulation. The canonical variables are promoted to operators acting on a Hilbert space, and the Poisson brackets to commutators. With our new covariant Hamiltonian formalism, we will now mimic these steps.

3.1 Quantization postulates

As the bracket $\{f, g\}$ that we have defined above has the same algebraic properties as the Poisson bracket, we promote it to a commutator of operators in exactly the same way,

$$\{f,g\} \quad \mapsto \quad -\mathrm{i}l^{d-1}[\hat{f},\hat{g}]. \tag{21}$$

According to a famous argument of Dirac [18], this is in fact the only consistent quantization postulate, if the quantum bracket is required to preserve its classical algebraic properties. Phase space functions f and g have been replaced by operators on some Hilbert space, denoted by a hat. The imaginary unit is required to imply that $-i[\cdot, \cdot]$ is self-adjoint for self-adjoint entries (with respect to the Hilbert space inner product which we will define below). In our units, where c = 1 and $\hbar = 1$, we have to introduce another independent length scale l, which we might choose to be the Planck length $l_{\rm P}$, to compensate the dimensions of the derivatives with respect to the canonical variables that appear in our Poisson bracket. This result does not depend on the dimension of the fields q^i ; it merely assumes the dimension of the Lagrangian L is $(length)^{-d}$. Note that the necessity of a fundamental length scale for quantization appears only on manifolds Σ of dimension d > 1.

Now we have to think about the vector field t^a in our bracket definition. The obvious choice seems to be a classical timelike vector field on Σ , with normalization N(d) = -1 for any dimension. However, this would have several undesirable consequences; firstly, no such vector field was included in the classical theory in the original formulation (2). Thus additional input would be necessary for the quantum theory. Such input would not be universal in the sense that the chosen timelike field could differ for different quantum systems under consideration. Secondly, this would amount to introducing a space-time split of Σ into the product of a family of timelike curves and their corresponding normal surfaces, thereby introducing all of the problems associated with the canonical procedure. Thus the aim of an intrinsically higher-dimensional quantization procedure on Σ would be lost. But what options are left now of choosing a vector field which is implicitly given on any Σ ?

To answer this question, we have to resort to some more geometry. On every curved background manifold Σ (admitting a spin structure) exists an algebra of Dirac matrices γ_a with the property that

$$\gamma_a \gamma_b + \gamma_b \gamma_a = 2g_{ab} \,. \tag{22}$$

As usual, these Dirac matrices are related to those of the local Lorentzian tangent spaces Γ_{μ} by the vielbeins e_{a}^{μ} as $\gamma_{a} = e_{a}^{\mu}\Gamma_{\mu}$. The vielbeins form the metric as $g_{ab} = e_{a}^{\mu}e_{b}^{\nu}\eta_{\mu\nu}$. The normalization of the Dirac matrices gives $\gamma_{a}\gamma^{a} = d$. This leads us to propose the following quantization postulate for the vector field t^{a} :

$$t^a \mapsto -\mathrm{i}n(d)\gamma^a$$
, (23)

which implies $N(d) = -dn(d)^2$. To satisfy the requirements N(1) = -1 and $t^{\sigma} = 1$ for the one-dimensional case, we note that the only Dirac matrix in d = 1 is $\Gamma^{\sigma} = i$, so that the normalization function n(d) must be chosen such that n(1) = 1. Otherwise n(d) is quite arbitrary and must be fixed by application of the theory, which remark also applies to the fundamental length scale l.

It is worth noting that the appearance of the Dirac matrices in this context has a historical parallel in Dirac's original derivation of the Dirac equation [19, 20], where a universal object with a covariant vector index was also required to fulfill the demands of covariance.

3.2 Quantum evolution – Dirac is Schrödinger

We will now motivate a quantum evolution equation based on our classical covariant Hamiltonian picture, which turns out to unify the Dirac and the Schrödinger equation.

The multi-symplectic phase space is spanned by the canonical variables q^i and p_i^a . Any "proper" phase space function f depends on the coordinates of the parameter space Σ only through these variables. For the operators \hat{f} associated to such phase space functions we now analyze the requirement that the classical evolution equation (19) holds in its quantum version as follows:

$$\begin{aligned} \mathrm{i}l^{d-1} \left[\hat{f}, \hat{H} \right] &- \mathrm{i}n(d) \left(\nabla \hat{f} \right) \\ &= \mathcal{S} \left(\frac{\widehat{\partial f}}{\partial p_i^a} \left(\mathrm{i}l^{d-1} \left[\hat{p}_i^a, \hat{H} \right] - \mathrm{i}n(d) \left(\nabla \hat{p}_i^a \right) \right) \right) \,. \end{aligned}$$

The operator S denotes a symmetrization of the canonical variables, which are now operators, and we use Feynman's shorthand notation $\nabla = \gamma^a \nabla_a$. Noting that $(\nabla \hat{f}) = [\nabla, \hat{f}]$ in the action on states, the above equation can be rewritten in the form

$$\left[\hat{f}, \hat{H} + n(d)l^{-d+1}\nabla\right] = \mathcal{S}\left(\frac{\partial \widehat{f}}{\partial p_i^a} \left[\hat{p}_i^a, \hat{H} + n(d)l^{-d+1}\nabla\right]\right).$$
(25)

This equation holds for all operators, if and only if $\hat{H} + n(d)l^{-d+1}\nabla$ is a constant independent of the canonical variables. For d = 1, this reduces to $\hat{H} + i\partial_{\sigma}$. To obtain the same result as in conventional quantum mechanics in this limit, we have to set $\hat{H} + n(d)l^{-d+1}\nabla = 0$. However, note that this type of derivation in quantum mechanics does not produce the Schrödinger equation, which is $\hat{H} - i\partial_{\sigma} = 0$, acting on Schrödinger picture states. This is because the quantization of the classical evolution equation leads to an operator equation valid in the Heisenberg picture. The unitary change of pictures is responsible for the change of signs.

We assume, as will be justified in Sect. 3.3 as it requires some development of the theory, that the same change of signs occurs here. Thus we finally arrive at the quantum evolution equation, as an equation acting on Σ -dependent states:

$$\left(\hat{H} - n(d)l^{-d+1}\nabla\right) |\psi(\sigma^a)\rangle = 0.$$
(26)

Note that the quantum evolution effectively does not require the terms appearing in the symmetrization operator, which thus need not be specified. This is an advantage because it is not consistently possible to do so even in conventional quantum mechanics: no map of phase space functions into an operator algebra exists, compatible with the Poisson bracket. An attempt to rectify this situation is made by deformation quantization, employing as operators formal power series in the Planck quantum \hbar ; see [21, 22] for reviews.

The above equation gives the operator \hat{H} the dimension of mass times l^{-d+1} . Supposing, in an expansion in terms of the canonical variables, that there is a constant term in \hat{H} , we find that both the Schrödinger and the Dirac equation follow from the same quantization procedure. The Schrödinger equation is relevant for a quantization of fields $x^i: \Sigma \cong \mathbb{R} \to \mathbb{R}^n$, and the Dirac equation corresponds to quantized fields on a parameter spacetime $\Sigma \cong M_{1,3}$. This will be further illustrated below. Here we only note that, in d > 1, the wave functions will automatically become spinors.

The quantum evolution equation in the form (26) has been conjectured before by Kanatchikov [6] and Navarro [23] on the basis of analogies between the Dirac equation and conventional quantum mechanics. Here we have presented for the first time a physically reasonable derivation of (26) from first principles, based solely on the two quantization postulates (21) and (23).

3.3 The local evolution operator and the Heisenberg picture

We shall now introduce the covariant Heisenberg picture, and in this context we will justify the remaining assumptions going into the derivation of the quantum evolution equation (26). To clarify the calculations we will use subscripts $_{\rm S}$ and $_{\rm H}$ for Schrödinger and Heisenberg picture quantities, respectively.

The first notion we need is that of an evolution operator $\hat{U}(\sigma, \sigma_0)$, with the help of which a Σ -dependent Schrödinger picture state may be written in terms of a Σ -independent Heisenberg picture state:

$$\left|\psi(\sigma)\right\rangle_{\rm S} = \hat{U}(\sigma, \sigma_0) \left|\psi(\sigma_0)\right\rangle_{\rm H} \,. \tag{27}$$

The consistency of expectation values requires U to be unitary in the sense $\hat{U}^{\#}\hat{U} = \mathbb{1}$ (cf. Sect. 3.5 below).

On curved parameter spaces Σ , such an evolution operator can only be defined locally, i.e., in a sufficiently small neighborhood of a point $p \in \Sigma$. If q is another point in this neighborhood, then there is a unique geodesic joining p and q. The corresponding evolution operator $\hat{U}(q, p)$ can be written as $\hat{U}(\sigma, \sigma_0)$ in a geodesic normal coordinate system. Substituting the above state expansion into the quantum evolution equation we find

Solving this equation to first order in an infinite simally small displacement $\delta\sigma$ then gives

$$\hat{U}(\sigma_0 + \delta\sigma, \sigma_0) = 1 + \frac{l^{d-1}}{dn(d)} \delta\sigma^a \gamma_a \hat{H}_{\rm S} \,. \tag{29}$$

The adjoint $\hat{U}^{\#}$, again to first order, follows from $(\gamma_a \hat{H}_S)^{\#} = -\hat{H}_S \gamma_a$. Hence \hat{U} is unitary, if and only if

$$\left[\gamma^a, \hat{H}_{\rm S}\right] = 0\,,\tag{30}$$

which we must require. (The examples below show that this relation usually holds.) The evolution operator for finite coordinate differences within the local neighborhood follows from the limiting procedure $\hat{U}(\sigma, \sigma_0) =$ $\lim (\hat{U}(\sigma, \sigma - \delta\sigma) \dots \hat{U}(\sigma_0 + \delta\sigma, \sigma_0))$ for $\delta\sigma \to 0$; in consequence, it is unitary as well.

We are now in the position to calculate the equation of motion for Heisenberg picture operators $\hat{f}_{\rm H} = \hat{U}^{\#} \hat{f}_{\rm S} \hat{U}$. Using the same steps as in conventional quantum mechanics yields

$$\nabla \hat{f}_{\mathrm{H}} - n(d)^{-1} l^{d-1} \left[\hat{f}_{\mathrm{H}}, \hat{H}_{\mathrm{H}} \right] = \left[\nabla_a \hat{U}^{\#}, \gamma^a \right] \hat{U} \hat{f}_{\mathrm{H}} \,. \tag{31}$$

The right hand side of this equation does not contribute. This is easily seen by noting that $\left[\nabla_a \hat{U}^{\#}, \gamma^a\right] = \left[\nabla_a \hat{U}, \gamma^a\right]^{\#}$ and using (29) to determine $\nabla_a \hat{U} \sim \gamma_a \hat{H}_{\rm S}$. Thus one finds $\left[\nabla_a \hat{U}, \gamma^a\right] \sim \left[\gamma_a, \hat{H}_{\rm S}\right]$, the vanishing of which was required by the existence of the Heisenberg picture. The Heisenberg equation of motion

$$n(d)l^{-d+1}\nabla \hat{f}_{\rm H} - \left[\hat{f}_{\rm H}, \hat{H}_{\rm H}\right] = 0$$
 (32)

follows. Using the same method as in the derivation of the quantum evolution equation in Sect. 3.2 one thus finds $\hat{H}_{\rm H} + n(d)l^{-d+1}\nabla = 0$ in the Heisenberg picture, fully justifying the change of sign we made in obtaining (26).

The Heisenberg equation of motion (32) will play an important role in showing that our theory indeed has the correct classical limit in Sect. 3.6 below.

3.4 Canonical operators in the Schrödinger picture

In the covariant Schrödinger picture, all operators, including the covariant Hamiltonian, act on states which are elements of some Hilbert space \mathcal{H} and depend on the coordinates of Σ , i.e. $|\psi(\sigma^a)\rangle$. We wish to find a realization of these operators acting on wave functions in an explicit Schrödinger representation; for this purpose we have to introduce a basis of \mathcal{H} , which is conveniently given by the states

$$|\mathbf{q}_{\alpha}\rangle = |\mathbf{q}\rangle \otimes e_{\alpha} \,, \tag{33}$$

where $|\mathbf{q}\rangle$ are eigenstates of the field operators \hat{q}^i , i.e. $\hat{q}^i |\mathbf{q}\rangle = q^i |\mathbf{q}\rangle$, and e_{α} are the canonical basis vectors of the representation space of the Dirac algebra. The dual states are given by

$$\langle^{\alpha} \mathbf{q} | = \langle \mathbf{q} | \otimes \omega^{\alpha} , \qquad (34)$$

where $\{\omega^{\alpha}\}$ is the dual basis of $\{e_{\alpha}\}$, such that the normalization condition becomes

$$\langle^{\alpha} \mathbf{q} \,|\, \tilde{\mathbf{q}}_{\beta} \rangle = \delta^{\alpha}_{\beta} \delta(\mathbf{q} - \tilde{\mathbf{q}}) \,. \tag{35}$$

In the basis $\{|\mathbf{q}_{\alpha}\rangle\}$ any state of the Hilbert space can be expanded as

$$|\psi\rangle = \int \mathrm{d}\mathbf{q} \,|\mathbf{q}_{\alpha}\rangle \,\psi^{\alpha}(\mathbf{q})\,.$$
 (36)

The components $\psi^{\alpha}(\mathbf{q}) = \langle {}^{\alpha}\mathbf{q} | \psi \rangle$ with respect to this basis give the spinorial Schrödinger picture wave function. In this notation we have suppressed the Σ -dependence; more precisely, one should write $\psi^{\alpha}(\sigma^{a};\mathbf{q})$. The identity operator on \mathcal{H} has a partition of the form

$$\mathbf{1} = \int \mathrm{d}\mathbf{q} \left| \mathbf{q}_{\alpha} \right\rangle \left\langle^{\alpha} \mathbf{q} \right| \,. \tag{37}$$

The canonical operators should satisfy the commutation relations

$$\left[\hat{q}^i, \hat{q}^j\right] = 0, \qquad (38a)$$

$$[\hat{p}_i, \hat{p}_i] = 0,$$
 (38b)

$$\left[\hat{q}^{i}, \hat{p}_{j}\right] = \mathrm{i} dn(d)^{2} l^{-d+1} \delta^{i}_{j}, \qquad (38\mathrm{c})$$

which follow from an application of the two quantization postulates to the classical Poisson bracket equations (16). It would seem to be convenient at this stage to remove the dimension dependence of the canonical commutation relations by setting $n(d) = 1/\sqrt{d}$, but we emphasize again that n(d) should be fixed by application. To study the action of the canonical operators on wave functions, we need the following matrix elements:

$$\langle^{\alpha}\mathbf{q} \,|\, \hat{p}_i \,|\, \tilde{\mathbf{q}}_{\beta} \rangle = \mathrm{i} dn(d)^2 l^{-d+1} \delta^{\alpha}_{\beta} \frac{\partial}{\partial \tilde{q}^i} \delta(\mathbf{q} - \tilde{\mathbf{q}}), \quad (39\mathrm{a})$$

$$\langle^{\alpha} \mathbf{q} \,|\, \gamma^{a} \,|\, \tilde{\mathbf{q}}_{\beta} \rangle = (\gamma^{a})^{\alpha}{}_{\beta} \delta(\mathbf{q} - \tilde{\mathbf{q}})\,, \tag{39b}$$

where the first identity follows from an expansion of $\langle {}^{\alpha}\mathbf{q} | [\hat{q}^{i}, \hat{p}_{i}] | \tilde{\mathbf{q}}_{\beta} \rangle$, using (38c). Now we act with our operators on arbitrary states, which yields

$$\hat{\mathbf{q}} |\psi\rangle = \int d\mathbf{q} |\mathbf{q}_{\alpha}\rangle \left(\mathbf{q}\psi^{\alpha}(\mathbf{q})\right) , \qquad (40a)$$

$$\hat{\mathbf{p}} |\psi\rangle = \int d\mathbf{q} |\mathbf{q}_{\alpha}\rangle \left(-\mathrm{i}dn(d)^{2}l^{-d+1}\frac{\partial}{\partial\mathbf{q}}\psi^{\alpha}(\mathbf{q})\right) , \qquad (40b)$$

$$\gamma^{a} \left| \psi \right\rangle = \int d\mathbf{q} \left| \mathbf{q}_{\alpha} \right\rangle \left((\gamma^{a})^{\alpha}{}_{\beta} \psi^{\beta}(\mathbf{q}) \right) \,. \tag{40c}$$

Thus \hat{q}^i and γ^a act multiplicatively on wave functions, whereas the \hat{p}_i essentially act as derivative operators. The commutation relations stated above are clearly satisfied.

A further important point is missing for a successful transition from the classical to the quantum theory. The classical covariant Hamiltonian depends on the phase space variables q^i and p_i^a , so that the Hamiltonian operator would seem to depend on the operators \hat{p}_i^a for which we have not yet given a representation. However, it is always possible to replace these operators by \hat{p}_i , as we will now show. Acting on wave functions the \hat{p}_i^a are realized by

$$\hat{p}_i^a \sim -n(d)l^{-d+1}\gamma^a \frac{\partial}{\partial q^i},$$
(41)

which may be derived from an application of our quantization postulates to the classical Poisson bracket $\{q^i, p_j^a\} = t^a \delta_j^i$. It follows that any occurrence of \hat{p}_i^a can be replaced by

$$\hat{p}_i^a = -\frac{\mathrm{i}}{dn(d)}\gamma^a \hat{p}_i \,, \tag{42}$$

so that the quantum Hamiltonian becomes effectively a function of the operators \hat{q}^i and \hat{p}_i . On one-dimensional Σ one reobtains $\hat{p}_i^{\sigma} = \hat{p}_i$ as in the classical theory.

In the case where the fields q^i form the coordinates of a target space manifold M, one must take care of appropriate integration measures in the state expansions, and of the fact that $\delta(\mathbf{q} - \tilde{\mathbf{q}})$ is a density. The appropriate Schrödinger representation would contain covariant, not partial, differentiation operators on M.

3.5 Hilbert space and probability interpretation

The Σ -dependent states $|\psi(\sigma^a)\rangle$ are elements of a Hilbert space \mathcal{H} . The essential algebraic structure on a Hilbert space is a scalar product, i.e., a bilinear form $\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$. We may define such a scalar product in terms of the wave functions corresponding to Hilbert space states:

$$\langle \psi | \phi \rangle = -i \int d\mathbf{q} \bar{\psi} \phi = -i \int d\mathbf{q} \psi^{\dagger} \Gamma^{0} \phi \,.$$
 (43)

Note that the appearance of the gamma matrix Γ^0 of the local Lorentzian tangent spaces guarantees that the scalar product maps to a diffeomorphism scalar of Σ . The spinor indices of the wave functions are suppressed, as are their Σ -and field-dependence.

The necessary requirement that the scalar product should return a scalar function on \varSigma results in its indefiniteness: indeed,

$$\langle \psi | \psi \rangle = -i \int d\mathbf{q} \psi^{\dagger} \Gamma^{0} \psi \neq \int d\mathbf{q} \psi^{\dagger} \psi ,$$
 (44)

where the Dirac matrix mixes the spinorial components to prevent a generically positive result. The indefiniteness is a feature of quantization on manifolds Σ of dimension d > 1. For d = 1, the non-equality above becomes an equality (and ψ^{\dagger} is simply the complex conjugate).

One of the consequences of this construction is the following: the self-adjoint operators with respect to our scalar product are no longer Hermitian with $\hat{O}^{\dagger} = \hat{O}$. By definition, self-adjoint operators satisfy $\langle \hat{O}\psi | \phi \rangle = \langle \psi | \hat{O}\phi \rangle$ for all ψ and ϕ . Here this implies \hat{O} is self-adjoint, if and only if

$$\hat{O}^{\#} \equiv -\Gamma^0 \hat{O}^{\dagger} \Gamma^0 = \hat{O} \,. \tag{45}$$

But self-adjoint operators are not guaranteed to have real eigenvalues because of the indefiniteness of the scalar product, which may produce null states with $\langle \psi | \psi \rangle = 0$. Another condition is needed: a self-adjoint operator is orthogonally diagonalizable with real eigenvalues if it is a so-called Pesonen operator satisfying $\langle \psi | \hat{O} \psi \rangle \neq 0$ for all null states ψ [24]. For the special case d = 1, we have $\Gamma^{\sigma} = i$ so that the relation above selects the Hermitian \hat{O} , as is the case in conventional quantum mechanics.

The standard interpretation of quantum mechanics interprets the squared modulus $|\psi|^2$ of the Schrödinger wave function ψ as a probability density. This is enabled by the fact that the Schrödinger equation guarantees the constancy of the total probability $\int d\mathbf{x} \psi^{\dagger} \psi$ in time. To give a similar interpretation here, we need a similar statement. Since the square $\langle \psi | \psi \rangle$ is no longer positive-definite for d > 1 and hence no longer admits a probability interpretation, we need to find another quantity that does. Consider the following vector current on Σ :

$$j^a = -\int \mathrm{d}\mathbf{q}\,\bar{\psi}\gamma^a\psi\,.\tag{46}$$

We assume that our covariant Hamiltonian has essentially real eigenvalues, meaning that it is self-adjoint with $\hat{H}^{\#} = -\Gamma^0 \hat{H}^{\dagger} \Gamma^0 = \hat{H}$. This is consistent because \hat{H} is directly related to $\gamma^a \nabla_a$, and we have $\gamma^{a\dagger} = \Gamma^0 \gamma^a \Gamma^0$ and Hermitian $i \nabla_a$. Then the Dirac form of relation (26) is sufficient to prove that j^a is conserved,

$$\nabla_a j^a = 0. \tag{47}$$

Locally, a conserved current implies a conserved charge: in normal coordinates on Σ ,

$$\partial_{\sigma^0} \int \mathrm{d}^{d-1} \sigma \, j^0 = 0 \,. \tag{48}$$

Thus we can interpret the integral of j^0 as the total probability to find the fields in any configuration **q** anywhere on the spatial part of Σ . This also means that

$$\rho(\sigma^a; \mathbf{q}) = -\bar{\psi}(\sigma^a; \mathbf{q})\gamma^0(\sigma)\psi(\sigma^a; \mathbf{q}), \qquad (49)$$

gives the probability density of finding the field configuration \mathbf{q} at a given point with coordinates σ^a of Σ . In normal coordinates, the probability density becomes $-\bar{\psi}\Gamma^0\psi = \psi^{\dagger}\psi$, and is positive-definite. In the one-dimensional case $\Sigma \cong \mathbb{R}$, we can always find global normal coordinates, so that we once again recover conventional quantum mechanics.

The wave function $\psi(\sigma^a; \mathbf{q})$ contains all the necessary information to reconstruct the Schrödinger wave functional of the conventional canonical approach in cases where the latter exists, as has been shown in [25, 26]. This suggests that the covariant canonical approach is at least as powerful as the conventional one; more powerful, in fact, since it works on backgrounds that do not allow the conventional spacetime foliation by spatial hypersurfaces.

3.6 Classical limit and Ehrenfest equations

To see how the classical limit emerges from our formalism, let us consider the following Ehrenfest-type theorem, arising from the expectation value of the Heisenberg equation of motion (32) above:

$$n(d)l^{-d+1}\nabla_a\left\langle\gamma^a\hat{f}\right\rangle = \left\langle\left[\hat{f},\hat{H}\right]\right\rangle.$$
(50)

Because the inner product is picture-independent, this equation in particular holds in the Schrödinger picture. Assuming now a classical covariant Hamiltonian of the form

$$H = -\frac{\alpha}{2}p_i^a p_a^i + V(q^i) \tag{51}$$

for constant α , one finds $\hat{H} = \alpha \hat{p}^i \hat{p}_i / (2dn(d)^2) + V(\hat{q}^i)$. We wish to evaluate the theorem for $\hat{f} \mapsto \hat{p}^j$ as well as for $\hat{f} \mapsto \gamma_a \hat{q}^j$. We use the commutator relations

$$[\hat{p}_j, \hat{H}] = -\mathrm{i}dn(d)^2 l^{-d+1} \frac{\partial V}{\partial q^j}(\hat{q}^i), \qquad (52\mathrm{a})$$

$$[\gamma_a \hat{q}^j, \hat{H}] = \mathrm{i}\alpha l^{-d+1} \gamma_a \hat{p}^j \tag{52b}$$

to arrive at the following equations:

$$\left\langle \frac{\partial H}{\partial q^j}(\hat{q}^i, \hat{p}_k^b) \right\rangle = -\nabla_a \left\langle \hat{p}_j^a \right\rangle, \tag{53a}$$

$$\left\langle \frac{\partial H}{\partial p_j^a}(\hat{q}^i, \hat{p}_k^b) \right\rangle = \nabla_a \left\langle \hat{q}^j \right\rangle.$$
 (53b)

Therefore, the classical covariant Hamiltonian field equations (7) are fulfilled within expectation values in the form of Ehrenfest equations. Interestingly, no choice of the normalizations of the length scale l or of n(d) was required to obtain this classical result, showing once more the consistency of the theory.

4 Elementary applications

In this section we will give several simple applications of the covariant canonical quantization method. This demonstrates the technique in some detail, but, more importantly, yields a number of interesting results: the Klein– Gordon equation arises as the wave equation of the relativistic point particle without any need to refer to the relativistic energy-momentum relation; the quantization of any bosonic field on an extended parameter space Σ with d > 1 creates spinorial wave functions; in particular, the Dirac equation emerges from the Klein–Gordon Lagrangian, along with the prediction of a fermion mass gap and a hierarchy of fermions that differ only by their masses.

4.1 Relativistic point particles – the Klein–Gordon equation

The simplest application of our quantization formalism is to the relativistic mechanics of a point particle. Completely side-stepping its usual derivation from the relativistic energy relation, we will find that the quantum wave equation is the Klein–Gordon equation.

Consider the following action for fields $x^i : \mathbb{R} \to M_{1,3}$ which describe the worldline embedding into a flat Minkowski spacetime,

$$S = \int d\sigma \sqrt{-g_{\sigma\sigma}} \frac{1}{2} \left(m_1 g^{\sigma\sigma} \nabla_\sigma x^i \nabla_\sigma x^j \eta_{ij} + m_2 \right) .$$
 (54)

Variation yields the equation of motion $\partial_{\sigma}(\sqrt{-g_{\sigma\sigma}} g^{\sigma\sigma}\partial_{\sigma}x^i) = 0$, and also the gravitational constraint $g^{\sigma\sigma}\nabla_{\sigma}x^i\nabla_{\sigma}x^j\eta_{ij} = m^2$. Both of these equations are needed to show that the above action is classically equivalent to the standard action of the relativistic point particle,

 $m \int d\sigma \sqrt{-\partial_{\sigma} x^i \partial_{\sigma} x^j \eta_{ij}}$, for two mass parameters m_1 and m_2 which satisfy $m_1 m_2 = m^2$.

The covariant momenta are $p_i^{\sigma} = m_1 g^{\sigma\sigma} \nabla_{\sigma} x^j \eta_{ji}$, and yield the covariant Hamiltonian $H = -\frac{1}{2m_1} g_{\sigma\sigma} p_i^{\sigma} p_j^{\sigma} \eta^{ij} -\frac{1}{2}m_2$. Using the Schrödinger representation of the momentum operators on wave functions returns the quantum wave equation

$$\left(-\frac{1}{2m_1}\Box - \frac{m_2}{2} - \mathrm{i}\partial_\sigma\right)\psi(\sigma; x^i) = 0\,,\tag{55}$$

where the box denotes the d'Alembertian on $M_{1,3}$. We still have to deal with the gravitational constraint on the classical momenta: in its quantum version it reads $(\Box + m^2)\psi = 0$. This can be satisfied consistently with the wave equation by choosing $\partial_{\sigma}\psi(\sigma; x^i) = 0$. The resulting wave function is then automatically independent of σ , and the equation for $\psi(x^i)$ becomes the Klein–Gordon equation on $M_{1,3}$.

The quantum wave equation is a Schrödinger equation with time parameter σ , but independence of the wave function of this parameter is forced by the constraint. In this sense, classical reparametrization invariance directly implies the Klein–Gordon equation.

4.2 Free bosonic strings – Weyl spinors

One of the most characteristic features of covariant canonical quantization is the fact that any bosonic field on a parameter space of dimension d > 1 produces spinor wave equations. To illustrate this point in the simplest setup, we consider free bosonic strings on a flat target space, given as maps $\Sigma \to M_{1,n}$ from the two-dimensional worldsheet Σ into Minkowski space $M_{1,n}$. We employ the Polyakov action

$$S = -\int_{\Sigma} \mathrm{d}^2 \sigma \sqrt{-g} \, \frac{1}{2} g^{ab} \partial_a \, X^i \partial_b X^j \eta_{ij} \,. \tag{56}$$

which is classically equivalent to the Nambu–Goto action that measures the area of the string worldsheet, if the gravitational constraint $g^{ab}g^{cd}\eta^*_{cd} = \eta^{*cd}$, where $\eta^*_{ab} = \partial_a X^i \partial_b X^j \eta_{ij}$ is the pull-back of η to the worldsheet, is implemented. The covariant momenta are derived as $p^a_i = -\partial^a X_i$ and give rise to $H = -p^a_i p^i_a/2$. This leads to the Schrödinger picture wave equation

$$\left(l^{-1}n(2)\Box + \gamma^a \partial_a\right)\psi(\sigma^b; X^\mu) = 0, \qquad (57)$$

where \Box denotes the target space d'Alembert operator on $M_{1,n}$. It is illustrative to use the separation ansatz $\psi = \Psi(\sigma^a)\Phi(X^{\mu})$ with spinorial Ψ for the wave function. This introduces a separation constant M, and generates the two separate equations

$$(\Box + lMn(2)^{-1}) \Phi = 0,$$
 (58a)

$$\gamma^a \partial_a - M) \Psi = 0. \tag{58b}$$

Thus the quantization of strings generates Weyl spinors on the two-dimensional worldsheet, whose mass M is linked to a Klein–Gordon equation on the target spacetime.

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As noted above, it is necessary to satisfy the gravitational constraint. Classically, we may rewrite it as $p^{ai}p_i^b - g^{ab}p_i^cp_c^2/2 = 0$, which is symmetric. Keeping the symmetry we hence find the Schrödinger representation

$$\left(-\gamma^{(a}\gamma^{b)}+g^{ab}\right)\hat{p}^{i}\hat{p}_{i}=0.$$
(59)

The expression in brackets is identically zero by the properties of the Dirac algebra. Surprisingly the constraint is satisfied automatically in the quantum theory. However, the quantization of the string in this formalism has no discernible relation to string theory, where the quantum requirement of the gravitational constraint leads to the Virasoro algebra.

4.3 Free scalar fields – the Dirac equation

The free scalar field $\phi: \Sigma_{1,3} \to \mathbb{R}$ on a four-dimensional Lorentzian spacetime $\Sigma_{1,3}$ with metric g is governed by the Lagrangian

$$L = -\frac{1}{2}g^{ab}\partial_a\phi\partial_b\phi - \frac{1}{2}m^2\phi^2.$$
 (60)

The covariant momenta follow as $\pi^a = -\partial^a \phi$ and yield $H = -\pi_a \pi^a/2 + m^2 \phi^2/2$. From quantization we hence obtain the Schrödinger picture wave equation

$$\left(-\frac{2n(4)}{l^3}\partial_{\phi}^2 + \frac{l^3m^2}{2n(4)}\phi^2 - \gamma^a\partial_a\right)\psi(\sigma^a;\phi) = 0.$$
 (61)

To illustrate the consequences of our theoretical construction, it is useful to consider a separation ansatz $\psi = \Psi(\sigma^a) \Phi(\phi)$ for the wave function, where only Ψ is taken spinorial. This introduces a separation constant M, and the wave equation generates two separate equations of the form

$$\left(-\frac{2n(4)}{l^3}\partial_{\phi}^2 + \frac{l^3m^2}{2n(4)}\phi^2\right)\Phi = M\Phi\,, \tag{62a}$$

$$\gamma^a \partial_a - M) \Psi = 0.$$
 (62b)

Thus the spacetime dependence of the wave function is described by a Dirac equation with mass M. However, this mass is not unconstrained: a spectrum of allowed masses is generated by the first equation, which is just the Schrödinger equation of a one-dimensional harmonic oscillator with frequency $\omega = 2m$. The mass spectrum is therefore given by

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$$M_k = m\left(2k+1\right) \tag{63}$$

with integer $k \geq 0$. While this spectrum does not look particularly appealing phenomenologically, it should be noted that we obtained the prediction of a mass hierarchy of otherwise identical Dirac particles from the non-interacting Klein–Gordon Lagrangian only. With the addition of interactions to the scalar action, more complex mass spectra could be generated, leading to the possibility of obtaining the generations of the standard model from a suitably tuned interacting scalar Lagrangian. Another important prediction from (62) is the existence of a mass gap for the fermions: M = 0 is generally not a solution if the harmonic potential $V(\phi) \sim \phi^2$ is replaced by a generic potential $V(\phi)$.

4.4 Local gauge invariance – gauge fields

We have seen that the quantization of pure scalar field models generates fermionic particles with an allowed mass spectrum given by the covariant Hamiltonian of the scalar field. Phenomenological relevance additionally requires these fermions to be charged. A mechanism to serve this purpose has been identified by Weyl [27] a long time ago, and we will now demonstrate its effect.

The basic observation underlying this mechanism is the invariance of the interpretationally relevant probability current $j^a = -i \langle \psi | \gamma^a | \psi \rangle$ defined in (46) under local phase shifts of the wave function, so-called gauge transformations. These are transformations $\psi \mapsto e^{ie\Lambda}\psi$ under a function $\Lambda : \Sigma \to \mathbb{R}$. The quantum evolution equation (26), however, is only invariant under global gauge transformations with constant Λ . If, in addition, local invariance is required, we have to amend this equation by the introduction of a gauge field:

$$\left(\hat{H} - n(d)l^{-d+1}(\nabla - \mathrm{i}e \mathcal{A})\right)|\psi\rangle = 0.$$
(64)

It now follows that if $|\psi\rangle$ is a solution of this equation, then so is the locally gauge transformed $e^{ie\Lambda} |\psi\rangle$, as long as the gauge field transforms at the same time as $A_a \mapsto A_a + \partial_a \Lambda$. The resulting equation is essentially the Dirac equation for particles of mass $\langle \hat{H} \rangle$ and charge e.

To make this statement more precise, observe that in order to speak about the spectrum of the theory we do not require knowledge about the probabilities for the original scalar fields, but only about the generated fermions. This means we may consider the integrated expectation value of the quantum evolution equation as a functional of ψ ,

$$S[\psi] = \int_{\Sigma} \mathrm{d}^{d} \sigma \left\langle \psi \right| \left(-n(d)^{-1} l^{d-1} \hat{H} + \nabla - \mathrm{i} e \,\mathcal{A} \right) \left| \psi \right\rangle \,, \tag{65}$$

in which the wave function's dependence on the original scalar fields is effectively integrated out. Indeed, if we assume the wave equation has been solved by a product ansatz $\psi = \Psi(\sigma^a)\Phi(\phi)$ as in the previous examples, we find

$$S_{\Phi}[\Psi] = \left(\int \mathrm{d}\phi \Phi^{\dagger} \Phi\right) \int_{\Sigma} \mathrm{d}^{d}\sigma \,\bar{\Psi} \left(\nabla - \mathrm{i}e \,\boldsymbol{A} - \tilde{M}\right) \Psi \,, \quad (66)$$

for one of the rescaled mass eigenvalues $\tilde{M} = n(d)^{-1}l^{d-1} \int d\phi \Phi^{\dagger} \hat{H} \Phi / \int d\phi \Phi^{\dagger} \Phi$ in the mass spectrum generated by the scalars' covariant Hamiltonian. So integrating out the original scalar field freedom, because it is not observable, returns precisely the Lagrangian theory for the Dirac field with mass \tilde{M} .

Now consider a multiplet of N scalar fields ϕ_i with a Lagrangian which is invariant under the action of some nonabelian subgroup G of SO(N). In this case, the covariant Hamiltonian will inherit the G-invariance, resulting in a degeneracy in the spectrum of the theory. The energy levels M_n can then be labelled by the irreducible representations of G, with the degeneracy of each level given by the dimension d_n of the irreducible representation under which it transforms. A solution of the quantum evolution equation can then be decomposed in terms of eigenfunctions of the covariant Hamiltonian:

$$\psi(\sigma,\phi) = \sum_{n=0}^{\infty} \sum_{\alpha=1}^{d_n} \Psi_{n,\alpha}(\sigma) \Phi_{n,\alpha}(\phi) \,. \tag{67}$$

Putting this decomposition into the definition of $S[\psi]$ above and using the orthogonality relation

$$\int_{\mathcal{M}} \mathrm{d}\phi \Phi_{n,\alpha}^{\dagger}(\phi) \Phi_{m,\beta}(\phi) = \delta_{m,n} \delta_{\alpha,\beta} \tag{68}$$

for the wave functions, we arrive at the action for Ψ

$$S[\Psi] = \sum_{n=0}^{\infty} \int_{\Sigma} \mathrm{d}\sigma \bar{\Psi}_{n,\alpha} \left(\nabla - \tilde{M}_n \right) \Psi_n^{\alpha} \,, \qquad (69)$$

where each kind of fermion has a mass M_n and is invariant under a $SU(d_n)$ symmetry in addition to the U(1) symmetry discussed above. Using the same arguments as before, these $SU(d_n)$ symmetries should also be gauged, giving rise to a spectrum of nonabelian gauge symmetries.

In the case of a finite scalar symmetry group G, there is only a finite number of irreducible representations, and correspondingly the gauge group of the fermionic theory then is a finite product of SU(N) gauge groups. For continuous G, an infinite product of SU(N) factors ensues. Groups that could give a standard model-like gauge group $SU(3) \times SU(2) \times U(1)$ (although we haste to point out that this simple model does not give the chiral couplings of the standard model) include the point groups T_d and O.

Hence, covariant canonical quantization with the additional requirement of local gauge invariance is able to produce, from a scalar field Lagrangian, all particles (so far) observed in Nature, namely fermions and gauge fields. While their masses are constrained by the covariant Hamiltonian of the original classical scalar field theory, the charges are additional input at the quantum level of the theory. In order to obtain a more complete theory, appropriate gauge-invariant dynamics for the gauge fields have to be added at this stage, which is a freedom that we have.

5 Discussion

Considering fields as maps from a parameter space Σ to a target space M, we have constructed a covariant quantization method that keeps the diffeomorphism invariance between the parameters of Σ intact. Covariant canonical quantization is based on the classical Hamiltonian theory developed by de Donder [1] and Weyl [2] which makes use of a finite-dimensional multi-symplectic phase space, where every field has a set of conjugate momenta associated to each of its partial derivatives. The classical theory is completely equivalent (in the sense of generating the same solutions) to the conventional Hamiltonian point of view, avoiding, however, the explicit breaking of diffeomorphism invariance that arises from singling out a time coordinate normal to an assumed foliation of Σ by spatial hypersurfaces.

We have introduced the notion of a covariant Poisson bracket within the classical theory, before applying two well-motivated quantization postulates. The first postulate replaces, according to Dirac's argument, the Poisson bracket of phase space functions by the commutator of corresponding operators acting on some Hilbert space. The second postulate is geometrically motivated: on parameter spacetimes Σ of dimension d > 1 it introduces the Clifford algebra of Dirac matrices into the quantum theory. The construction is such that covariant canonical quantization coincides with conventional canonical quantization in d = 1, i.e., when the fields depend only on time.

The two quantization postulates, applied to the classical de Donder–Weyl theory, for the first time allow for the derivation of a quantum evolution equation in terms of the covariant Hamiltonian, which had been conjectured before on the mere basis of analogies [6, 7]. This evolution equation effectively unifies the Dirac and the Schrödinger equations. We have further developed the theory in the covariant Schrödinger picture, including a discussion of the representation of the field and multi-momentum operators, and the relevant Hilbert space. Diffeomorphism invariance requires an indefinite inner product on the Hilbert space, whose consequences for the diagonalizability of operators and their eigenvalues have been discussed. We have also provided a probability interpretation for the fields' wave function.

Further development of the theory could progress in several directions. One of the obvious questions concerns the Heisenberg picture for the theory. The formal solution for the evolution operator follows from (29) as the path-ordered exponential $U(\sigma, \sigma_0) \sim \mathcal{P} \exp\left(l^{d-1}/(dn(d))\right)$

 $\int_{\sigma_0}^{\sigma} H\gamma_a d\xi^a$). As such it is only locally defined, and pathdependent, at least on generic curved spacetimes Σ where we had to specify the path along which the exponent is integrated by using geodesic normal coordinates on sufficiently small neighborhoods. This raises questions about the possibility of developing scattering theory in these cases. Another question is that of the quantization of gravity. Although we have made use of gravitational constraints in two of the examples, it is not so clear how the theoretical setup could be consistent with additional dynamics for the background metric on the parameter space Σ .

We have discussed a number of elementary applications of the formalism with some surprising and very interesting results. The quantization of the relativistic point particle immediately yields as quantum wave equation the Klein– Gordon equation, without conceptually employing the relativistic energy momentum relation. Though there is no readily discernible connection to string theory, it is interesting to note that the quantization of bosonic strings produces Weyl spinors on the worldsheet whose mass is linked to a Klein–Gordon equation on the target space. This fact expresses one of the most characteristic features of covariant canonical quantization, namely that the quantization of any field on Σ with d > 1 produces a spinorial wave equation.

We have shown that a purely scalar classical Lagrangian can produce, upon quantization, a theory of Dirac fermions interacting with gauge fields. The latter come into the theory by requiring the local gauge invariance of the interpretationally relevant probability current also on the level of the wave equation. This means that the basic equations of the quantum field theory of the standard model may emerge from a classical scalar field theory as wave equations. Several interesting results are obtained along with this mechanism.

The emergence of spinor fields as a purely quantum phenomenon by passes the usual need for a semi-classical treatment of the Dirac equation, which emerges as a fully quantum equation from the very beginning. More intriguingly, on the phenomenological side, the procedure of covariant canonical quantization provides a new mechanism to unify particles of different masses, which leads to an (at least qualitative) explanation of the generations of the standard model in terms of a self-interacting scalar field. It should be noted that in this framework fermionic masses are generated without a Higgs mechanism. Instead, the mass and self-interaction of the underlying scalar field manifest themselves by generating a mass spectrum for the effective fermion field which is the spacetime part of the scalar field's quantum wave function.

It is interesting to speculate where a scalar model complicated enough to yield the standard model upon quantization could come from in the first place. One possibility seems to be the compactification of a higherdimensional bosonic, maybe gravitational, theory. Such compactifications generally produce a large number of scalar fields as shape moduli of the internal manifold, with self-interactions through some effective potential. If such a potential had a minimum, one would expect it at some negative value, due to a geometric no-go theorem [28] (see also the discussion in [29]), thus generating a discrete mass spectrum for the fermionic fields in the quantum theory which could have phenomenological relevance. More speculatively still, the fact that the quantization of a purely scalar classical theory necessarily leads to a fermionic quantum theory might be indicating some sort of semiclassical supersymmetry at work behind the scenes.

Covariant canonical quantization clearly does not replace conventional quantum field theory; rather it adds a first quantization to the usual procedure, which then literally becomes a second quantization: first, a scalar model generates spinorial quantum wave equations which, after integrating out the unobservable scalar degrees of freedom, become the classical equations of motion underlying the standard model. Then the quantization of these equations proceeds in standard quantum field theoretical fashion. The intriguing result of this investigation is the fact that the standard model's classical equations of motion for fermions and gauge fields, along with the prediction of discrete mass spectra of identically charged particles, are generated from the quantization of a purely scalar classical field theory. This gives reason to hope that covariant canonical quantization might find further use and applications.

Acknowledgements. MNRW thanks Klaus Fredenhagen and Stefan Hofmann for very useful discussions. He acknowledges financial support from the German Research Foundation (DFG), the German Academic Exchange Service (DAAD), and the European RTN program MRTN-CT-2004-503369. GMvH acknowledges partial financial support from the Natural Sciences and Engineering Research Council of Canada and the Government of Saskatchewan.

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