

BSc Thesis Applied Mathematics - Applied Physics

A classical treatment of scalar electrodynamics

Gauge theory in the port-Hamiltonian framework

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Abstract

The charged, massive Klein-Gordon field is a scalar field with a global U(1)-gauge symmetry. It is coupled to the Maxwellian electromagnetic field to get a system that has a local U(1)-gauge symmetry. We study the classical field theory of the Klein-Gordon field coupled to the electromagnetic field on a curved spacetime. The spacetime is foliated into spacelike hypersurfaces, each corresponding to a single "time", such that a Hamiltonian theory may be formulated. Hamilton's equations of motion and the gauge symmetries are worked out for the Klein-Gordon-Maxwell system under the assumption that the total energy of the system is constant. Port-Hamiltonian theory is used to reformulate the dynamics in a way that allows for the treatment of energy exchange with the environment. In the port-Hamiltonian formulation, however, the gauge symmetries are obscured.

 $Keywords\colon$ Gauge theory, Classical field theory, Port-Hamiltonian theory, scalar electrodynamics

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1 Introduction

A gauge theory is a closed system that exhibits arbitrary functions in its dynamic equations, even after a systematic algorithm for their elimination has been executed. The direct implication of the presence of these arbitrary functions is that a single physical state corresponds to multiple, equivalent, mathematical solutions to the dynamic equations of the system. Port-Hamiltonian theory extends Hamiltonian theory to open systems that can exchange energy with their environment via ports that encode power coming in to or going out of the system. Interconnecting ports in an overall power-preserving way one can model complex composite systems. In this work, a first step towards formulating an open gauge theory using the language of port-Hamiltonian theory is made by formulating the dynamics of a gauge theory in a port-Hamiltonian way.

As a central test case, we will consider the gauge theory of a massive, charged Klein-Gordon field coupled to the electromagnetic field. We will treat the system on a curved spacetime. The charged Klein-Gordon field is a scalar field of which the quantized version describes charged pions. We will, however, keep the analysis exclusively classical.

In general, gauge theories are best understood from the point of view of Hamiltonian dynamics. We start from the Lagrangian formulation of field theory and work our way to a Hamiltonian formulation. Hamilton's formalism requires a sense of time evolution. Extra structure is needed on spacetime to be able to write down evolutionary equations. Once the extra structure has been prepared, the evolutionary equations of the Klein-Gordon-Maxwell system are worked out. The evolutionary equations contain an arbitrary function because there is an inherent constraint present in the system such that the Hamiltonian is not uniquely determined.

We apply a systematic algorithm, called the Dirac algorithm, to try to eliminate the arbitrary function from the dynamics, but we find that arbitrary function is pertinent in the dynamic equations. What is more, to ensure that the dynamic equations preserve the inherent constraint, a second constraint must be added. The constraints are combined into a single conserved object that encodes the gauge symmetries of the system. Finally, the gauge system, which is inherently closed, is formulated in a port-Hamiltonian way. Although the port-Hamiltonian description provides possibilities to extend the closed system to an open system, the gauge symmetries are obscured.

In section 2 we provide the necessary constructions for doing classical Hamiltonian field theory on a curved spacetime. The section starts with a treatment of the Lagrangian formulation of field theory. To talk about evolutionary equations, a (3 + 1)-decomposition of spacetime is made. The (3 + 1)-decomposition consists in foliating the spacetime with spacelike hypersurfaces, each hypersurface corresponding to a single "time". This foliation turns out to be the appropriate extra structure needed for evolutionary equations. Finally, Hamiltonian theory field theory for closed systems is provided using the Poisson bracket. In section 3 the key features of gauge theories are worked out for point particle theory. In particular, the Dirac algorithm and the construction of the gauge generator are discussed. Section 3 concludes by discussing the electromagnetic field on Minkowski space, which is a gauge theory. This example is used to show how to interpret the point particle constructions in the setting of a field theory.

In section 4 we get to the closed Klein-Gordon-Maxwell system. First the Hamiltonian formulation of this field theory is constructed. The equations of motion are calculated explicitly. Next, using the constructions from section 3, the gauge generator is calculated. Finally, in section 5 the port-Hamiltonian view of modeling open systems is introduced and we revisit the closed Klein-Gordon-Maxwell system using a port-Hamiltonian approach.

2 Classical field theory on curved spacetime

In this section, we review the Lagrangian and Hamiltonian formulation of classical field theory on a general spacetime. A spacetime is a four-dimensional manifold equipped with a Lorentzian metric. The action functional is presented as the integral of the Lagrangian density over the region of spacetime under consideration. The physical configurations of the fields on spacetime are those configurations that extremize the action functional. Field configurations that extremize the action are solutions to the Euler-Lagrange equations. In order to talk about dynamics, the spacetime manifold must be foliated by spacelike hypersurfaces, each hypersurface corresponding to a single "time". Hamilton's equations of motion encode how the fields change along curves transverse to these spacelike hypersurfaces, thus providing the dynamic equations for the fields. The Lagrangian and Hamiltonian formulation of field theory are connected through a partial Legendre transform. In this section, we will assume that the Legendre transform is invertible. We will also assume that the systems under consideration are closed in a sense that will be clarified when we deal with Hamiltonian theory.

2.1 Lagrangian field theory

In this subsection we provide the fundamental notions of Lagrangian field theory on a curved spacetime. We start out by considering the theory of a scalar field ϕ on a fourdimensional smooth manifold M equipped with a Lorentzian metric g. The Euler-Lagrange equations will be derived from the action using variational principles. The constructions given in this subsection can be extended to hold also for fields of other tensorial type, in particular, for covector fields.

We restrict our attention to a region $\mathscr{V} \subset M$ in the spacetime manifold enclosed by its boundary $\partial \mathscr{V}$. Assume without real loss of generality that \mathscr{V} is the domain of a coordinate chart (\mathscr{V}, x) . If this is not the case, the usual constructions with a smooth atlas apply.

In Lagrangian field theory, we are given a Lagrangian density $\mathscr{L}(\phi, (\partial/\partial x^m)\phi)$,¹ which is a weight-one scalar density² on \mathscr{V} that depends on the field ϕ and its partial derivatives. The action functional $S[\phi]$ is

$$S[\phi] = \int_{\mathscr{V}} \mathscr{L}\left(\phi, \frac{\partial}{\partial x^m}\phi\right) \, dx^0 \wedge \dots \wedge dx^3.$$

The Lagrangian density can be decomposed as the product of the square root of the metric determinant $\sqrt{-g}$ and a scalar function \mathscr{L}_{scalar} , that is,

$$\mathscr{L} = \mathscr{L}_{scalar} \sqrt{-g}.$$

With this decomposition, the action integral can be computed in the chart (\mathcal{V}, x) in the usual way

$$S[\phi] = \int_{x(\mathscr{V})} d^4 \alpha \, \left(\sqrt{-g} \circ x^{-1}\right)(\alpha) \, \mathscr{L}_{scalar}(\phi \circ x^{-1}, \partial_m(\phi \circ x^{-1}))(\alpha).$$

In the remainder of this subsection we will use a more concise notation for the the action integral in the chart (\mathcal{V}, x) by letting an upper (x) indicate the chart representative of an

¹Latin indices run from 0 to 3, Greek indices run from 1 to 3.

²Any object whose components under a change of coordinates pick up the same Jacobian factor as $(\sqrt{-\det g})^w$ (apart from the usual transformation matrices for each tensor component) is called a tensor density of weight w.

object. For the action functional this amounts to

$$S[\phi] = \int_{x(U)} d^4 \alpha \sqrt{-g}^{(x)}(\alpha) \mathscr{L}_{scalar}\left(\phi^{(x)}, \partial_m \phi^{(x)}\right)(\alpha).$$

We want to find the physical field configuration of the scalar field ϕ inside the region \mathscr{V} when ϕ is specified on the boundary $\partial \mathscr{V}$. The action principle states that the physical field configuration of ϕ is one that extremizes the action. A particular configuration ϕ extremizes the action when adding any infinitesimal variation $\delta \phi$ to ϕ leaves the action unchanged to first order, which is to say

$$S[\phi + \delta\phi] - S[\phi] = O(\epsilon^2),$$

where we take the variation $\delta\phi$ to be of the form $\delta\phi = \epsilon v$, where $v \in C^{\infty}(\mathscr{V})$ is an arbitrary scalar field and ϵ is an infinitesimal parameter. We require that v vanishes on the boundary $\partial\Sigma$ such that $\phi + \delta\phi$ satisfies the same boundary conditions as ϕ .

In the chart (\mathscr{V}, x) , we can expand the Lagrangian density \mathscr{L} in powers of ϵ around ϕ . For the action evaluated at $\phi + \delta \phi$ this yields

$$\begin{split} S[\phi + \delta\phi] &= \int_{x(\mathscr{V})} d^4 \alpha \sqrt{-g}^{(x)} \mathscr{L}_{scalar} \left(\phi^{(x)} + \epsilon \, v^{(x)}, \partial_m \left(\phi^{(x)} + \epsilon \, v^{(x)} \right) \right) \\ &= \int_{x(\mathscr{V})} d^4 \alpha \left[\sqrt{-g}^{(x)} \mathscr{L}_{scalar} \left(\phi^{(x)}, \partial_m \phi^{(x)} \right) \\ &+ \sqrt{-g}^{(x)} \frac{\partial \mathscr{L}_{scalar}}{\partial \phi} \left(\phi^{(x)}, \partial_m \phi^{(x)} \right) \epsilon \, v^{(x)} \\ &+ \sqrt{-g}^{(x)} \frac{\partial \mathscr{L}_{scalar}}{\partial \left(\partial_m \phi \right)} \left(\phi^{(x)}, \partial_m \phi^{(x)} \right) \epsilon \, \partial_m v^{(x)} + O\left(\epsilon^2 \right) \right]. \end{split}$$

Integrating the last term by parts, we find that, to first order, the change in the action due to variation $\delta\phi$ is

$$\begin{split} S[\phi + \delta\phi] - S[\phi] &= \int_{x(\mathscr{V})} d^4\alpha \, \left(\epsilon \, v^{(x)}\right) \left[\sqrt{-g}^{(x)} \frac{\partial \mathscr{L}_{scalar}}{\partial \phi} \left(\phi^{(x)}, \partial_m \phi^{(x)}\right) \\ &- \partial_m \left(\sqrt{-g}^{(x)} \frac{\partial \mathscr{L}_{scalar}}{\partial (\partial_m \phi)} \left(\phi^{(x)}, \partial_m \phi^{(x)}\right) \right) \right] \\ &+ \int_{x(\mathscr{V})} d^4\alpha \, \partial_m \left(\sqrt{-g}^{(x)} \frac{\partial \mathscr{L}_{scalar}}{\partial (\partial_m \phi)} \left(\phi^{(x)}, \partial_m \phi^{(x)}\right) \epsilon \, v^{(x)} \right). \end{split}$$

By the divergence theorem, the last integral becomes an integral over the boundary. The boundary integral vanishes by the requirement that v be zero on the boundary.

From the arbitrariness of v it follows that $S[\phi + \delta \phi] - S[\phi] = 0$ if and only if

$$\frac{\partial \mathscr{L}_{scalar}}{\partial \phi} - \frac{1}{\sqrt{-g}} \frac{\partial}{\partial x^m} \left(\sqrt{-g} \frac{\partial \mathscr{L}_{scalar}}{\partial \left((\partial/\partial x^m) \phi \right)} \right) = 0.$$
(2.1)

To see this, note that if equation 2.1 holds, then $S[\phi + \delta \phi] - S[\phi]$ for every $\delta \phi$. Conversely, suppose that equation 2.1 does not hold, then at some point in \mathscr{V} the left hand side is not zero, say positive. By smoothness, the left hand side of 2.1 is then positive in an open neighbourhood of that point. We can choose v to be a positive, smooth function with support contained in this open neighbourhood, but then $S[\phi + \delta \phi] - S[\phi] > 0$. We conclude that for $S[\phi + \delta \phi] - S[\phi]$ to be zero for all $\delta \phi$, equation 2.1 must hold. Equation 2.1 is known as the Euler-Lagrange equation for a scalar field.

One can also derive the Euler-Lagrange equations for the component functions of tensor fields in this way. For a (0, 1)-tensor, i.e. a covector field, $A = A_n dx^n$, the Euler-Lagrange equations are given componentwise by

$$\frac{\partial \mathscr{L}_{scalar}}{\partial A_n} - \frac{1}{\sqrt{-g}} \frac{\partial}{\partial x^m} \left(\sqrt{-g} \frac{\partial \mathscr{L}_{scalar}}{\partial \left(\left(\partial / \partial x^m \right) A_n \right)} \right) = 0.$$

2.2 (3+1)-decomposition of spacetime

Recall that Hamilton's equations in classical mechanics are given by

$$\dot{p} = -\frac{\partial H}{\partial q}$$
 and $\dot{q} = \frac{\partial H}{\partial p}$

The left hand sides of these equations are time derivatives. Hamilton's equations thus describe *evolution in time*. If we want to construct such evolutionary equations on our spacetime manifold, a foliation of the spacetime manifold into spacelike hypersurfaces is needed. Each hypersurface corresponds to a single "time" and time evolution of a field establishes itself as the change of the field along curves transverse to the leaves. In this section, we provide the appropriate extra structure on a general spacetime required for Hamiltonian dynamics.

A foliation of a spacetime M into spacelike hypersurfaces $\Sigma_t \subset M$ is a one-parameter family of smooth embeddings

$$X_t: \Sigma \to M,$$

for $t \in \mathbb{R}$ and some *fixed* three-dimensional manifold Σ such that

- (F.1) $\Sigma_t \coloneqq X_t(\Sigma)$ are the leaves of the foliation,
- (F.2) For every $p \in M$, there is a unique pair (s,t) with $t \in \mathbb{R}$ and $s \in \Sigma$ such that $p = X_t(s)$,
- (F.3) For every vector $V \in T_s \Sigma$ tangent to Σ and every $t \in \mathbb{R}$, the pushforward $X_{t*}V \in T_{X_t(s)}M$ of V along X_t is spacelike with respect to g.

Now suppose that we are given a closed region $\mathscr{V} \subseteq M$ of spacetime with a boundary $\partial \mathscr{V}$ that can be decomposed as

$$\partial \mathscr{V} = \mathscr{B}_i \cup \mathscr{B} \cup \mathscr{B}_f \,,$$

where \mathscr{B} is a timelike submanifold and \mathscr{B}_i and \mathscr{B}_f are spacelike submanifolds, all necessarily of codimension one, of the spacetime manifold M. Let $X_t : \Sigma \to \mathscr{V}$ for $t \in [t_i, t_f]$ be a foliation of \mathscr{V} into spacelike hypersurfaces such that

$$X_{t_i}(\Sigma) = \mathscr{B}_i$$
 and $X_{t_f}(\Sigma) = \mathscr{B}_f$

as well as

$$X_t(\partial \Sigma) \subset \mathscr{B}$$
 for all $t \in (t_i, t_f)$,

hold in addition to properties (F.1), (F.2) and (F.3), see figure 1.



FIGURE 1: Foliation of spacetime into spacelike hypersurfaces.

Let us assume for simplicity that all of Σ can be covered by a single coordinate chart (Σ, y) . The coordinate maps y^{α} on Σ induce a canonical basis for the tangent space $T_s \Sigma$ at $s \in \Sigma$ consisting of the vectors

$$\left(\frac{\partial}{\partial y^1}\right)_s$$
, $\left(\frac{\partial}{\partial y^2}\right)_s$ and $\left(\frac{\partial}{\partial y^3}\right)_s$.

In turn, for every $t \in \mathbb{R}$, the pushforwards

$$(e_{\alpha})_{X_t(s)} \coloneqq X_{t*} \left(\frac{\partial}{\partial y^{\alpha}}\right)_s \in T_{X_t(s)} \Sigma_t$$

of the basis vectors $(\partial/\partial y^{\alpha})_s$ for $T_s\Sigma$ constitute a basis for $T_{X_t(s)}\Sigma_t$.

We want to extend the set $\{(e_{\alpha})_{X_t(s)}\}$ to a basis for $T_{X_t(s)}\mathcal{V}$. One possible way to do this is to choose a covector $(n)_{X_t(s)} \in T^*_{X_t(s)}\mathcal{V}$ that satisfies

(n.1) $(n)_{X_t(s)} \left((e_\alpha)_{X_t(s)} \right) = 0,$

(n.2)
$$g^{-1}((n)_{X_t(s)}, (n)_{X_t(s)}) = 1$$

(n.3) $(e_0)_{X_t(s)} \coloneqq g^{-1}((n)_{X_t(s)}, \cdot)$ is future-directed.

In other words, the vector $(e_0)_{X_t(s)}$ is the *future-directed normal vector* of the hypersurface. The vectors $\{(e_0)_{X_t(s)}, (e_\alpha)_{X_t(s)}\}$ form a basis for $T_{X_t(s)}\mathcal{V}$. This basis constitutes a (3+1)-decomposition of the tangent space $T_{X_t(s)}\mathcal{V}$.

It is crucially important to note that, in general, every coordinate map $x: \mathscr{V} \to \mathbb{R}^4$ will yield

$$e_0 \neq \frac{\partial}{\partial x^0} \,,$$

even though

$$e_{\alpha} = \frac{\partial}{\partial x^{\alpha}}$$

can be achieved for $\alpha = 1, 2, 3$. That is to say that the basis $\{(e_0)_{X_t(s)}, (e_\alpha)_{X_t(s)}\}$ of $T_{X_t(s)}\mathcal{V}$ is not coordinate-induced, but only frame-induced. Nevertheless, it is useful to consider the frame-induced components \bar{g}_{ab} of the spacetime metric which, using properties (n.1) and (n.2), are readily seen to be

$$\bar{g}_{ab} = g(e_a, e_b) = \begin{pmatrix} 1 & 0 \\ 0 & h_{\alpha\beta} \end{pmatrix}$$

where $h_{\alpha\beta} \coloneqq g(e_{\alpha}, e_{\beta})$, however, is coordinate induced. Note that the pullbacks of the metric g along the maps X_t yield a one-parameter family of metrics h_t on Σ . The metrics h_t are Riemannian metrics. Furthermore, by choosing the coordinate chart (\mathcal{V}, x) such that $x^{\alpha}(X_t(s)) = y^{\alpha}(s)$, we have $(h_t)_{\alpha\beta}(s) = h_{\alpha\beta}(X_t(s))$.

In order to devise a (3 + 1)-decomposition of the spacetime metric in terms of components that indeed are induced by coordinates, we will now replace the troublesome e_0 basis vector at each $X_t(s)$ by another vector that is transverse to the hypersurfaces Σ_t and is already defined in terms of the foliation maps X_t . The maps X_t induce a congruence of curves γ_s in \mathscr{V} transverse to Σ_t , where for every $s \in \Sigma$ we have a curve

$$\gamma_s : [t_i, t_f] \to \mathscr{V}, \qquad t \mapsto \gamma_s(t) \coloneqq X_t(s).$$

Now consider a point $p \in \mathscr{V}$. Recall that by (F.2) there is a unique pair (s, t) such that $p = X_t(s)$. Define the vector field T on \mathscr{V} by

$$T_p = T_{X_t(s)} \coloneqq \dot{\gamma}_s(t).$$

The set of vectors $\{T_p, (e_\alpha)_p\}$ is a basis for the tangent space $T_p \mathscr{V}$ and this basis is coordinate induced. In particular, the chart maps x^a that satisfy

$$x^{0}(p) = x^{0}(X_{t}(s)) = t$$
 and $x^{\alpha}(p) = x^{\alpha}(X_{t}(s)) = y^{\alpha}(s),$ (2.2)

are the ones that induce the $\{T_p, (e_\alpha)_p\}$ basis for the tangent space.

Since T_p is a tangent vector at the point p it may written as a linear combination of the vectors $\{(e_0)_p, (e_\alpha)_p\}$. We write this linear combination as

$$T_{X_t(s)} = N_t(s)(e_0)_{X_t(s)} + N_t^{\alpha}(s)(e_{\alpha})_{X_t(s)},$$

where the scalar $N_t : \Sigma \to \mathbb{R}$ is called the *lapse* and $N_t^{\alpha} : \Sigma \to \mathbb{R}$ are the components of a vector field on Σ called the *shift*.

At the point $p = X_t(s)$, the components of the metric g may also be expressed using the $\{T_p, (e_\alpha)_p\}$ basis, which is manifestly coordinate-induced. In terms of the lapse, the shift and the induced metric, we obtain

$$g_{ab}(X_t(s)) = \begin{pmatrix} N_t^2(s) + N_t^{\alpha}(s)N_t^{\beta}(s)(h_t)_{\alpha\beta}(s) & N_t^{\beta}(s)(h_t)_{\alpha\beta}(s) \\ N_t^{\alpha}(s)(h_t)_{\alpha\beta}(s) & (h_t)_{\alpha\beta}(s) \end{pmatrix}$$

for the components of the metric with respect to the chart (\mathcal{V}, x) . From this expression one can see that

$$\det g(p) = N_t^2(s) \det h_t(s),$$

and hence

$$\sqrt{-\det g} = N_t \sqrt{-\det h_t}.$$

Using block matrix formulae for the inverse of a matrix, it can be shown that g^{-1} has the matrix representation

$$g^{ab}(X_t(s)) = \begin{pmatrix} \frac{1}{N_t^2(s)} & -\frac{N_t^\beta(s)}{N_t^2(s)} \\ -\frac{N_t^\alpha(s)}{N_t^2(s)} & (h_t)^{\alpha\beta}(s) + \frac{N_t^\alpha(s)N_t^\beta(s)}{N_t^2(s)} \end{pmatrix}.$$

The coordinate representation g_{ab} of the metric and g^{ab} of the inverse metric are instrumental for doing explicit calculations. Moreover, note that the pullback of the weight-one density $\sqrt{-g}$ on \mathscr{V} along X_t yields the weight-one density $N_t\sqrt{-h_t}$ on Σ . This fact allows for a proper formulation of integrals in coordinates restricted to the spacelike hypersurface Σ_t as integrals over Σ .

2.3 Fields in the (3+1)-decomposition

We have worked out the (3+1)-decomposition of the metric in the previous subsection. In this subsection, we show how scalar and covector fields on \mathscr{V} induce fields on Σ . The fields on Σ will be subject to "time evolution". They are precisely the ones we need to formulate a Hamiltonian theory.

Consider the (3+1)-decomposition of \mathscr{V} characterised by the embeddings

$$X_t: \Sigma \to \mathscr{V},$$

such that $X_{t_i}(\Sigma) = \mathscr{B}_i, X_{t_f}(\Sigma) = \mathscr{B}_f$ and, for every $t \in (t_i, t_f), X_t(\partial \Sigma) \subset \mathscr{B}$. We assume that Σ can be covered by a chart (Σ, y) . For \mathscr{V} we choose a coordinate chart (\mathscr{V}, x) such that the coordinate maps x^m satisfy the relations 2.2.

Now, let $\phi : \mathscr{V} \to \mathbb{R}$ be scalar field on \mathscr{V} . The scalar field ϕ on \mathscr{V} induces a oneparameter family of scalar fields $\phi_t : \Sigma \to \mathbb{R}$, where ϕ_t is defined as the pull-back of ϕ along X_t , i.e.

$$\phi_t := X_t^*(\phi) = \phi \circ X_t.$$

Intuitively, a velocity field ϕ_t on Σ should tell us how ϕ_t changes at at each point when slightly increasing the parameter t. To make this notion precise, let us define the velocity $\dot{\phi}_t$ as the pullback along X_t of the Lie derivative along T, that is

$$\dot{\phi}_t := X_t^*(\mathcal{L}_T \phi)$$

In fact, in the chosen coordinate system, taking the Lie derivative along T is the same as taking the zeroth partial derivative $\partial/\partial x^0$ of ϕ .

The scalar field ϕ on \mathscr{V} thus induces two scalar fields on Σ , ϕ_t and ϕ_t that contain the same information as the original field ϕ in a neighbourhood of the hypersurface Σ_t .

For a covector field $A : \mathscr{V} \to T^*\mathscr{V}$ we have to do some more work. The covector field Aon \mathscr{V} induces a one-parameter family of covector fields $A_t : \Sigma \to T^*\Sigma$ on Σ , where $A_t := X_t^*(A)$. In the chart (\mathscr{V}, x) , we suggestively write A in components as $A = A_0 dx^0 + A_\mu dx^\mu$. The components of A_t are then given by

$$(A_t)_{\mu}(s) = \left(X_t^*(A)\left(\frac{\partial}{\partial y^{\mu}}\right)\right)(s) = A\left(X_{t*}\left(\frac{\partial}{\partial y^{\mu}}\right)_s\right) = A\left(\left(\frac{\partial}{\partial x^{\mu}}\right)_{X_t(s)}\right) = A_{\mu}(X_t(s)),$$

where we have used that the charts satisfy 2.2.

In pulling back A we have exactly lost the zeroth component of A. Note, however, that the component A_0 is totally unimpressed by a change of coordinates on Σ . Indeed, recall that the vector field T on \mathscr{V} is defined without any reference to the coordinates on Σ . We find that the zeroth component of A provides a one-parameter family of a scalar fields $(A_0)_t$ on Σ , defined by

$$(A_0)_t := A_0 \circ X_t.$$

To establish velocities of A_t and $(A_0)_t$ we compute the pullback along X_t of the Lie derivative of A along T. In the (3+1)-decomposed coordinates on \mathscr{V} , the Lie derivative of A along T can be computed using Cartan's magic formula. Let V be an arbitrary smooth

vector field on \mathscr{V} , then at the point $p = X_t(s)$ we have

$$\begin{aligned} (\mathcal{L}_T A)_p V_p &= \iota_T (dA)_p V_p + d(\iota_T (A))_p V_p \\ &= (dA_p) (T_p, V_p) + d(A(T))_p V_p \\ &= \left(\sum_{\mu=1}^3 \left\{ \frac{\partial A_\mu}{\partial x^0} - \frac{\partial A_0}{\partial x^\mu} \right\} \right)_p dx_p^\mu V_p + \left(\frac{\partial A_0}{\partial x^0} dx^0 + \frac{\partial A_0}{\partial x^\mu} dx^\mu \right)_p V_p \\ &= \frac{\partial A_m}{\partial x^0} (p) dx_p^m V_p. \end{aligned}$$

That is, the Lie derivative of A is the covector field on \mathscr{V} with components $\partial A_m / \partial x^0$. The velocity of A_t is then defined by

$$\dot{A}_t := X_t^*(\mathcal{L}_T A) = \left(\frac{\partial A_\mu}{\partial x^0} \circ X_t\right) dy^\mu.$$

Analogously, we define the velocity of the scalar field $(A_0)_t$ as

$$(\dot{A}_0)_t := \frac{\partial A_0}{\partial x^0} \circ X_t.$$

In components, the velocities \dot{A}_0 and \dot{A}_t can thus be computed by taking the partial derivatives with respect to x^0 of the component functions. In the remainder, we shall always use charts on (\mathcal{V}, x) and (Σ, y) such that the relations 2.2 are satisfied such that the constructions given in this subsection apply.

2.4 Hamiltonian field theory for closed systems

With the Lagrangian formalism and the (3+1)-decomposition in place, we are in a position to state the Hamiltonian formulation of field theory on a curved spacetime. The velocities of the fields are replaced by momenta via a partial Legendre transformation. The Hamiltonian is established as a functional of the fields and their momenta. In this subsection, we assume that the Legendre transform is invertible. The next section on gauge theory is dedicated to the the case of a non-invertible Legendre transform. The main result of this subsection will be to present Hamilton's equations for a closed system in terms of the Poisson bracket.

Let us again start by considering a scalar field

$$\phi:\mathscr{V}\to\mathbb{R}.$$

We assume a (3+1)-decomposition of \mathscr{V} and a Lagrangian density $\mathscr{L}(\phi, (\partial/\partial x^m)\phi)$, with respect to the (3+1)-decomposed coordinates (\mathscr{V}, x) , are given. The Lagrangian density \mathscr{L} on \mathscr{V} gives rise to a one-parameter family of weight-one scalar densities $\mathscr{L}_t\left(\phi_t, \dot{\phi}_t, (\partial/\partial y^\mu)\phi_t\right)$ on Σ . Making use of the lapse and the induced metric, the densities \mathscr{L}_t may be written in terms of the scalars $(\mathscr{L}_{scalar})_t$ as

$$\mathscr{L}_t = (\mathscr{L}_{scalar})_t N_t \sqrt{-h_t}.$$

The scalars $(\mathscr{L}_{scalar})_t : \Sigma \to \mathbb{R}$ are defined in the familiar way as $(\mathscr{L}_{scalar})_t := X_t^* (\mathscr{L}_{scalar})$.

The momentum π_t is defined to be

$$\pi_t(\phi_t, \dot{\phi}_t, (\partial/\partial y^{\mu})\phi_t) = \frac{\partial}{\partial \dot{\phi}_t} \mathscr{L}_t(\phi_t, \dot{\phi}_t, (\partial/\partial y^{\mu})\phi_t),$$

indeed, since \mathscr{L}_t is a density of weight +1 and ϕ_t is density of weight 0, the momenta π_t form a one-parameter family of weight-one scalar densities on Σ . Just like the Lagrangian density, the momentum π_t may be decomposed as the product of a scalar field $(\pi_{scalar})_t$ and a density factor $N_t \sqrt{-h_t}$. The momentum π_t thus has an explicit t dependence via the density factor. From here on out, we will work exclusively with the fields and momenta on Σ . To make the notation less cumbersome, we will, in principle, not write their subscript t anymore. Furthermore, we will employ the shorthand ∂_{μ} for the vector field $\partial/\partial y^{\mu}$.

The Lagrangian energy density \mathscr{E}_t is a weight-one scalar density on Σ that depends on ϕ , $\dot{\phi}$ and $(\partial/\partial y^{\mu})\phi$. It is defined as

$$\mathscr{E}_t\left(\phi, \pi\left(\phi, \dot{\phi}, \partial_\mu \phi\right), \partial_\mu \phi\right) = \pi\left(\phi, \dot{\phi}, \partial_\mu \phi\right) \dot{\phi} - N_t \sqrt{-h_t} \,\mathscr{L}_t\left(\phi, \dot{\phi}, \partial_\mu \phi\right).$$

The Hamiltonian density \mathscr{H}_c is a weight-one scalar density that depends on ϕ , π and $\partial_{\mu}\phi$ and satisfies

$$\mathscr{E}_t = \mathcal{F}L^*(\mathscr{H}_t),$$

where $\mathcal{F}L$ is the partial Legendre transform taking $\dot{\phi}$ to π , i.e.

$$\mathcal{F}L(\phi, \dot{\phi}, \partial_{\mu}\phi) = \left(\phi, \pi(\phi, \dot{\phi}, \partial_{\mu}\phi), \partial_{\mu}\phi\right).$$

If the Legendre transform is invertible, then we may write $\dot{\phi}$ as function of ϕ , π and $\partial_{\mu}\phi$. In that case, the Hamiltonian density is simply equal to

$$\mathscr{H}_{t}\left(\phi,\pi,\partial_{\mu}\phi\right) = \pi \,\dot{\phi}\left(\phi,\pi,\partial_{\mu}\phi\right) - N_{t}\sqrt{-h_{t}}\,\mathscr{L}_{t}\left(\phi,\dot{\phi}\left(\phi,\pi,\partial_{\mu}\phi\right),\partial_{\mu}\phi\right).$$

In terms of the Hamiltonian density, we define the Hamiltonian functional

$$H[\phi,\pi](t) = \int_{\Sigma} \mathscr{H}_t(\phi,\pi,\partial_\mu\phi) \, dy^1 \wedge dy^2 \wedge dy^3$$

Let us provide Hamilton's equations of motion for the scalar field ϕ on a stationary spacetime. For a stationary spacetime there exists a (3 + 1)-decomposition in which the lapse, shift and induced metric are independent of t. We take that (3 + 1)-decomposition. The momentum π_t is then no longer explicitly dependent on t. Hamilton's equations now follow analogous to the Euler-Lagrange equations from variation of the action.

Under the assumption of an invertible Legendre transform the action can be expressed in terms of the Hamiltonian density as

$$S[\phi,\pi] = \int_{t_i}^{t_f} \int_{\Sigma} \left[\pi \dot{\phi} \left(\phi,\pi,\partial_{\mu}\phi\right) - \mathscr{H}_t\left(\phi,\pi,\partial_{\mu}\phi,t\right) \right].$$

The field ϕ and momentum π extremize the action if

$$\delta S = S[\phi + \delta\phi, \pi + \delta\pi] - S[\phi, \pi] = 0,$$

where $\delta\phi$ and $\delta\pi$ are variations such that $\delta\phi$ vanishes on the boundary of Σ . We do not require $\delta\pi$ to vanish on the boundary. A similar derivation to the one performed for the Euler-Lagrange equations shows that $\delta S = 0$ if and only if³

$$\dot{\phi} = \frac{\partial \mathscr{H}_t}{\partial \pi}$$
 and $\dot{\pi} = -\frac{\partial \mathscr{H}_t}{\partial \phi} + \partial_\mu \left(\frac{\partial \mathscr{H}_t}{\partial (\partial_\mu \phi)}\right).$ (2.3)

³The variations are performed explicitly in [6].

These are Hamilton's equations of motion for a scalar field.

For a closed system, we may use the Poisson bracket, as introduced in appendix B, to formulate Hamilton's equations of motion in an alternative way. A system is closed if on any given solution to Hamilton's equations, the Hamiltonian functional is constant as a function of t. For the Hamiltonian of a scalar field this amounts to

$$\frac{d}{dt}\left(H[\phi,\pi]\right) = 0,$$

for any solution $(\phi(s,t), \pi(s,t))$ to 2.3. Note that for a general curved spacetime, there are no such solutions because of the explicit *t*-dependence of the Hamiltonian. A Hamiltonian theory on a general curved spacetime is thus inherently *open*. On a stationary spacetime, however, there is a (3+1) decomposition, such that the explicit *t* derivative of the Hamiltonian is zero. Choosing that (3+1)-decomposition, as we did when deriving Hamilton's equations, the *t*-derivative of the Hamiltonian on the solution (ϕ_t, π_t) is zero when

$$\int d^3y \left[\partial_{\nu} \left(\frac{\partial \mathscr{H}_t}{\partial (\partial_{\nu} \phi)}(y) \dot{\phi}(y) \right) \right] = 0.$$

On a stationary spacetime, a closed system is one for which this integral vanishes. Physically, the vanishing of this integral means that no energy enters or leaves the system via its timelike boundary.⁴

Finally, we find that Hamilton's equations as given in 2.3 are equivalent to

$$\dot{\phi}(s) = \{\phi(s), H\}$$
 and $\dot{\pi}(s) = \{\pi(s), H\}$ for all $s \in \Sigma$,

where

$$\phi(s) = \phi[\delta_{y(s)}] := \int \phi(y^{-1}(\alpha))\delta_{y(s)}(\alpha) d^3\alpha.$$

Let us stress that the Poisson bracket formulation is only valid for closed systems on stationary spacetime with the appropriate (3 + 1)-decomposition in which the lapse, shift and induced metric independent of the parameter t.

If the Lagrangian (additionally) depends on a covector field A on Σ , then one can also construct the momentum E conjugate to A. The momentum E is a vector density of weight +1 with components

$$E^{\nu} := \frac{\partial}{\partial (\dot{A})_{\nu}} (\mathscr{L}_t).$$

Following the same construction of the Hamiltonian density and doing the variation of the action componentwise, one finds Hamilton's equations for the components of A_t and E_t to be

$$(\dot{A})_{\nu} = \frac{\partial \mathscr{H}_t}{\partial E^{\nu}} \quad \text{and} \quad (\dot{E})^{\nu} = -\frac{\partial \mathscr{H}_t}{\partial A_{\nu}} + \partial_{\mu} \left(\frac{\partial \mathscr{H}_t}{\partial (\partial_{\mu} A_{\nu})}\right),$$

or, in terms of the Poisson bracket,

$$\dot{A}_{\nu}(s) = \{A_{\nu}(s), H\}$$
 and $\dot{E}^{\nu}(s) = \{E^{\nu}(s), H\}$ for all $s \in \Sigma$.

⁴See appendix A for a discussion of the integral and the boundary terms.

3 Review of gauge theory

In this section, we provide the mathematical framework for gauge theories. A gauge theory is a closed system described by a Lagrangian whose Hessian with respect to the generalized velocities is singular, so that the Hamiltonian still contains arbitrary functions even after a systematic algorithm for the elimination of these arbitrary functions has been executed. The theory is developed in detail for systems with a finite-dimensional phase space. The key constructions carry over to field theory. The electromagnetic field in Minkowski spacetime turns out to be a gauge theory and it is presented as an example at the end of this section.

3.1 Singular Lagrangians and primary constraints

Let us consider a system with a finite-dimensional configuration space Q. The Lagrangian

$$L: TQ \to \mathbb{R}, \qquad (q, v) \mapsto L(q, v)$$

is called singular if the Hessian matrix with respect to the velocities

$$W_{ij} = \frac{\partial^2 L}{\partial v^i \partial v^j},$$

is singular. The Legendre transform

$$\mathcal{F}L: TQ \to T^*Q, \qquad (q, v) \mapsto (q, \hat{p}(v)),$$

where

$$\hat{p}_j(v) = \frac{\partial L}{\partial v^j}(q, v),$$

of such a singular Lagrangian, is not invertible.

Assume that the rank deficiency of the Hessian W_{ij} is equal to some integer k < n constant throughout the tangent bundle TQ. If k is not constant throughout TQ, we restrict our attention to a region of TQ where it is. In the coordinates (q^i, v^j) on TQ, the differential of $\mathcal{F}L$ can be represented by the $2n \times 2n$ matrix

$$d(\mathcal{F}L)_{(q,v)} = \begin{pmatrix} \mathrm{Id}_n & 0\\ * & W_{ij}(q,v) \end{pmatrix}$$

The upper $n \times 2n$ rectangle has rank n and the rank of the lower $n \times 2n$ rectangle is equal to the rank of W_{ij} , which is n - k. In total, the rank of $d(\mathcal{F}L)_{(q,v)}$ is then equal to 2n - k. By the rank theorem⁵, we can, locally, find k independent functions

$$\psi_1, \ldots, \psi_k : T^*Q \to \mathbb{R}^{2n}$$

such that

$$(q,p) \in \operatorname{Im}_{\mathcal{F}L}(TQ) \iff \psi_1(q,p) = 0, \dots, \psi_k(q,p) = 0.$$

The functions ψ_1, \ldots, ψ_k are called the *primary constraints*. Their vanishing defines a surface of codimension k in T^*Q to which the dynamics are restricted. This surface is referred to as the constrained surface.

A foliation of TQ is defined where each leaf is the preimage of a point $(q, p) \in \text{Im}_{\mathcal{F}L}(TQ)$ under the Legendre map. The leaves are surfaces in TQ of codimension 2n - k. A basis

 $^{{}^{5}}$ Theorem 4.12 in [5].

 $\Gamma_i^{(q)}$ of vector fields tangent to the leaf preim_{*FL*}(q, p), is provided in terms of the primary constraints:

$$\Gamma_i^{(q)} = \left(\frac{\partial \psi_i}{\partial p_j}\right)_{(q,\hat{p}(v))} \frac{\partial}{\partial v^j},$$

see [7] for a proof.

The canonical Hamiltonian is defined as the function $H_c : T^*Q \to \mathbb{R}$ such that $\mathcal{F}L^*(H_c) = E$, where $E(q, v) = v^m q_m - L(q, v)$ is the Lagrangian energy. On the image of the Legendre transform, the canonical Hamiltonian is well-defined, since the Lagrangian energy E is in fact constant on every leaf preim_{$\mathcal{F}L$}(q, p) of the foliation. To see this, we act on E with the vector fields Γ_i :

$$\begin{split} \Gamma_i E(q,v) &= \left(\frac{\partial \psi_i}{\partial p_j}\right)_{(q,\hat{p}(q,v))} \frac{\partial}{\partial v^j} \left(v^m \hat{p}_m(q,v) - L(q,v)\right) \\ &= \left(\frac{\partial \psi_i}{\partial p_j}\right)_{(q,\hat{p}(v))} \left(\hat{p}_j(q,v) + v^m \frac{\partial \hat{p}_m}{\partial v^j}(q,v) - \frac{\partial L}{\partial v^j}(q,v)\right) \\ &= \left(\frac{\partial \psi_i}{\partial p_j}\right)_{(q,\hat{p}(v))} v^m \frac{\partial \hat{p}_j}{\partial v^m}(q,v) \\ &= \left(\frac{\partial \psi_i \circ \mathcal{F}L}{\partial v^m}\right)_{(q,v)} v^m \\ &= 0. \end{split}$$

In the second line we have assumed that the Lagrangian is smooth such that the Hessian $\partial \hat{p}_m / \partial v^j$ is symmetric. The last step follows because the constraints are, by definition, constant on the image of the Legendre transform.

Although the canonical Hamiltonian is uniquely defined on $\mathcal{F}L(TQ)$, on the entire phase space T^*Q it is only defined up to an arbitrary linear combination of the primary constraints ψ_i since $\mathcal{F}L^*\psi_i = 0$ for $i = 1, \ldots, k$. In particular, suppose that we have found H_c that satisfies the requirement $\mathcal{F}L^*H_c = E$, then $H_c + v^i\psi_i$, for $v^i(q, p; t)$ arbitrary functions on T^*Q that may depend on time, is as good a canonical Hamiltonian as the H_c we calculated. This leads us to the definition of the *total Hamiltonian* $H_T := H_c + v^i\psi_i$. The ambiguity in the definition of the total Hamiltonian is at the root of gauge symmetry.

3.2 Classifying constraints and the Dirac algorithm

In the case of regular Lagrangian,⁶ once the Hamiltonian is found the equations of motion are formulated in terms of the Poisson bracket as

$$\dot{q} = \{q, H\}$$
 and $\dot{p} = \{p, H\}.$ (3.1)

It turns out that in the singular case, equations 3.1 remain to be true when we replace H by H_T . The dynamics are completely described by the following system of differential and algebraic equations:

$$\begin{cases} \dot{q} = \{q, H_T\} = \{q, H_c\} + v^i \{q, \psi_i\} \\ \dot{p} = \{p, H_T\} = \{p, H_c\} + v^i \{p, \psi_i\} \\ 0 = \psi_i \end{cases}$$
(3.2)

 $^{6}\mathrm{A}$ regular Lagrangian is one with an invertible Hessian matrix.

The splitting of the brackets in the first two lines is justified by the Leibniz identity for the Poisson bracket and the observation that $\{q, v_i\}\psi_i = 0$ on a solution curve, since on a solution curve the constraints $\psi_i = 0$ are satisfied.

Let us stress that equations 3.2 encompass the complete time evolution of the system. However, the differential equations are intertwined with the algebraic equations. There is a more enlightening way to represent the contents of equations 3.2, in which the differential and algebraic equations have been disentangled. This disentangling is done by applying the Dirac algorithm. The key steps of the Dirac algorithm are discussed in the remainder of this subsection.

We start out by defining the time evolution vector field X_H by

$$X_H = \frac{\partial}{\partial t} + \{\cdot, H_c\} + v^i \{\cdot, \psi_i\},$$

where $\partial/\partial t$ has been included to account for explicit time dependencies. Suppose we have a solution curve $\gamma : \mathbb{R} \to T^*Q$ such that on γ equations 3.2 hold. On this solution curve it holds, in particular, that $\psi_i = 0$ for $i = 1, \ldots, k$. Therefore, acting with the time evolution vector field X_H on ψ_i along the curve γ we get zero. From this observation, we deduce the so-called *consistency conditions*

 $X_H(\psi_i)|_{\gamma(t)} = 0$, for all solution curves γ and all $i = 1, \dots, k$.

Computing the consistency conditions explicitly, we have

$$0 = X_H(\psi_j)|_{\gamma(t)} = \{\psi_j, H_c\}|_{\gamma(t)} + v^i \{\psi_j, \psi_i\}|_{\gamma(t)}.$$
(3.3)

Here enters the crucial step of splitting the constraints into two classes, first class and second class. We start by defining first class functions with respect to a set of constraint functions.

Definition 1. Given a set of constraint functions ψ_1, \ldots, ψ_k , a function $f: T^*Q \to \mathbb{R}$ is called first class with respect to ψ_1, \ldots, ψ_k if

$$\{f, \psi_i\} =_{\psi=0} 0 \quad for \ i = 1, \dots, m.$$

The " $\psi = 0$ " below the equality sign indicates that the equality sign is required to hold only on the surface in T^*Q defined by the simultaneous vanishing of the constraint functions ψ_i . A constraint ψ_i is called first class if it is a first class function, that is, when $\{\psi_i, \psi_j\} = 0$ for $j = 1, \ldots, k$. A constraint which is not first class is called second class. Let us relabel the indices of the primary constraints such that for $i \leq p$ the constraints are first class and for i > p the constraints are second class. It can be shown that the matrix of the Poisson brackets of the second class constraints

$$M_{ij} = \{\psi_i, \psi_j\}, \qquad i, j > p,$$

is invertible.

With this classification of the constraints, we are ready to systematically treat the consistency conditions. It turns out that the second class constraints determine some of the arbitrary functions v^i . In particular, from 3.3 it follows that

$$v^i = M^{ij} \{ \psi_j, H_c \}, \qquad i, j > p.$$

The total Hamiltonian can then be redefined to be

$$H_T = H_c + M^{bj} \{ \psi_j, H_c \} \psi_b + v^a \psi_a = H^{(1)} + v^a \psi_a,$$

where b runs over the primary second class constraints and a over the primary first class constraints and $H^{(1)} = H_c + M^{bj} \{\psi_j, H_c\} \psi_b$.

For a first class constraint ψ_i , the right hand side of condition 3.3 becomes

 $\{\psi_i, H_c\}|_{\gamma(t)}.$

If this is already zero for any curve $\gamma(t)$ in the constraint surface, nothing needs to be done. If that is not the case, then $\tilde{\psi}_i := \{\psi_i, H_c\}$ must be included in the set of constraint functions. The new constraints $\tilde{\psi}_i$ coming up in this way are called *secondary constraints*. Suppose that in total we identify m secondary constraints. We rename the secondary constraints to $\psi_{k+1}, \ldots, \psi_{k+m}$ and append them to the list of primary constraints as to obtain the total set of constraint $\{\psi_1, \ldots, \psi_{k+m}\}$. This concludes the first iteration of the Dirac algorithm.

Let us review what was done. We have first classified the constraints as either first or second class. The second class constraints have eliminated some of the arbitrary functions and in the process led us to define $H^{(1)}$. Some of the first class gave rise to new, secondary, constraints that extended our list of existing constraints. The dynamics may be now be in terms of $H^{(1)}$ and the new set of constraints as

$$\begin{cases} \dot{q} = \{q, H^{(1)}\} + v^a \{q, \psi_a\} \\ \dot{p} = \{p, H^{(1)}\} + v^a \{p, \psi_a\} \\ 0 = \psi_i \quad \text{for } i = 1, \dots, k + m \end{cases}$$
(3.4)

Again, we have a Hamiltonian $H^{(1)}$, arbitrary functions v^a and a set of constraints $\psi_1, \ldots, \psi_{k+m}$. We can classify the constraints with respect to the new set into first and second class constraints and work out the consistency relations. We repeat this process until no new constraints come up. When that is the case, we have a final Hamiltonian H', a final set of constraints ψ_1, \ldots, ψ_M and, possibly, arbitrary functions v^a . The final form of the dynamic equations is

$$\begin{cases} \dot{q} = \{q, H'\} + v^a \{q, \psi_a\} \\ \dot{p} = \{p, H'\} + v^a \{p, \psi_a\} \\ 0 = \psi_i, \quad i = 1, \dots, M \end{cases}$$
(3.5)

The differential equations only contain brackets with the primary first class constraints ψ_a . Furthermore, one can check that the Hamiltonian H' is first class. In this form, the algebraic and differential equations are disentangled. If one constructs an initial condition that satisfies the constraints, then the differential equations will automatically preserve the constraints since H' and the ψ_a are first class. That is, one can first solve the algebraic equations and after that, one only has to worry about solving the differential equations.

3.3 Gauge transformations from generating functions

A gauge transformation maps a solution of the dynamic equations to another, infinitesimally close, solution with the same initial conditions. Gauge transformation are canonical transformations in the sense that a dynamical quantity g is taken to $g + \{g, G\}$, where G is a function called the gauge generator. In this subsection, we give the definition of a gauge generator and provide a general ansatz for finding them.

Before we can state the definition of a gauge generator, we need to introduce the concept of a strong equality, as devised by Dirac (see [2]). A function f is said to be strongly equal to zero

$$f \equiv 0$$

with respect to a set of constraints denoted by ψ if both f and its partial derivatives, $\frac{\partial f}{\partial q^i}$ and $\frac{\partial f}{\partial p_j}$, vanish on the constrained surface. Furthermore, a function f is strongly equal to another function g if $f - g \equiv_{\psi=0} 0$.

With this terminology, a gauge generator $G: T^*Q \times \mathbb{R} \to \mathbb{R}$ is a function that satisfies three conditions:

(G.1) G(t) is first class,

(G.2)
$$\frac{\partial G}{\partial t}(t) + \{G(t), H'\} \equiv_{\psi=0} \mathbf{pfcc},$$

(G.3) $\{G(t), \psi_a\} \underset{\psi=0}{\equiv} \mathbf{pfcc},$

where ψ_a are the primary constraints and **pfcc** denotes a linear combination of the primary first class constraints. The gauge generator is required first class such that constraints are preserved under a gauge transformation. Properties (G.2) and (G.3) are chosen such that the gauge generator itself is a conserved quantity, but note that it is a conserved quantity of a special type as the time evolution of the gauge generator is in fact *strongly* equal to zero.⁷

So, how do we find the gauge generator of a system? One way is to use an ansatz of the form

$$G(t) = G_0\xi(t) + G_1\dot{\xi}(t) + \dots + G_N\xi^{(N)}(t), \qquad (3.6)$$

where N is the total number of first class constraints and ξ is an arbitrary function of time. Plugging the ansatz into (G.3), and using that $\xi(t)$ is an arbitrary function of time, we find that

$$\{G_i, \psi_a\} \underset{\psi=0}{\equiv} \mathbf{pfcc}$$

must hold for i = 1, ..., N. If we plug in the ansatz to (G.2), then we find

$$G_0 \dot{\xi} + \dots + G_N \xi^{(N+1)} + \xi \{G_0, H'\} + \dot{\xi} \{G_1, H'\} + \dots + \xi^{(N)} \{G_N, H'\} \underset{\psi=0}{\equiv} \mathbf{pfcc}.$$

Collecting like terms in $\xi^{(n)}$ and noting the arbitrariness of ξ , we conclude that G must satisfy

$$\{G_0, H'\} \underset{\psi=0}{\equiv} \mathbf{pfcc},\tag{3.7}$$

$$G_n \equiv_{\psi=0} -\{G_{n+1}, H'\} + \mathbf{pfcc} \quad \text{for } n = 0, 1, \dots, N-1$$
 (3.8)

$$G_N \underset{\eta \models 0}{\equiv} \mathbf{pfcc.}$$
 (3.9)

The last equation sets G_N to be a linear combination of primary first class constraints. The rest of the G_n are determined recursively by 3.8. Under certain conditions, given in [4], equation 3.7 is also satisfied and one is sure that the ansatz yields a gauge generator. However, even without such conditions, one could still use the ansatz by setting G_N equal to a primary first class constraint and performing the recursion. Doing so, one finds a function G and as long as (G.1), (G.2) and (G.3) are satisfied, G is indeed a gauge generator.

⁷A precise motivation for the properties (G.2) and (G.3) is given in [7].

3.4 The electromagnetic field as a gauge theory

The analysis of gauge theories so far has been performed for systems with a finitedimensional phase space. The constructions provided extend to field theory when the field theory of interest is formulated in terms of the Poisson bracket. As an example, we will work out the gauge symmetries of the electromagnetic field in a Minkowski spacetime using a gauge generator.

We consider the electromagnetic field with potential $A: M \to T^*M$ in a Minkowski spacetime M. Minkowski spacetime can be covered by a single canonical chart in which the metric η is a diagonal matrix $\eta = \text{diag}(1, -1, -1, -1)$. The Lagrangian density for the electromagnetic field is

$$\mathscr{L} = -\frac{1}{4}\eta^{am}\eta^{nb}F_{ab}F_{mn},$$

where $F_{mn} = \partial_m A_n - \partial_n A_m$ are the components of the electromagnetic field tensor F and η^{ab} are the components of the inverse metric which are the same as the components η_{ab} of the metric. In field theory, the Hessian with respect to the velocities is computed with the variational derivative:

$$W^{mn} = \frac{\delta^2 \mathscr{L}}{\delta(\partial_0 A_m) \delta(\partial_0 A_n)}.$$

Since F_{mn} is anti-symmetric $F_{00} = 0$ and, hence, $W^{m0} = W^{0n} = 0$. Working out the rest of the components of the Hessian, we find that, altogether, it is singular with corank 1.

A (3+1)-decomposition of M is trivially established by taking

$$X_t : \mathbb{R}^3 \to \mathbb{R}^4, \qquad (y^1, y^2, y^3) \mapsto (t, y^1, y^2, y^3).$$

We require that the foliation is such that $t = x^0$. Going over to the Hamiltonian formulation, we must first compute the momenta E^0 conjugate to A_0 and E^{μ} conjugate to A_{μ} . The momentum E^0 is directly seen to be

$$E^0 = \frac{\partial \mathscr{L}}{\partial (\partial_0 A_0)} = 0$$

and the components E^{μ} are

$$E^{\mu} = \frac{\partial \mathscr{L}}{\partial (\partial_0 A_{\mu})} = -\frac{1}{2} \eta^{am} \eta^{nb} F_{ab} \left(\delta^0_m \delta^\mu_n - \delta^0_n \delta^\mu_m \right) = \eta^{a\mu} \eta^{0b} F_{ab} = F^{\mu 0}.$$

Note that the conjugate momenta E^{μ} of A_{μ} are the components of the electric field. In the process of calculating the momenta we have already found the primary constraint. The primary constraint ψ_1 is a function of the fields, momenta and their gradients and it is given by

$$\psi_1(A_0, \partial_\mu A_0, E^0, A_\nu, \partial_\mu A_\nu, E^\nu) = E^0.$$

The constraint ψ_1 is a scalar field on Σ . It is useful to define the functional $\Psi_1[v_1]$ as a smeared version of the constraint function ψ_1 :

$$\Psi_1[v_1] = \int d^3y \, v_1\psi_1 \, .$$

Take note that the integral is only over the spatial variables. After a bit of manipulation, the canonical Hamiltonian can be seen to be

$$H_c = \int d^3y \left[\frac{1}{4} \eta^{\alpha\mu} \eta^{\nu\beta} F_{\alpha\beta} F_{\mu\nu} - \frac{1}{2} \eta_{\mu\nu} E^{\mu} E^{\nu} + E^{\mu} \partial_{\mu} A_0 \right].$$

The total Hamiltonian is given in terms of H_c and $\Psi_1[v_1]$, with v_1 an arbitrary function

$$H_T = H_c + \Psi_1[v_1].$$

We assume that the system is closed such that the Poisson bracket formulation of the dynamics applies. The dynamic equations in the form of equation 3.2 are given by

$$\begin{cases} \dot{A}_m(s) &= \{A_m(s), H_c\} + \{A_m(s), \Psi_1[v_1]\} \\ \dot{E}^m(s) &= \{E^m(s), H_c\} + \{E^m(s), \Psi_1[v_1]\} \\ 0 &= \psi_1(s) \end{cases}$$

We now perform the first iteration of the Dirac algorithm. The time evolution operator is

$$X_H = \frac{\partial}{\partial t} + \{\cdot, H_c\} + \{\cdot, \Psi_1[v_1]\}$$

Working out the consistency relation $X_H \psi_1(s) = 0$, we find the secondary constraint

$$\psi_2(s) := \{\psi_1(s), H_c\} = \partial_\mu E^\mu(s).$$

The two constraints ψ_1 and ψ_2 are both first class and no more constraints come up. The canonical Hamiltonian is first class with respect to ψ_1 and ψ_2 . The final form of the dynamic equations is then

$$\begin{cases} \dot{A}_m(s) &= \{A_m(s), H_c\} + \{A_m(s), \Psi_1[v_1]\} \\ \dot{E}^m(s) &= \{E^m(s), H_c\} + \{E^m(s), \Psi_1[v_1]\} \\ 0 &= \psi_1(s) \\ 0 &= \psi_2(s) \end{cases}.$$

The ansatz for the gauge generator in 3.6 has to be slightly modified. The G_i are no longer functions, but they become *functionals* of $\xi^{(i)}$. There are two first class constraints, so the ansatz takes the form

$$G(t) = G_0[\xi](t) + G_1[\xi](t),$$

where $G_i[\xi^{(i)}] = \int \mathcal{G}_i(A_n, E^n, \partial_\mu A_n) \xi^{(i)}(y, t) d^3y$. From 3.9, we know that the functional G_1 must be a primary constraint. There is only one primary constraint, so we have to take

$$G_1 = \Psi_1.$$

It then follows immediately form 3.8 that

$$G_0 = -\Psi_2.$$

In its full form the gauge generator is given by

$$G(t) = -\Psi_2[\xi](t) + \Psi_1[\dot{\xi}](t) = \int d^3y \left[E^0(y)\dot{\xi}(y,t) - (\partial_\mu E^\mu)(y)\xi(y,t) \right].$$

Indeed, this G(t) generates the familiar U(1)-gauge symmetry of the electromagnetic potential:

$$\delta A_0 = \{A_0, G\} = \xi$$
 and $\delta A_\mu = \{A_\mu, G\} = \partial_\mu \xi.$

4 The gauge theory of interacting Klein-Gordon and Maxwell fields

We study the classical dynamics of a charged scalar field interacting with the Maxwellian electromagnetic field on a curved spacetime. It turns out that this is a gauge theory. We start from the Lagrangian formulation of the theory. Some heavy calculational work must be performed to obtain the Hamiltonian. Once the Hamiltonian formulation has been established in the form of equations 3.2, we apply the Dirac algorithm to work out the constraints. Finally, we use the ansatz 3.6 to find the gauge generator of the system.

4.1 The locally gauge invariant Lagrangian

In this subsection, we set up the Lagrangian of a charged, massive scalar field coupled to the electromagnetic field. The scalar field we consider is the Klein-Gordon field. The bare Klein-Gordon field has a global gauge symmetry that is compatible with the local gauge symmetry of the electromagnetic field. To make the global gauge symmetry of the Klein-Gordon field into a local gauge symmetry, the Klein-Gordon field must be coupled to the electromagnetic field. The Lagrangian that describes the coupled system of the Klein-Gordon field interacting with the electromagnetic field is the main result of this subsection. As preparation for the step into Hamiltonian dynamics, we will (3 + 1)-decompose the Lagrangian.

Let (M, g) be a spacetime manifold. We restrict our attention to a region $\mathscr{V} \subseteq M$ that is bounded by closed hypersurface $\partial \mathscr{V}$. We assume that \mathscr{V} can be covered by a single chart (\mathscr{V}, x) . If not, the usual constructions using a smooth atlas for M apply. In this region, consider a complex, massive, charged Klein-Gordon field

$$\phi:\mathscr{V}\to\mathbb{C}.$$

with Lagrangian density

$$\mathscr{L}_{KG}(\phi,\partial_m\phi,\phi^*,\partial_m\phi^*) = \sqrt{-g} \left[g^{ab} \partial_a \phi^* \partial_b \phi - M^2 \phi^* \phi \right]$$

The complex conjugate ϕ^* of ϕ is treated as an independent field on \mathscr{V} .⁸ The Lagrangian density \mathscr{L}_{KG} is invariant under the global gauge transformation

$$\bar{\phi} = e^{iQ\Lambda}\phi$$
 and $\bar{\phi}^* = e^{-iQ\Lambda}\phi^*$,

for some constant Λ . This gauge symmetry corresponds to applying a global phase shift to the Klein-Gordon field.

To make this global gauge symmetry into a local one would mean that we replace the constant Λ by a function $\lambda : \mathscr{V} \to \mathbb{R}$. As given, \mathscr{L}_{KG} is not locally gauge invariant. Indeed, if we plug in $\bar{\phi} = e^{iQ\lambda}\phi$ and $\bar{\phi}^* = e^{-iQ\lambda}\phi^*$ to \mathscr{L}_{KG} extra terms show up. However, by coupling to a covector field with dynamics that are invariant under the transformation

$$\bar{A}_m = A_m + \partial_m \lambda,$$

it turns out that we can make a locally gauge invariant Lagrangian density for the Klein-Gordon field. The potential

$$A:\mathscr{V}\to T^*\mathscr{V},$$

⁸Equivalently, one could take the real and imaginary parts of ϕ as the independent fields.

of the electromagnetic field has precisely this symmetry. Of course, the electromagnetic field also has its own Lagrangian density

$$\mathscr{L}_{EM} = -\sqrt{-g} \, \frac{1}{4} g^{am} g^{bn} F_{ab} F_{mn}.$$

Note that the Lagrangian density for the electromagnetic field is already locally gauge invariant. It turns out that the locally gauge invariant Lagrangian density for the Klein-Gordon coupled to the electromagnetic field is given by

$$\mathscr{L}[A,\phi,\phi^*] = \sqrt{-g} \left[-\frac{1}{4} g^{ma} g^{bn} \left(\frac{\partial}{\partial x^a} A_b - \frac{\partial}{\partial x^b} A_a \right) \left(\frac{\partial}{\partial x^m} A_n - \frac{\partial}{\partial x^n} A_m \right) + g^{mn} \left(\frac{\partial}{\partial x^m} + iQA_m \right) \phi^* \left(\frac{\partial}{\partial x^n} - iQA_n \right) \phi - M^2 \phi^* \phi \right].$$

$$(4.1)$$

We have written the Lagrangian density as a functional of the fields, but in coordinates, the Lagrangian density can be considered a function of the field components and their partial derivatives.

Now assume that we have made a (3 + 1)-decomposition of $\mathscr V$ characterised by the embeddings

$$X_t: \Sigma \to \mathscr{V},$$

for $t \in [t_i, t_f]$ such that $X_{t_i}(\Sigma) = \mathscr{B}_i, X_{t_f}(\Sigma) = \mathscr{B}_f$ and $X_t(\partial \Sigma) \subset \mathscr{B}$ for every $t \in (t_i, t_f)$. The usual assumption that that Σ can be covered by a chart (Σ, y) is in effect. It is furthermore assumed that the chart (\mathcal{V}, x) is the one that satisfies 2.2.

We want to write the Lagrangian density as a function of the time derivatives and the spatial derivatives of the fields on Σ . The first step is to split the full contractions in 4.1 over the Latin indices into full contractions over only Greek indices. The result is:

$$\begin{split} \mathscr{L}[A,\phi,\phi^*] &= \sqrt{-g} \bigg[-\frac{1}{4} g^{\mu\alpha} g^{\beta\nu} (\partial_\alpha A_\beta - \partial_\beta A_\alpha) (\partial_\mu A_\nu - \partial_\nu A_\mu) \\ &- g^{\mu 0} g^{\beta\nu} (\partial_0 A_\beta - \partial_\beta A_0) (\partial_\mu A_\nu - \partial_\nu A_\mu) \\ &- \frac{1}{2} g^{00} g^{\beta\nu} (\partial_0 A_\beta - \partial_\beta A_0) (\partial_0 A_\nu - \partial_\nu A_0) \\ &- \frac{1}{2} g^{0\alpha} g^{0\nu} (\partial_\alpha A_0 - \partial_0 A_\alpha) (\partial_0 A_\nu - \partial_\nu A_0) \\ &+ g^{00} (\partial_0 \phi^* \partial_0 \phi + i Q A_0 \phi^* \partial_0 \phi - i Q A_0 \phi \partial_0 \phi^* + Q^2 A_0 A_0 \phi \phi^*) \\ &+ g^{\mu 0} (\partial_\mu \phi^* \partial_0 \phi + i Q A_\mu \phi^* \partial_0 \phi - i Q A_0 \phi \partial_\mu \phi^* + Q^2 A_\mu A_0 \phi \phi^*) \\ &+ g^{\mu\nu} (\partial_\mu \phi^* \partial_\nu \phi + i Q A_0 \phi^* \partial_\nu \phi - i Q A_\nu \phi \partial_0 \phi^* + Q^2 A_\mu A_\nu \phi \phi^*) - M^2 \phi^* \phi \bigg]. \end{split}$$

In this expression, the shorthand notation ∂_{α} for $\frac{\partial}{\partial x^{\alpha}}$ and ∂_0 for $\frac{\partial}{\partial x^0}$ is used. Using the results of section 2, we can give the Lagrangian density on Σ at time t in terms of the induced fields. We must then replace the derivatives with respect to x^0 by

the velocity fields on Σ . Doing so, we obtain

$$\begin{split} \mathscr{L}_{t}[(A_{0})_{t},A_{t},\phi_{t},\phi_{t}^{*}] &= N\sqrt{-h} \bigg[-\frac{1}{4}g^{\mu\alpha}g^{\beta\nu}(\partial_{\alpha}A_{\beta}-\partial_{\beta}A_{\alpha})(\partial_{\mu}A_{\nu}-\partial_{\nu}A_{\mu}) \\ &-g^{\mu0}g^{\beta\nu}(\dot{A}_{\beta}-\partial_{\beta}A_{0})(\partial_{\mu}A_{\nu}-\partial_{\nu}A_{\mu}) \\ &-\frac{1}{2}g^{00}g^{\beta\nu}(\dot{A}_{\beta}-\partial_{\beta}A_{0})(\dot{A}_{\nu}-\partial_{\nu}A_{0}) \\ &-\frac{1}{2}g^{0\alpha}g^{0\nu}(\partial_{\alpha}A_{0}-\dot{A}_{\alpha})(\dot{A}_{\nu}-\partial_{\nu}A_{0}) \\ &+g^{00}(\dot{\phi}^{*}\dot{\phi}+iQA_{0}\phi^{*}\dot{\phi}-iQA_{0}\phi\dot{\phi}^{*}+Q^{2}A_{0}A_{0}\phi\phi^{*}) - M^{2}\phi^{*}\phi \\ &+g^{\mu0}(\partial_{\mu}\phi^{*}\dot{\phi}+iQA_{\mu}\phi^{*}\dot{\phi}-iQA_{0}\phi\partial_{\mu}\phi^{*}+Q^{2}A_{\mu}A_{0}\phi\phi^{*}) \\ &+g^{0\nu}(\dot{\phi}^{*}\partial_{\nu}\phi+iQA_{\mu}\phi^{*}\partial_{\nu}\phi-iQA_{\nu}\phi\dot{\phi}^{*}+Q^{2}A_{\mu}A_{\nu}\phi\phi^{*}) \\ &+g^{\mu\nu}(\partial_{\mu}\phi^{*}\partial_{\nu}\phi+iQA_{\mu}\phi^{*}\partial_{\nu}\phi-iQA_{\nu}\phi\partial_{\mu}\phi^{*}+Q^{2}A_{\mu}A_{\nu}\phi\phi^{*}) \bigg], \end{split}$$

where all objects are on Σ and the inverse metric components are functions of lapse, shift and h_t . The Lagrangian L can now be taken as

$$L = \int_{\Sigma} \mathscr{L}_t \, dy^1 \wedge d^2 y \wedge dy^3.$$

4.2 Hamiltonian of interacting Klein-Gordon-Maxwell system

With the Lagrangian and the (3 + 1)-decomposition at our disposal, we are ready to compute the Hamiltonian. The first step is to compute the momenta conjugate to the fields on Σ . A single primary constraint will come up in this computation. Then, the Lagrangian energy is defined in terms of the fields, their gradients and the time derivatives. The Hamiltonian is computed such that its pullback along the Legendre transform equals the Lagrangian energy.

Let us set E^{ρ} to be the momentum for A_{ρ} and E^{0} to be the momentum for A_{0} . We let π and π^{*} denote be the momenta for ϕ and ϕ^{*} , respectively. Let us first compute E^{ρ} . At the point s, we have

$$E^{\rho}(s) := \frac{\delta L}{\delta \dot{A}_{\rho}(s)} = \frac{\partial \mathscr{L}_{t}}{\partial \dot{A}_{\rho}}(s)$$

Hence, the components with respect to the chart (Σ, y) of the weight-one vector density E conjugate to the covector field A on Σ are

$$E^{\rho} = \left[g^{\mu 0} g^{\rho \nu} (\partial_{\nu} A_{\mu} - \partial_{\mu} A_{\nu}) + g^{00} g^{\rho \nu} (\partial_{\nu} A_{0} - \dot{A}_{\nu}) + g^{\mu 0} g^{\rho 0} (\dot{A}_{\mu} - \partial_{\mu} A_{0}) \right] N_{t} \sqrt{-h_{t}}.$$

Now consider the momentum E^0 conjugate to A_0 . It is immediately seen from the the Lagrangian density that

$$E^0 = 0,$$

since the Lagrangian density does not contain the term \dot{A}_0 . We have thus found the primary constraint

$$\psi_1(A_0, E^0, \partial_\mu A_0, \partial_\mu E^0, \dots) = E^0.$$

This is the only primary constraint that comes up. Note again that the primary constraint ψ_1 is function of the fields, the momenta and their gradients and, in this case, it happens to be a very simply function.

Now to find π we vary L with respect to ϕ . At the point s, we have that

$$\pi(s):=\frac{\delta L}{\delta \dot{\phi}(s)}=\frac{\partial \mathscr{L}_t}{\partial \dot{\phi}}(s)$$

So, explicitly, the canonical momentum π conjugate to the scalar field ϕ is

$$\pi = \left[g^{00} (\dot{\phi}^* + iQA_0 \phi^*) + g^{\mu 0} (\partial_\mu \phi^* + iQA_\mu \phi^*) \right] N_t \sqrt{-h_t} \,.$$

A similar computation provides the canonical momentum π^* conjugate to the scalar field ϕ^* . Doing the computation one finds that the π^* is really the complex conjugate of π , so the notation is justified. The momenta π and π^* are weight-one scalar densities.

We have defined the Lagrangian on Σ and we have found the canonical momenta. We are now in position to compute the Hamiltonian. Denote by $\mathcal{F}L$ the partial Legendre transform that maps the velocities to the momenta. The canonical Hamiltonian density \mathcal{H}_c is defined such that

$$\mathcal{F}L^*\mathscr{H}_c = \mathscr{E},$$

where

$$\mathscr{E}[A_0, A_\alpha, \phi, \phi^*, \dot{A}_0, \dot{A}_\alpha, \dot{\phi}, \dot{\phi}^*] = \left(E^0 \dot{A}_0 + E^\alpha \dot{A}_\alpha + \pi \dot{\phi} + \pi^* \dot{\phi}^* - \mathscr{L}_t \right)$$

is the Lagrangian energy density. In the Lagrangian energy density, the momenta are functions of the fields and the velocities. To obtain the Hamiltonian we should get rid of the velocities and replace them by the momenta. Getting rid of $\dot{\phi}$ and $\dot{\phi}^*$ is easy. The defining relation between $\dot{\phi}$ and π can be inverted to yield

$$\dot{\phi}(A_0, E^0, A_\alpha, E^\alpha, \phi, \pi, \phi^*, \pi^*) = \frac{\pi^* - g^{\mu 0} N_t \sqrt{-h_t} (\partial_\mu \phi - iQA_\mu \phi)}{g^{00} N_t \sqrt{-h_t}} + iQA_0 \phi,$$

and similarly,

$$\dot{\phi}^*(A_0, E^0, A_\alpha, E^\alpha, \phi, \pi, \phi^*, \pi^*) = \frac{\pi - g^{\mu 0} N_t \sqrt{-h_t} (\partial_\mu \phi^* + i Q A_\mu \phi^*)}{g^{00} N_t \sqrt{-h_t}} - i Q A_0 \phi^*.$$

Replacing the velocities of the electromagnetic field by the E^0 and E^{μ} is not so straightforward. Consider the terms in the Lagrangian energy that contain time derivatives of the covector field A on Σ and rewrite them in terms of the momenta and spatial derivatives. To keep track of indices, we abandon the upper dot as the time derivative for a moment and instead write a ∂_0 . The terms in the Lagrangian energy that contain $\partial_0 A_{\mu}$ are

$$E^{\alpha}\partial_{0}A_{\alpha} - \left\{ -\frac{1}{4}g^{\mu\alpha}g^{\beta\nu}(\partial_{\alpha}A_{\beta} - \partial_{\beta}A_{\alpha})(\partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}) - g^{\mu0}g^{\beta\nu}(\partial_{0}A_{\beta} - \partial_{\beta}A_{0})(\partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}) - \frac{1}{2}g^{00}g^{\beta\nu}(\partial_{0}A_{\beta} - \partial_{\beta}A_{0})(\partial_{0}A_{\nu} - \partial_{\nu}A_{0}) - \frac{1}{2}g^{0\alpha}g^{0\nu}(\partial_{\alpha}A_{0} - \partial_{0}A_{\alpha})(\partial_{0}A_{\nu} - \partial_{\nu}A_{0})\right\}N_{t}\sqrt{-h_{t}}.$$

We start by adding $\partial_{\alpha}A_0 - \partial_{\alpha}A_0$ and after some manipulation using the explicit expression for the components of E, we find that the above terms can be written as

$$E^{\alpha}\partial_{\alpha}A_{0} + \left\{\frac{E^{\alpha}}{2N_{t}\sqrt{-h_{t}}}(\partial_{0}A_{\alpha} - \partial_{\alpha}A_{0}) + \frac{1}{2}g^{\mu0}g^{\beta\nu}(\partial_{0}A_{\beta} - \partial_{\beta}A_{0})(\partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}) + \frac{1}{4}g^{\mu\alpha}g^{\beta\nu}(\partial_{\alpha}A_{\beta} - \partial_{\beta}A_{\alpha})(\partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu})\right\}N_{t}\sqrt{-h_{t}}$$

From this expression the velocities can be eliminated by recognizing that acting on E with the metric yields

$$g_{\alpha\rho}E^{\rho} = \left\{g^{\mu0}F_{\alpha\mu} + g^{00}(\partial_0A_{\alpha} - \partial_{\alpha}A_0)\right\}N_t\sqrt{-h_t}.$$

And hence, by rearranging the terms we have that

$$\left(\partial_0 A_\alpha - \partial_\alpha A_0\right) = -\frac{1}{g^{00}} \left(\frac{g_{\alpha\rho} E^{\rho}}{N_t \sqrt{-h_t}} + g^{\mu 0} F_{\mu\alpha}\right).$$

The right hand side is independent of velocities. Plugging this results into the terms under investigation we thus find, again after some manipulation, that they reduce even further to a velocity independent expression

$$E^{\alpha}\partial_{\alpha}A_{0} - \frac{E^{\alpha}g_{\alpha\rho}E^{\rho}}{2g^{00}N_{t}\sqrt{-h_{t}}} - \frac{E^{\alpha}g^{\mu0}F_{\mu\alpha}}{g^{00}} + \left\{\frac{g^{\mu0}g^{\alpha\nu}g^{0\beta}F_{\alpha\beta}F_{\mu\nu}}{2g^{00}} + \frac{1}{4}g^{\mu\alpha}g^{\beta\nu}F_{\alpha\beta}F_{\mu\nu}\right\}N_{t}\sqrt{-\det h_{t}}$$

So now, we found velocity independent expressions for all the terms in the Lagrangian energy density that originally contained the velocities. In particular, we can now express the Lagrangian energy in terms of the momenta instead of the velocities. That yields the canonical Hamiltonian. Expressing all the velocity terms in terms of the momenta and simplifying the expressions we find that the canonical Hamiltonian densit is given by

$$\begin{aligned} \mathscr{H}_{c} &= E^{\alpha} \partial_{\alpha} A_{0} - \frac{E^{\alpha} g_{\alpha\rho} E^{\rho}}{2g^{00} N_{t} \sqrt{-h}} - \frac{E^{\alpha} g^{\mu 0} F_{\mu \alpha}}{g^{00}} \\ &+ \left\{ \frac{g^{\mu 0} g^{\alpha \nu} g^{0\beta} F_{\alpha\beta} F_{\mu \nu}}{2g^{00}} + \frac{1}{4} g^{\mu \alpha} g^{\beta \nu} F_{\alpha\beta} F_{\mu \nu} \right\} N_{t} \sqrt{-h} + \frac{\pi \pi^{*}}{g^{00} N_{t} \sqrt{-h}} \\ &+ i Q A_{0} (\pi \phi - \pi^{*} \phi^{*}) - \frac{g^{\mu 0}}{g^{00}} (\pi (\partial_{\mu} \phi - i Q A_{\mu} \phi) + \pi^{*} (\partial_{\mu} \phi^{*} + i Q A_{\mu} \phi^{*})) \\ &+ \frac{g^{\mu 0} g^{0 \nu} N_{t} \sqrt{-h}}{g^{00}} (\partial_{\mu} \phi^{*} + i Q A_{\mu} \phi^{*}) (\partial_{\nu} \phi - i Q A_{\nu} \phi) \\ &- g^{\mu \nu} N_{t} \sqrt{-h} (\partial_{\mu} \phi^{*} + i Q A_{\mu} \phi^{*}) (\partial_{\nu} \phi - i Q A_{\nu} \phi) + M^{2} \phi^{*} \phi N_{t} \sqrt{-h}. \end{aligned}$$

The canonical Hamiltonian density is determined up to the product of an arbitrary function v with the primary constraint density ψ_1 . This yields the total Hamiltonian density $\mathscr{H}_T = \mathscr{H}_c + v\psi_1$ and the total Hamiltonian functional

$$H_T = \int_{\Sigma} \mathscr{H}_T \, dy^1 \wedge dy^2 \wedge dy^3 = \int_{\Sigma} \left[\mathscr{H}_c + v\psi_1 \right] \, dy^1 \wedge dy^2 \wedge dy^3.$$

As presented, the Hamiltonian density looks messy. The expression can be cleaned up considerably by making the inverse metric components explicit. Doing so, we find that the total Hamiltonian density can be brought into the more compact form

$$\mathscr{H}_{T} = E^{\alpha} \partial_{\alpha} A_{0} - \frac{Nh_{\alpha\beta} E^{\alpha} E^{\beta}}{2\sqrt{-h}} + N^{\mu} E^{\alpha} F_{\mu\alpha} + \frac{1}{4} h^{\mu\alpha} h^{\beta\nu} F_{\alpha\beta} F_{\mu\nu} N \sqrt{-h} + \frac{N\pi\pi^{*}}{\sqrt{-h}} + iQA_{0}(\pi\phi - \pi^{*}\phi^{*}) + N^{\mu} \left(\pi D_{\mu}\phi + \pi^{*} D_{\mu}^{*}\phi^{*}\right) - h^{\mu\nu} N \sqrt{-h} D_{\mu}^{*} \phi^{*} D_{\nu} \phi + M^{2} \phi^{*} \phi N \sqrt{-h} + v \psi_{1} ,$$

where $D_{\mu} = \partial_{\mu} - iQA_{\mu}$ is the covariant derivative.

Next, we can express the $F_{\mu\nu}$ in terms of the magnetic field components B^{κ} using the Levi-Civita symbol

$$F_{\mu\nu} = -\epsilon_{\mu\nu\kappa}B^{\kappa},$$

where $\epsilon_{123} = 1$. The Levi-Civita symbol $\epsilon_{\mu\nu\kappa}$ is a tensor density of weight -1. Since $F_{\mu\nu}$ is a real tensor, the B^{κ} must be a tensor density of weight +1. This suits us well, since we also have that E^{μ} is a tensor density of weight +1. Multiplying the Levi-Civita symbol by the weight-one scalar density $\sqrt{-h}$, we obtain the Levi-Civita tensor

$$\omega_{\mu\nu\kappa} \coloneqq \sqrt{-h} \,\epsilon_{\mu\nu\kappa}.$$

The Levi-Civita tensor and the magnetic field are related by

$$F_{\mu\nu}\sqrt{-h} = -\omega_{\mu\nu\kappa}B^{\kappa}.$$

This representation is useful since we can raise and lower indices of ω with the metric h. Using the magnetic field components, the fourth term in the Hamiltonian can then be brought into a more enlightening form,

$$\begin{split} \frac{1}{4}h^{\mu\alpha}h^{\beta\nu}F_{\alpha\beta}F_{\mu\nu}N\sqrt{-h} &= \frac{N}{4\sqrt{-h}}h^{\mu\alpha}h^{\beta\nu}\omega_{\mu\nu\kappa}B^{\kappa}\omega_{\alpha\beta\lambda}B^{\lambda}\\ &= \frac{N}{4\sqrt{-h}}h_{\kappa\rho}\omega^{\alpha\beta\rho}\omega_{\alpha\beta\lambda}B^{\kappa}B^{\lambda}\\ &= -\frac{Nh_{\kappa\lambda}B^{\kappa}B^{\lambda}}{2\sqrt{-h}}, \end{split}$$

where we contracted the ω 's in the last line using

$$\omega^{\alpha\beta\rho}\omega_{\alpha\beta\lambda} = \frac{\operatorname{sgn}(\det h)}{|\det h|} \epsilon^{\alpha\beta\rho}\epsilon_{\alpha\beta\lambda} = -2\delta_{\lambda}^{\rho}.$$

The third term in the Hamiltonian can also be written in terms of the magnetic field as

$$N^{\mu}E^{\alpha}F_{\mu\alpha} = -N^{\mu}E^{\alpha}\epsilon_{\mu\alpha\kappa}B^{\kappa}$$

With all these simplifications in order, we may present the total Hamiltonian density as

$$\mathscr{H}_{T} = E^{\alpha}\partial_{\alpha}A_{0} - \frac{Nh_{\alpha\beta}E^{\alpha}E^{\beta}}{2\sqrt{-h}} - N^{\mu}\epsilon_{\mu\alpha\beta}E^{\alpha}B^{\beta} - \frac{Nh_{\alpha\beta}B^{\alpha}B^{\beta}}{2\sqrt{-h}} + \frac{N\pi\pi^{*}}{\sqrt{-h}} + iQA_{0}(\pi\phi - \pi^{*}\phi^{*}) + N^{\mu}\left(\pi D_{\mu}\phi + \pi^{*}D_{\mu}^{*}\phi^{*}\right) - h^{\mu\nu}N\sqrt{-h}D_{\mu}^{*}\phi^{*}D_{\nu}\phi + M^{2}\phi^{*}\phi N\sqrt{-h} + v\psi_{1}.$$

In the pure electromagnetic terms we recognize $E^2 + B^2$, positive, since $h_{\alpha\beta}$ is negative definite. The third term encodes energy in the electromagnetic field due to the curvature of the underlying spacetime. The importance of the first term $E^{\alpha}\partial_{\alpha}A_0$ will become clear in the next subsection. In the Klein-Gordon terms we recognize $|\pi|^2$, $M^2|\phi|^2$ and $|D_{\mu}\phi|^2$ which all look like reasonable energy terms. Also for the Klein-Gordon field there is a term involving the shift. Of course, the electromagnetic field and the Klein-Gordon field are coupled via the covariant derivative D_{μ} . In addition, they are coupled by an explicit term that represents the product of the charge density with the scalar potential A_0 .

4.3 Hamilton's equations of motion

In this subsection we discuss some of the equations of motion of the Klein-Gordon-Maxwell system. We will see that one of Maxwell's inhomogeneous equations, in particular, the Ampère-Maxwell equation comes up as one of the equations of motion. We will also identify Gauss' law as a secondary constraint.

Recall from section 3 that for a closed system the equations of motion are given by 3.2. Under the assumption of a closed system, we can work out the Poisson brackets to find that we are dealing with the system of differential and algebraic equations given by

$$\begin{split} \dot{E}^{0} &= -\left(\frac{\partial \mathscr{H}_{T}}{\partial A_{0}} - \partial_{\nu} \frac{\partial \mathscr{H}_{T}}{\partial(\partial_{\nu} A_{0})}\right) & \dot{A}_{0} &= \frac{\partial \mathscr{H}_{T}}{\partial E^{0}} \\ \dot{E}^{\mu} &= -\left(\frac{\partial \mathscr{H}_{T}}{\partial A_{\mu}} - \partial_{\nu} \frac{\partial \mathscr{H}_{T}}{\partial(\partial_{\nu} A_{\mu})}\right) & \dot{A}_{\mu} &= \frac{\partial \mathscr{H}_{T}}{\partial E^{\mu}} \\ \dot{\pi} &= -\left(\frac{\partial \mathscr{H}_{T}}{\partial \phi} - \partial_{\nu} \frac{\partial \mathscr{H}_{T}}{\partial(\partial_{\nu} \phi)}\right) & \dot{\phi} &= \frac{\partial \mathscr{H}_{T}}{\partial \pi} \\ \dot{\pi}^{*} &= -\left(\frac{\partial \mathscr{H}_{T}}{\partial \phi^{*}} - \partial_{\nu} \frac{\partial \mathscr{H}_{T}}{\partial(\partial_{\nu} \phi^{*})}\right) & \dot{\phi}^{*} &= \frac{\partial \mathscr{H}_{T}}{\partial \pi^{*}} \end{split}$$

subject to $E^0 = 0$.

Direct computation of the right hand sides of these equations leads us to explicit equations of motion. The explicit equations of motion are listed in appendix C. There are three equations that deserve special attention. The first of which is the equation for \dot{A}_0 . There is a single term in the total Hamiltonian density that contains E^0 , namely, the arbitrary multiple of the constraint. The velocity of A_0 is thus given by

$$\dot{A}_0 = v,$$

where v is an arbitrary function. In other words, the time evolution of A_0 is arbitrary, and hence, physically insignificant. Gauge theories are often said to have more degrees of freedom then are physically necessary, and, indeed, A_0 has turned out to be such a redundant degree of freedom. In fact, since $E^0 = 0$ for every physical solution, E^0 itself is also a redundant degree of freedom of the system.

The second equation that is interesting to consider is the time derivative of the E^{μ} , that is, as we have seen, the time derivative of the components of the electric field density. The equation of motion for E^{μ} is

$$\begin{split} \dot{E}^{\mu} &= -N_t^{\mu} i Q \left(\pi^* \phi^* - \pi \phi \right) + i Q h^{\mu\nu} N_t \sqrt{-h} \left(\phi^* D_{\nu} \phi - \phi D_{\nu}^* \phi^* \right) \\ &+ E^{\mu} \partial_{\rho} N_t^{\rho} + N_t^{\rho} \partial_{\rho} E^{\mu} - N_t^{\mu} \partial_{\rho} E^{\rho} - E^{\rho} \partial_{\rho} N_t^{\mu} + \partial_{\rho} (h^{\kappa\rho} h^{\mu\nu} F_{\kappa\nu} N_t \sqrt{-h}) \end{split}$$

This expression is complicated because of all the lapses and shifts flying around. Let us interpret the equation under the assumption that the shift is zero, which can be achieved for so-called static spacetimes. Using the Levi-Civita tensor, we can also rewrite the last term using the magnetic field density to obtain

$$\dot{E}^{\mu} = iQh^{\mu\nu}\sqrt{-h}\left(\phi^*D_{\nu}\phi - \phi D_{\nu}^*\phi^*\right) - \partial_{\rho}(\omega^{\rho\mu\sigma}B_{\sigma}).$$

Note that $\partial_{\rho}(\omega^{\rho\mu\sigma}B_{\sigma})$ are the components of $-\nabla \times \vec{B}$ and $iQh^{\mu\nu}\sqrt{-h}(\phi^*D_{\nu}\phi - \phi D_{\nu}^*\phi^*)$ is equal to minus the spatial components of the Noether conserved current of the locally gauge invariant Klein-Gordon field in flat spacetime. The Noether conserved quantity of the Klein-Gordon field is the electric charge. Denoting the Noether conserved current of

the Klein-Gordon field by J^{μ} , the conservation law $\partial_{\mu}J^{\mu}$ is equivalent to the continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{J}$$

which comes up in the vector calculus formulation of electrodynamics. The zeroth component of the Noether current is the charge density, while the spatial components of the Noether current are the components of the current vector \vec{J} . We thus find that the equations of motion for E^{μ} in flat spacetime are equivalent to

$$\frac{\partial}{\partial t}\vec{E} = \nabla \times \vec{B} - \vec{J},$$

which is the Ampère-Maxwell equation in the language of vector calculus.

The final equation we will consider in this section, and that is absolutely crucial to investigate, is, of course, the time derivative of E^0 . The primary constraint ψ_1 is equal to E^0 , so the consistency relation tells us that

$$\dot{E}^{0} = 0.$$

Computating Hamilton's equation for \dot{E}^0 shows, however, that,

$$\dot{E}^0=\partial_
u E^
u-iQ\left(\phi\pi-\phi^*\pi^*
ight).$$

We have thus found a secondary constraint

$$\psi_2 := \partial_\nu E^\nu - iQ \left(\phi \pi - \phi^* \pi^*\right).$$

There are no more primary constraints to check for consistency, so ψ_2 is the only secondary constraint that comes up at this stage.

The secondary constraint is, in fact, the remaining inhomogeneous Maxwell equation. The term $\partial_{\nu}E^{\nu}$ is equivalent to the divergence of the electric field. Furthermore, the zeroth component of the Noether conserved current is $iQ(\phi g^{0m}D_m^*\phi^* - \phi^*g^{0m}D_m\phi)$. Looking at the expressions we have for the momenta π and π^* , we see that we have $\pi = (g^{00}D_0^*\phi^* + g^{0\mu}D_{\mu}^*\phi^*)N\sqrt{-h}$ and $\pi^* = (g^{00}D_0\phi + g^{0\mu}D_{\mu}\phi)N\sqrt{-h}$. Hence, $iQ(\phi\pi - \phi^*\pi^*)$ is the zeroth component of the Noether conserved current, i.e. the charge density. The secondary constraint is thus equivalent to Gauss' equation.

4.4 The gauge symmetries

We have performed the first iteration of the Dirac algorithm in the previous section. In this section, we perform the second iteration starting from the system with Hamiltonian H_c and constraints ψ_1 and ψ_2 . We will find that no more constraints come up. Subsequently, the gauge generator is constructed using the ansatz 3.6. From the gauge generator we recover the expected gauge symmetries of the fields.

At this stage in the Dirac algorithm, we have two constraints ψ_1 and ψ_2 . The constraint ψ_1 appears with an arbitrary factor v in the total Hamiltonian density. In the total Hamiltonian functional we integrate over $v\psi_1$. This suggests we define the constraint functionals

$$\Psi_1[v_1] = \int_{\Sigma} E^0 v_1 \, dy^1 \wedge dy^2 \wedge dy^3,$$

and

$$\Psi_2[v_2] = \int_{\Sigma} \left[\left(\partial_{\nu} E^{\nu} - iQ(\phi \pi - \phi^* \pi^*) \right) v_2 \right] dy^1 \wedge dy^2 \wedge dy^3,$$

where v_1 and v_2 are arbitrary functions.

Let us explicitly perform the next iteration of the Dirac algorithm to check if more constraints come up. First, we classify the two constraints that we have as either first class or second class. By the skew-symmetry of the Poisson bracket, they must of course be of the same class. The classification is readily done since ψ_1 only depends on E^0 , but ψ_2 does not depend on A^0 . We thus already conclude that

$$\{\Psi_1[v_1], \Psi_2[v_2]\} = 0.$$

The bracket of the constraints vanishes, therefore both constraints are first class. The arbitrary function in the total Hamiltonian remains and, in particular, the canonical Hamiltonian is not modified.

We should now perform the consistency check. For this, we must compute the bracket of $\Psi_2[v_2]$ with H_c . For general v_2 and on a solution to the dynamics, the bracket is given by

$$\{\Psi_2[v_2], H_c\} = \int d^3w \left[\frac{\delta\Psi_2[v_2]}{\delta A_m(w)} \frac{\delta H_c}{\delta E^m(w)} - \frac{\delta\Psi_2[v_2]}{\delta E^m(w)} \frac{\delta H_c}{\delta A_m(w)} \right. \\ \left. + \frac{\delta\Psi_2[v_2]}{\delta\phi(w)} \frac{\delta H_c}{\delta\pi(w)} - \frac{\delta\Psi_2[v_2]}{\delta\pi(w)} \frac{\delta H_c}{\delta\phi(w)} \right. \\ \left. + \frac{\delta\Psi_2[v_2]}{\delta\phi^*(w)} \frac{\delta H_c}{\delta\pi^*(w)} - \frac{\delta\Psi_2[v_2]}{\delta\pi^*(w)} \frac{\delta H_c}{\delta\phi^*(w)} \right]$$

The first term is obviously zero. The second term is nonzero for m = 1, 2, 3. For these indices we get⁹

$$-\int d^3w \frac{\delta \Psi_2[v_2]}{\delta E^{\mu}(w)} \frac{\delta H_c}{\delta A_{\mu}(w)} = -\int d^3w \left[-\left(\partial_{\nu} \frac{\partial(v_2 \,\psi_2)}{\partial(\partial_{\nu} E^{\mu})}\right) \left(\frac{\partial \mathscr{H}_c}{\partial A_{\mu}} - \partial_{\kappa} \frac{\partial \mathscr{H}_c}{\partial(\partial_{\kappa} A_{\mu})}\right) \right]$$
$$= -\int d^3w \left[\partial_{\nu} \left(v_2 \delta^{\nu}_{\mu}\right) \dot{E}^{\mu} \right]$$
$$= \int d^3w \, v_2 \, \partial_{\nu} \dot{E}^{\nu},$$

where we used integration by parts in the last step under the assumption that v_2 is zero on the boundary such that the boundary term vanishes. The other terms can be computed by a similar calculation. Altogether, the resulting bracket is

$$\{\Psi_2[v_2], H_c\} = \int d^3w \left[v_2(w) \partial_\mu \dot{E}^\mu(w) - iQv_2(w) \left(\pi(w) \dot{\phi}(w) + \phi(w) \dot{\pi}(w) - \pi^*(w) \dot{\phi}^*(w) - \phi^*(w) \dot{\pi}^*(w) \right) \right].$$

Using Hamilton's equations of motion we can explicitly calculate the terms. For the

⁹See appendix B an account of (computation of) functional derivatives.

electric field term we have from Hamilton's equation of motion that

$$\begin{aligned} \partial_{\mu}\dot{E}^{\mu} &= \partial_{\mu}\bigg(-N_{t}^{\mu}iQ\left(\pi^{*}\phi^{*}-\pi\phi\right)+iQh^{\mu\nu}N_{t}\sqrt{-h}\left(\phi^{*}D_{\nu}\phi-\phi D_{\nu}^{*}\phi^{*}\right) \\ &+E^{\mu}\partial_{\rho}N_{t}^{\rho}+N_{t}^{\rho}\partial_{\rho}E^{\mu}-N_{t}^{\mu}\partial_{\rho}E^{\rho}-E^{\rho}\partial_{\rho}N_{t}^{\mu}+\partial_{\rho}(h^{\kappa\rho}h^{\mu\nu}F_{\kappa\nu}N_{t}\sqrt{-h})\bigg) \\ &=\partial_{\mu}\bigg(-N_{t}^{\mu}iQ\left(\pi^{*}\phi^{*}-\pi\phi\right)+iQh^{\mu\nu}N_{t}\sqrt{-h}\left(\phi^{*}D_{\nu}\phi-\phi D_{\nu}^{*}\phi^{*}\right)\bigg) \\ &+\partial_{\mu}\partial_{\rho}(E^{\mu}N^{\rho})-\partial_{\mu}\partial_{\rho}(N^{\mu}E^{\rho})+\partial_{\mu}\partial_{\rho}(h^{\kappa\rho}h^{\mu\nu}F_{\kappa\nu}N_{t}\sqrt{-h}) \\ &=\partial_{\mu}\bigg(-N_{t}^{\mu}iQ\left(\pi^{*}\phi^{*}-\pi\phi\right)+iQh^{\mu\nu}N_{t}\sqrt{-h}\left(\phi^{*}D_{\nu}\phi-\phi D_{\nu}^{*}\phi^{*}\right)\bigg).\end{aligned}$$

where the last terms vanish since full contraction of the symmetric $\partial_{\mu}\partial_{\rho}$ with objects that are anti-symmetric in the indices μ and ρ yields zero. For the Klein-Gordon field terms we find that, again using Hamilton's equations,

$$iQ\left(\pi\dot{\phi} + \phi\dot{\pi} - \pi^{*}\dot{\phi}^{*} - \phi^{*}\dot{\pi}^{*}\right) = iQ\partial_{\mu}(N^{\mu}\pi\phi - N^{\mu}\pi^{*}\phi^{*}) - iQ\partial_{\mu}(h^{\mu\nu}N_{t}\sqrt{-h}[\phi D_{\nu}^{*}\phi^{*} - \phi^{*}D_{\nu}\phi]).$$

Upon combining the terms we find that

$$\{\psi_2(y), H_c\} = 0.$$

The Dirac algorithm thus terminates at this point. So that is it, the primary constraint ψ_1 and the secondary constraint ψ_2 are the only constraints that come up and they are both first class.

We take the ansatz 3.6 for the gauge generator. Since we only have one primary first class constraint, there is (up to signs) just one choice for the gauge generator. We choose the signs such that the ansatz for G(t) becomes

$$G(t) = \int d^3y \left[E^0(y) \frac{\partial \Lambda}{\partial t}(y,t) - \left[(\partial_\nu E^\nu)(y) - iQ(\phi\pi - \phi^*\pi^*)(y) \right] \Lambda(y,t) \right],$$

where

$$\Lambda: \Sigma \times [t_i, t_f] \to \mathbb{R}$$

is arbitrary. To see that G is indeed a gauge generator, we check the conditions as stated in section 3:

- 1. G(t) is first class with respect to ψ_1 and ψ_2 .
- 2. $\frac{\partial G}{\partial t} + \{G, H_c\} \equiv \mathbf{pfcc}$
- 3. $\{G, \psi_1(y)\} \equiv \mathbf{pfcc},$

where the strong equalities are taken with respect to the constraints ψ_1 and ψ_2 . For the first condition, we compute the brackets of G with $\Psi_1[v_1]$ and $\Psi_2[v_2]$. This results in

$$\{G, \Psi_1[v_1]\}(t) = 0, \{G, \Psi_2[v_2]\}(t) = 0,$$

both brackets vanish for all possible field configurations, even for $E^0 \neq 0$, thus G is first class and condition 1 is satisfied. Moreover, the vanishing of the bracket of G with $\Psi_1[v_1]$ for every possible field configuration already verifies condition 3. It remains to check condition 2. We have that

$$\begin{split} \{G, H_c\}(t) &= \int d^3y \bigg[-\frac{\delta H_c}{\delta A_0(y)} \frac{\partial \Lambda}{\partial t}(y, t) - \frac{\delta H_c}{\delta A_\mu(y)} (\partial_\mu \Lambda)(y, t) \\ &+ iQ\Lambda(y, t) \left(\pi(y) \frac{\delta H_c}{\delta \pi(y)} - \phi(y) \frac{\delta H_c}{\delta \phi(y)} - \pi^*(y) \frac{\delta H_c}{\delta \pi^*(y)} + \phi^*(y) \frac{\delta H_c}{\delta \phi^*(y)} \right) \bigg], \end{split}$$

All these variational derivatives have once been computed to find the equations of motion which are listed in appendix C. Using the explicit formulae, and integrating the second term by parts we find that it cancels with the third term.

The partial derivative of G(t) with respect to t hits the explicit time dependence of G(t), which is only in Λ , so

$$\frac{\partial G}{\partial t}(t) = \int d^3y \left[E^0(y) \frac{\partial^2 \Lambda}{\partial t^2}(y,t) - \left[(\partial_\nu E^\nu)(y) - iQ(\phi\pi - \phi^*\pi^*)(y) \right] \frac{\partial \Lambda}{\partial t}(y,t) \right].$$

Combining the bracket and the explicit time derivative we find

$$\frac{\partial G}{\partial t}(t) + \{G, H_c\}(t) = \int d^3y \left[E^0(y) \frac{\partial^2 \Lambda}{\partial t^2}(y, t) \right].$$

Rearranging the terms and employing the definition of the constraint functional Ψ_1 , we have that for all possible field configurations, including the ones where $E^0 \neq 0$,

$$\frac{\partial G}{\partial t}(t) + \{G, H_c\}(t) - \Psi_1\left[\frac{\partial^2 \Lambda}{\partial t^2}\right](t) = 0.$$

This ensures the strong equality, and, hence, condition 2 is satisfied. We conclude that

$$G(t) = \int d^3y \left[E^0(y) \frac{\partial \Lambda}{\partial t}(y,t) - \left[(\partial_\nu E^\nu)(y) - iQ(\phi\pi - \phi^*\pi^*)(y) \right] \Lambda(y,t) \right], \qquad (4.2)$$

indeed constitutes a gauge generator.

With the gauge generator at our disposal, we can easily compute the gauge transformations that it induces. The gauge transformations of the potential and the Klein-Gordon field are found to be:

$$(\delta A_0(y))(t) = \{A_0(y), G(t)\} = \frac{\delta G}{\delta E^0(y)} = (\partial_0 \Lambda)(y, t), (\delta A_\mu(y))(t) = \{A_\mu(y), G(t)\} = \frac{\delta G}{\delta E^\mu(y)} = (\partial_\mu \Lambda)(y, t)$$

and

$$(\delta\phi(y))(t) = \{\phi(y), G(t)\} = \frac{\delta G(t)}{\delta\pi(y)} = iQ\Lambda(y, t)\phi(y).$$

The gauge transformations for the A_m are of the form

$$\bar{A}_m(y)(t) = A_m(y)(t) + (\partial_m \Lambda)(y, t).$$

For ϕ the gauge transformations look like

$$\bar{\phi}(y)(t) = \phi(y)(t) + iQ\Lambda(y,t)\phi(y)(t) = e^{iQ\Lambda(y,t)}\phi(y)(t) + O(\Lambda^2).$$

To first order, we get all the gauge symmetries that we expect from the local gauge principle. In particular, we have found that the gauge symmetries of the interacting Klein-Gordon and Maxwell fields are given by *simultaneous* transformations, both depending on the same function Λ .

5 A port-Hamiltonian theory of the Klein-Gordon-Maxwell system

The theory of Hamiltonian mechanics developed so far deals with closed systems. In this section, we introduce the port-Hamiltonian view of dynamics which is an extension of Hamiltonian dynamics that allows for the description of open systems by encoding the energy exchange of a system with its environment in so-called ports. A port consists of a pair of algebraically dual variables whose intrinsic dual product yields a power. Power preserving interconnections of systems are achieved by connecting ports via a Dirac structure that encodes the redistribution of power. We provide a port-Hamiltonian description of the closed system constituted by the Klein-Gordon field coupled to the electromagnetic field. By introducing extra ports one could open up the system, but we will not do so here.

5.1 Dirac structure over a linear space

At the core of port-Hamiltonian theory is the Dirac structure. Dirac structures provide a generalization of the symplectic structure in Hamiltonian dynamics. In particular, Dirac structures generalize the Poisson bracket. Physically, a Dirac structure represents a power preserving interconnection of different systems. This interconnection of different systems is characterised by two algebraically dual variables called the flow f and the effort e. The 2-tuple (f, e) constitutes a port. The power transmitted through this port is given by the dual product of the effort and flow, written as P = e(f).¹⁰ The details are provided in this subsection.

Let us work towards the definition of a Dirac structure. We start by considering a linear space \mathcal{F} . The flows f are elements of \mathcal{F} . The efforts e are linear functionals

$$e:\mathcal{F}\to\mathbb{R}$$

that is, they are elements of the linear dual space \mathcal{F}^* . A port configuration (f, e) is an element of the linear space $\mathcal{F} \oplus \mathcal{F}^*$. The pairing P of the flow and effort (f, e) is given by

$$P: \mathcal{F} \oplus \mathcal{F}^* \to \mathbb{R}, \qquad (f, e) \mapsto e(f).$$

Note that because of the linear structures on \mathcal{F} and \mathcal{F}^* , the map P is linear. The physical interpretation of P(f, e) is as the power transmitted through the port with configuration (f, e). In terms of the pairing P we may define a symmetric bilinear form

$$\langle \langle \cdot, \cdot \rangle \rangle : (\mathcal{F} \oplus \mathcal{F}^*) \times (\mathcal{F} \oplus \mathcal{F}^*) \to \mathbb{R},$$

by

$$\langle\langle(f,e),(f',e')\rangle\rangle \coloneqq P(f,e') + P(f',e) = e'(f) + e(f') + e(f'$$

We are now ready to state the definition of a Dirac structure D over the linear space \mathcal{F} .

Definition 2. A Dirac structure D over a linear space \mathcal{F} is a linear subspace

$$D \subset \mathcal{F} \oplus \mathcal{F}^*,$$

such that

$$D = D^{\perp},$$

where D^{\perp} is the orthogonal complement of D with respect to the bilinear form $\langle \langle \cdot, \cdot \rangle \rangle$.

¹⁰It is customary to write this natural pairing as $\langle e|f\rangle$ (see [3]). This notation has the danger of being interpreted as an inner product, since it is used like that in quantum mechanics. The natural pairing is, however, the dual product, not the inner product. We will therefore avoid the bra-ket notation for the dual product.

Indeed, this definition gives us the desired power preservation. Consider an arbitrary flow-effort pair $(f, e) \in D$. Since $(f, e) \in D$, we also have that $(f, e) \in D^{\perp}$. That implies that

$$\langle \langle (f, e), (f, e) \rangle \rangle = 2e(f) = 0,$$

i.e. P(f,e) = e(f) = 0. The condition that $D = D^{\perp}$ also ensures that all (f,e) that are power preserving are included in D. A proof of this in the case of a finite-dimensional linear space \mathcal{F} is given in [3].

5.2 Some fundamental ports

In the previous subsection we used (f, e) to denote a port and we defined the Dirac structure as all of the power preserving port configurations (f, e). The flows f were taken from an abstract linear space \mathcal{F} and the efforts e from the dual space \mathcal{F}^* . In this subsection, we will refine this view. In particular, we will decompose the linear space \mathcal{F} in a direct sum of smaller linear spaces. Each smaller space will correspond to a physically different mechanism of power transfer.

In general, the one port (f, e) can build up from four different ports, which represent four physically distinct types of power transfer. There are two ports that deal with *internal* power distribution and two ports that deal with *external* power distribution. The internal ports are the storage port S and the resistive port \mathcal{R} . For our purposes, the only internal port that we need is the storage port. The configurations of the storage port will be denoted $(f_S, e_S) \in \mathcal{F}_S \oplus \mathcal{F}_S^*$. The external ports are the interaction port \mathcal{I} and the control port \mathcal{C} , their port variables are $(f_I, e_I) \in \mathcal{F}_I \oplus \mathcal{F}_I^*$ and $(f_C, e_C) \in \mathcal{F}_C \oplus \mathcal{F}_C^*$, respectively.

Let us first discuss the storage port. The storage port on the Dirac structure is interconnected to the port of the energy storage of the system, which is a finite-dimensional manifold $\mathscr X$ together with a function

$$H:\mathscr{X}\to\mathbb{R}$$

The function H generally has the interpretation of the total energy of the system. The pairing of the flow and effort variables of the energy storage then deserves the interpretation of the change in stored energy of the system, i.e. the power coming into the system. Consider a solution curve

$$X: \mathbb{R} \to \mathscr{X}.$$

The change in energy of the system over time on this solution curve at a certain time t_0 is given by

$$\left. \frac{d}{dt} (H \circ X) \right|_{t=t_0} = (dH)_{X(t_0)} \dot{X}(t_0).$$

Note that $\dot{X}(t_0)$ is an element of $T_{X(t_0)} \mathscr{X}$ and $(dH)_{X(t_0)}$ is an element of $T^*_{X(t_0)} \mathscr{X}$. We take the tangent spaces $T_x \mathscr{X}$ as the spaces of flows of the energy storage and the cotangent spaces $T^*_x \mathscr{X}$ as the effort spaces. The flow and effort spaces are thus modulated by the current state $x \in \mathscr{X}$. The power preserving interconnection of the port of the energy storage and the storage port on the Dirac structure is established by setting

$$f_S(t) = -\dot{X}(t)$$
 and $e_S(t) = (dH)_{X(t)}$,

for each time t. In figure 2, a Dirac structure coupled to an energy storage is displayed. The interconnection of the port variables is encoded in the 0 and the Id. The 0 indicates that the sum of f_S and \dot{X} is zero and the Id indicates that e_S equals $(dH)_X$.



FIGURE 2: Dirac structure coupled to energy storage. The relation $e_S = (dH)_X$ is indicated by "Id" and the relation $f_S + \dot{X} = 0$ is indicated by "0". The external ports have not been connected to anything.

One could have a Dirac structure with only a storage port. This would be the case for a closed system. However, when we add external ports we can also describe open systems. The flow is then given by $(f_S, f_I, f_C) \in \mathcal{F}_S \oplus \mathcal{F}_I \oplus \mathcal{F}_C$ and the effort is $(e_S, e_I, e_C) \in \mathcal{F}_S^* \oplus \mathcal{F}_I^* \oplus \mathcal{F}_C^*$. The power preserving feature of the Dirac structure results in the balance equation

$$e_S(f_S) + e_I(f_I) + e_C(f_C) = 0,$$

which with the coupling of the storage port to the energy storage can be written as an energy balance

$$\frac{d}{dt}(H \circ X) = e_C(f_C) + e_I(f_I),$$

on a solution curve X. The Dirac structure D of the total system is now a linear subspace of the direct sum of all flow and effort spaces, i.e.

$$D \subset (\mathcal{F}_S \oplus \mathcal{F}_S^*) \oplus (\mathcal{F}_C \oplus \mathcal{F}_C^*) \oplus (\mathcal{F}_I \oplus \mathcal{F}_I^*).$$

The symmetric pairing $\langle \langle \cdot, \cdot \rangle \rangle_{SCI}$ is directly obtained from the pairings on the storage, control and interaction spaces as

$$\langle \langle (f_S, e_S, f_C, e_C, f_I, e_I), (f'_S, e'_S, f'_C, e'_C, f'_I, e'_I) \rangle \rangle_{SCI} = \\ \langle (f_S, e_S), (f'_S, e'_S) \rangle \rangle_S + \langle \langle (f_C, e_C), (f'_C, e'_C) \rangle \rangle_C + \langle \langle (f_I, e_I), (f'_I, e'_I) \rangle \rangle_I$$

where $\langle \langle \cdot, \cdot \rangle \rangle_S : (\mathcal{F}_S \oplus \mathcal{F}_S^*) \times (\mathcal{F}_S \oplus \mathcal{F}_S^*) \to \mathbb{R}$, and so on. The Dirac structure is then defined by the requirement that $D = D^{\perp}$ with respect to the bilinear form $\langle \langle \cdot, \cdot \rangle \rangle_{SCI}$.

5.3 The Dirac structure of a gauge theory

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In section 3 we have found that, after completing the Dirac algorithm, the dynamic equations of a gauge theory were given in terms of a first class Hamiltonian H' and primary first class constraints. Additionally, the initial conditions had to satisfy a set of algebraic constraints. Since the Hamiltonian H' was first class, all consistency conditions were satisfied. In this section, we show that the dynamic equations as given in 3.5 together with the consistency relations give rise to a Dirac structure. The constructions are done for a system with a finite-dimensional phase space. Consider a closed system with an n-dimensional configuration space Q. Suppose that we have performed the Dirac algorithm for the closed system and have found the final equations of motion to be provided componentwise by

$$\begin{cases} \dot{q}^m &= \{q^m, H'\} + v^a \{q^m, \psi_a\} \\ \dot{p}_m &= \{p_m, H'\} + v^a \{p_m, \psi_a\} \\ 0 &= \psi_i, \quad i = 1, \dots, M \end{cases}$$

where m = 1, ..., n. Recall that in the context of a finite-dimensional phase space, the Poisson bracket takes two functions $f, g \in C^{\infty}(T^*Q)$ and maps them to a new function

$$\{f,g\} = \sum_{m=1}^{n} \frac{\partial f}{\partial q^m} \frac{\partial g}{\partial p_m} - \frac{\partial g}{\partial q^m} \frac{\partial f}{\partial p_m}.$$

One can work out the Poisson brackets of the q^m and p_m with the first class Hamiltonian H' to be

$$\{q^m, H'\} = \frac{\partial H'}{\partial p_m}$$
 and $\{p_m, H'\} = -\frac{\partial H'}{\partial q^m}.$

Thus, using a column vector of partial derivatives of H', the dynamic equations can be presented as

$$\begin{bmatrix} \dot{q}^{1} \\ \vdots \\ \dot{p}_{n} \end{bmatrix} = \begin{pmatrix} 0 & \mathrm{Id}_{n} \\ -\mathrm{Id}_{n} & 0 \end{pmatrix} \begin{bmatrix} \frac{\partial H'}{\partial q^{1}} \\ \vdots \\ \frac{\partial H'}{\partial p_{n}} \end{bmatrix} + \begin{pmatrix} \{q^{1}, \psi_{1}\} & \cdots & \{q^{1}, \psi_{A}\} \\ \vdots & & \vdots \\ \{p_{n}, \psi_{1}\} & \cdots & \{p_{n}, \psi_{A}\} \end{pmatrix} \begin{bmatrix} v^{1} \\ \vdots \\ v^{A} \end{bmatrix},$$
(5.1)

where A is the total number of primary first class constraints.

In port-Hamiltonian theory, it is known that the set

$$D = \{ (f, e) \in \mathcal{F} \times \mathcal{F}^* \, | \, f = Je + C\lambda, \quad C^*e = 0 \},$$

where J is skew-symmetric, $C: \mathcal{V} \to \mathcal{F}$ for some linear space \mathcal{V} and $\lambda \in \mathcal{V}$ is arbitrary, is a Dirac structure.¹¹ The dynamic equations as given in 5.1 correspond to the equation $f = Je + C\lambda$ in a particular way. In the previous subsection, we have established the modulated flow and effort of a system with one storage port to be $f = -\dot{X}$ and $e = (dH)_X$, where now X(t) = (q(t), p(t)). We recover equation 5.1 from $f = Je + C\lambda$ by setting

$$J = \begin{pmatrix} 0 & -\mathrm{Id}_n \\ \mathrm{Id}_n & 0 \end{pmatrix}, \qquad C = -\begin{pmatrix} \{q^1, \psi_1\} & \cdots & \{q^1, \psi_A\} \\ \vdots & & \vdots \\ \{p_n, \psi_1\} & \cdots & \{p_n, \psi_A\} \end{pmatrix} \qquad \text{and} \qquad \lambda = \begin{bmatrix} v^1 \\ \vdots \\ v^A \end{bmatrix}.$$

The condition $C^*e = 0$ becomes

$$\begin{pmatrix} \{q^1, \psi_1\} & \cdots & \{q^1, \psi_A\} \\ \vdots & & \vdots \\ \{p_n, \psi_1\} & \cdots & \{p_n, \psi_A\} \end{pmatrix}^T \begin{bmatrix} \frac{\partial H'}{\partial q^1} \\ \vdots \\ \frac{\partial H'}{\partial p_n} \end{bmatrix} = 0.$$
 (5.2)

A close investigation of equation 5.2 reveals that it is already satisfied, in fact, it is equivalent to the consistency conditions of the primary first class constraints. Indeed, the

¹¹See the discussion on the *constrained input-output representation* for Dirac structures in [3].

condition in 5.2 is actually a set of A equations. We work out the first equation explicitly. Having done the matrix multiplication, the left hand side of the first equation states

$$\{q^1,\psi_1\}\frac{\partial H'}{\partial q^1} + \dots + \{p_n,\psi_1\}\frac{\partial H'}{\partial p_n} = \frac{\partial \psi_1}{\partial p_1}\frac{\partial H'}{\partial q^1} + \dots - \frac{\partial \psi_1}{\partial q^n}\frac{\partial H'}{\partial p_n} = \{H',\psi_1\}.$$

Since the Hamiltonian H' is first class, the bracket with ψ_1 already vanishes. We conclude that equation 5.1 together with the additional equation 5.2 defines a modulated Dirac structure over the linear spaces $T_{(q,p)}Q$. Together with the total set of constraints ψ_1, \ldots, ψ_M , the Dirac structure defined by 5.1 and 5.2 is equivalent to equations 3.5.

5.4 Klein-Gordon-Maxwell as a port-Hamiltonian system

For the closed Klein-Gordon-Maxwell system, we have calculated all the equations of motion and the gauge generator. In this section, we will revisit the Klein-Gordon-Maxwell system from a port-Hamiltonian point of view. In order to avoid unnecessary technical complications, we restrict attention to stationary spacetimes and we assume that the 3 + 1-decomposition has been chosen such that the lapse, shift and induced metric are independent of the parameter t. We start out by revisiting the storage port in the case of a field theory. Subsequently, we describe the closed system consisting of the Klein-Gordon field coupled to the electromagnetic field with one storage port. The secondary constraint will come up in a natural way when representing the Dirac structure in a constrained input-output representation.

We have developed the storage port in the case of a finite-dimensional state space. The Klein-Gordon-Maxwell system, however, is a field theory and therefore has an infinite-dimensional state space. The Hamiltonian is no longer an ordinary *function* on some finite-dimensional state state space, but a *functional* on the infinite-dimensional space of all possible field configurations. The energy storage (\mathcal{X}, H) of the system is thus given by an infinite-dimensional space of field configurations \mathcal{X} and a functional $H : \mathcal{X} \to \mathbb{R}$.

In order to motivate the choice of storage port variables, let us consider the Hamiltonian of a real Klein-Gordon field. On a solution $(\phi(s,t),\pi(s,t))$ the time derivative of the Hamiltonian can be computed using the chain rule for functional derivatives to be

$$\frac{d}{dt}\left(H[\phi,\pi]\right)(t) = \int d^3y \left[\frac{\delta H}{\delta\phi(y)}[\phi,\pi](y,t)\dot{\phi}(y,t) + \frac{\delta H}{\delta\pi(y)}[\phi,\pi](y,t)\dot{\pi}(y,t)\right].$$

Following the same reasoning as in the finite-dimensional case, we should define the flow f_S and effort e_S at a point $s \in \Sigma$ to be

$$f_S(s) := -\begin{bmatrix} \dot{\phi}(s) \\ \dot{\pi}(s) \end{bmatrix}$$
 and $e_S(s) := \begin{bmatrix} \delta H / \delta \phi(s) \\ \delta H / \delta \pi(s) \end{bmatrix}$.

Recall from appendix B that, for a closed system, the variational derivatives of H are computed as

$$\frac{\delta H}{\delta \phi(y)} = \frac{\partial \mathscr{H}}{\partial \phi}(y) - \partial_{\nu} \frac{\partial \mathscr{H}}{\partial (\partial_{\nu} \phi)}(y) \quad \text{and} \quad \frac{\delta H}{\delta \pi(y)} = \frac{\partial \mathscr{H}}{\partial \pi}(y),$$

since the Hamiltonian density does not depend on the derivatives of the momentum. Since the momentum π and the Hamiltonian density \mathscr{H} are weight-one densities, we have the flow $f_S \in C^{\infty}(\Sigma) \oplus D(\Sigma) =: \mathcal{F}_S$ and the effort $e_S \in D(\Sigma) \oplus C^{\infty}(\Sigma)$. The efforts can be considered elements of the dual space \mathcal{F}^* to $C^{\infty}(\Sigma) \oplus D(\Sigma)$ when we associate to a density σ the functional $i(\sigma)[f] = \int_{\Sigma} \sigma f dy^1 \wedge dy^2 \wedge dy^3$ and we associate to a function g the functional $j(g)[\eta] = \int_{\Sigma} \eta f dy^1 \wedge dy^2 \wedge dy^3$ via maps

$$i: D(\Sigma) \to (C^{\infty}(\Sigma))^*$$
 and $j: C^{\infty}(\Sigma) \to (D(\Sigma))^*$.

We define a pairing

$$P: C^{\infty}(\Sigma) \oplus D(\Sigma) \oplus D(\Sigma) \oplus C^{\infty}(\Sigma) \to \mathbb{R}, \qquad \left(\begin{bmatrix} f \\ \sigma \end{bmatrix}, \begin{bmatrix} \eta \\ g \end{bmatrix} \right) \mapsto \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^3 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 \wedge dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^1 \wedge dy^2 \wedge dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 \wedge dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 \wedge dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 \wedge dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f + g\sigma \right] \, dy^2 + \frac{1}{2} \int_{\Sigma} \left[\eta f +$$

The bilinear form $\langle \langle \cdot, \cdot \rangle \rangle$ is defined in terms of the pairing P in the usual way.

Let us now turn to the Klein-Gordon-Maxwell system. We have the canonical Hamiltonian $H_c[A_0, E^0, A, E, \phi, \pi, \phi^*, \pi^*]$ and the total Hamiltonian $H_T = H_c + \Psi_1[v_1]$, where

$$\Psi_1[v_1] = \int d^3y \,\psi_1(A_0, E^0, \dots)(y)v_1(y, t)$$

is a linear functional of a one-parameter family of arbitrary functions $v_1(\cdot, t) : \Sigma \to \mathbb{R}$. Running the same spiel with calculating the time derivative using the chain rule for variational derivatives as above, we are led to define

$$\tilde{f}_{S}(s) := - \begin{bmatrix} A_{0}(s) \\ \dot{A}_{\mu}(s) \\ \phi(s) \\ \dot{\phi}(s) \\ \dot{\phi}^{*}(s) \\ \dot{E}^{0}(s) \\ \dot{E}^{\mu}(s) \\ \dot{\pi}(s) \\ \dot{\pi}^{*}(s) \end{bmatrix} \quad \text{and} \quad \tilde{e}_{S}(s) := \begin{bmatrix} \delta H_{T}/\delta A_{0}(s) \\ \delta H_{T}/\delta A_{\mu}(s) \\ \delta H_{T}/\delta \phi(s) \\ \delta H_{T}/\delta \phi(s) \\ \delta H_{T}/\delta E^{0}(s) \\ \delta H_{T}/\delta E^{0}(s) \\ \delta H_{T}/\delta \pi^{*}(s) \end{bmatrix} = \begin{bmatrix} \delta H_{c}/\delta A_{0}(s) \\ \delta H_{c}/\delta A_{\mu}(s) \\ \delta H_{c}/\delta \phi(s) \\ \delta H_{c}/\delta \phi(s) \\ \delta H_{c}/\delta E^{0}(s) \\ \delta H_{c}/\delta \pi^{*}(s) \end{bmatrix} + v_{1}(s) \begin{bmatrix} 0 \\ \mathbf{0}_{3\times 1} \\ 0 \\ 1 \\ \mathbf{0}_{3\times 1} \\ \mathbf{0}_{3\times 1} \\ \mathbf{0}_{3\times 1} \\ \mathbf{0}_{3\times 1} \\ \delta H_{T}/\delta \pi^{*}(s) \end{bmatrix}$$

where every component of the vector and covector fields is in a separate entry of the column vectors.

Hamilton's equations tell us that the pointwise flow $f_S(s)$ and effort $\tilde{e}_S(s)$ as given above are related through the skew symmetric matrix

$$J = \begin{pmatrix} 0 & \mathrm{Id}_6 \\ -\mathrm{Id}_6 & 0 \end{pmatrix},$$

where $Id_6 = diag(1, 1, 1, 1, 1, 1)$, as

$$-\tilde{f}_S(s) = J\tilde{e}_S(s).$$

Working out the matrix multiplication, this relation can be expressed as

$$-f_S(s) = Je_S(s) + Cv_1(s),$$

where $f_S(s) = \tilde{f}_S(s)$, $e_S(s)$ is the column vector of variational derivatives of H_c and C is the 12 × 1 column vector with a 1 in the first entry and 0's in the other entries.

For the moment, we restrict our attention the equations for \dot{A}_0 and \dot{E}^0 . That is, we consider the pointwise equation

$$\begin{bmatrix} \dot{A}_0(s) \\ \dot{E}^0(s) \end{bmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{bmatrix} \delta H_c / \delta A_0(s) \\ \delta H_c / \delta E^0(s) \end{bmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} v_1(s).$$

Recall that A_0 is a scalar field on Σ and E^0 is a scalar density of weight +1. Given that \mathscr{H}_c is a weight +1 scalar density, this implies that $\delta H_c/\delta A_0$ is a weight +1 scalar density and $\delta H_c/\delta E^0$ is scalar field. Inspired by the results of the previous section, we propose a Dirac structure.

Theorem 1. The set $D \subset C^{\infty}(\Sigma) \oplus D(\Sigma) \oplus D(\Sigma) \oplus C^{\infty}(\Sigma)$ given by

$$D = \left\{ (f, e) \mid -f = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} e + \lambda \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} 1 & 0 \end{pmatrix} e = 0 \right\},$$

where λ is some arbitrary $C^{\infty}(\Sigma)$ -function, is a Dirac structure. That is, $D = D^{\perp}$, where the orthogonal complement is taken with respect to the symmetric pairing $\langle \langle \cdot, \cdot \rangle \rangle$.

Proof. To condense the notation, we will treat f and e as column vectors, similar to how we treated them in the definition of the pairing earlier in this subsection. In particular, we set

$$f = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$$
 and $e = \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}$,

where $f_1, e_2 \in C^{\infty}(\Sigma)$ and $f_2, e_1 \in D(\Sigma)$.

Showing that $D \subset D^{\perp}$ is straightforward. Take (f, e) and (f', e') in D. It follows that

$$\begin{split} \langle \langle (f,e), (f',e') \rangle \rangle &= \int d^3y \left[e(y)^T f'(y) + e'^T(y) f(y) \right] \\ &= \int d^3y \left[-e^T(y) J e'(y) \right. \\ &\left. -e^T(y) C \lambda'(y) - e'^T(y) J e(y) - e'^T(y) C \lambda(y) \right] \\ &= 0, \end{split}$$

since J is anti-symmetric and $e^T(C\lambda) = C^T(e)\lambda = 0$.

It remains to show that $D^{\perp} \subset D$. To this end, take an element $(f, e) \in D^{\perp}$. For arbitrary $(f', e') \in D$, we then have that the symmetric pairing of (f, e) and (f', e') vanishes. Moreover, using the defining features of $(f', e') \in D$, we obtain

$$0 = \langle \langle (f, e), (f', e') \rangle \rangle = \int d^3y \left[e^T(y) f'(y) + e^{\prime T}(y) f(y) \right] \\ = \int d^3y \left[-e^T(y) J e'(y) - e^T(y) C \lambda'(y) + e^{\prime T}(y) f(y) \right],$$

Rearranging the terms we have

$$\int d^{3}y \left[-e^{T}(y)(J^{T}e(y) - f(y)) - e^{T}(y)C\lambda'(y) \right] = 0.$$

The objects λ' and e' are independent. Suppose we take e' = 0, then still for arbitrary λ' it should hold that the integral vanishes. Hence, we have that $C^T e(s) = 0$ for any $s \in \Sigma$. Next, we realize that the constraint on e' dictates that $e'_1 = 0$ and e'_2 can be chosen arbitrarily. Moreover, $C^T e(s) = 0$ implies that $e_1 = 0$. For $\lambda' = 0$, the above integral thus becomes

$$\int d^3y \left[-\begin{bmatrix} 0 & e_2'(y) \end{bmatrix} \left(\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{bmatrix} 0 \\ e_2(y) \end{bmatrix} - \begin{bmatrix} f_1(y) \\ f_2(y) \end{bmatrix} \right) \right] = 0.$$

This integral vanishes for all $e'_2(y)$ if and only if $f_2(y) = 0$ and $-e_2(y) - f_1(y) = \lambda(y)$ for some arbitrary λ . That is, (f, e) satisfies the pointwise conditions of the Dirac structure, i.e. $(f, e) \in D$.

This concludes the proof that D is a Dirac structure.

The proof easily extends to the case of the full Klein-Gordon-Maxwell system with an adequate pairing for covector fields and weight-one vector densities. We may thus write down the Dirac structure for the closed Klein-Gordon-Maxwell to be all (f_S, e_S) , such that

$$-\begin{bmatrix}\dot{A}_{0}(s)\\\dot{A}_{\mu}(s)\\\dot{\phi}(s)\\\dot{\phi}(s)\\\dot{\phi}(s)\\\dot{e}^{*}(s)\\\dot{E}^{0}(s)\\\dot{E}^{\mu}(s)\\\dot{\pi}(s)\\\dot{\pi}(s)\\\dot{\pi}^{*}(s)\end{bmatrix} = \begin{pmatrix} 0 & \mathrm{Id}_{4}\\ -\mathrm{Id}_{4} & 0 \end{pmatrix} \begin{bmatrix} \delta H_{c}/\delta A_{0}(s)\\\delta H_{c}/\delta A_{\mu}(s)\\\delta H_{c}/\delta \phi(s)\\\delta H_{c}/\delta \phi(s)\\\delta H_{c}/\delta \phi^{*}(s)\\\delta H_{c}/\delta E^{0}(s)\\\delta H_{c}/\delta E^{\mu}(s)\\\delta H_{c}/\delta \pi^{*}(s)\end{bmatrix} + \lambda \begin{pmatrix} 1\\0\\\vdots\\\end{pmatrix}, \quad (1 & 0 & \cdots) \begin{bmatrix} \delta H_{c}/\delta A_{0}(s)\\\delta H_{c}/\delta A_{\mu}(s)\\\delta H_{c}/\delta \phi(s)\\\delta H_{c}/\delta \phi^{*}(s)\\\delta H_{c}/\delta E^{0}(s)\\\delta H_{c}/\delta \pi^{*}(s)\end{bmatrix} = 0,$$

holds pointwise and $\lambda \in C^{\infty}(\Sigma)$ is arbitrary.

With this result, we have verified that the system with storage flow and effort as given above constitutes a Dirac structure when introducing an additional constraint. Notice that the necessary constraint is precisely the secondary constraint that we got in our standard analysis following the Dirac algorithm, namely, $\delta H_c/\delta A_0 = 0$. Moreover, only the primary constraint is explicitly present in the dynamics. We have thus successfully captured the Hamiltonian dynamics of the closed Klein-Gordon-Maxwell system in the language of port-Hamiltonians and Dirac structures. Although we now have the equations of motion and the constraints, it is not at all obvious how the gauge symmetries come up in the port-Hamiltonian formulation.

6 Conclusions

Starting from the locally gauge invariant Lagrangian describing the Klein-Gordon field coupled to the electromagnetic field, we have developed the full classical Hamiltonian description of the Klein-Gordon-Maxwell system on a stationary spacetime. Going from Lagrangian theory to Hamiltonian theory required us to make a (3 + 1)-decomposition of spacetime so that we could talk about dynamics. The Dirac algorithm has been executed to find all constraints of the theory. From the constraints, we have constructed the gauge generator. The gauge generator, indeed, generated the expected gauge symmetries. All this was done under the assumption that no energy entered the system through the timelike boundary. As a preparation to extend the theory to include boundary energy flow, or even other sources of energy, we have made a port-Hamiltonian description of the closed system. To obtain the Dirac structure for the closed system required using the dynamic equations and the consistency conditions. Although the port-Hamiltonian approach allows to treat more general system, the gauge symmetries are obscured.

The explicit equations of motion listed in appendix C and discussed in section 4.3 describe the dynamics of the coupling of the scalar Klein-Gordon field and the electromagnetic field in full detail. One of the equations of motion that was derived has been recognized as the Ampère-Maxwell equation. Furthermore, Gauss' equation has come up as a constraint.

The gauge symmetries of the electromagnetic field and the Klein-Gordon field an sich were already known when constructing the locally gauge invariant Lagrangian. The gauge generator as given in equation 4.2 verified these local gauge symmetries. What was not already present at the start is how other dynamical quantities would change under the gauge transformations. With the gauge generator at hand, these transformations can now be worked out easily by just computing the relevant Poisson brackets.

The closed Klein-Gordon-Maxwell system has been fully understood in terms of dynamics and gauge symmetries. Finally, we have made a first step towards describing the open Klein-Gordon-Maxwell system by constructing the Dirac structure for the closed system. Although the Dirac structure provides the equations of motion, it is not obvious how to retrieve the gauge symmetries. To derive the gauge symmetries, one should study infinitesimal variations of the arbitrary functions that are present in the Dirac structure.

There are at least two ways in which the port-Hamiltonian view could provide further insights. The first is that energy flow through the boundary can be included by adding a boundary port. Some research has been done in this direction in [8], however, this approach is not suitable for field theories such as the Klein-Gordon-Maxwell system. To discover what form the boundary port should take, one should compute the energy balance without assuming that the boundary terms vanish. The boundary term needs to be taken as the pairing of the boundary flow and boundary effort. The storage flow and storage effort should remain as we have established them for the closed system.

Port-Hamiltonian theory could also help to understand the coupling of the Maxwell field and the Klein-Gordon field by taking two separate energy storages and Dirac structures, one for the electromagnetic field and one for the locally gauge invariant Klein-Gordon field. Studying the coupling in that way as a coupling of two Dirac structures will provide further insight in the interplay of the two fields.

A Integration on manifolds with a metric

We often want to perform integrals over manifolds with a metric. The only objects that can be integrated on a manifold are differential forms of top-degree. In coordinates, this results in weight-one densities being the only objects that can be properly integrated.

Let M be a smooth n-dimensional manifold with a metric g. Integration on M is defined only for differential forms of top-degree n. For simplicity, we assume that M can be covered by a single chart (M, x). Essentially no generality is lost, since with a smooth atlas and partition of unity arguments we can treat the case in which M is not covered by one chart. Let ω be a top form on M. There is a unique weight-one density $f^{(x)}: M \to \mathbb{R}$ such that $\omega = f^{(x)} dx^1 \wedge \cdots \wedge dx^n$. The integral of ω over M is defined as

$$\int_M \omega = \int_M f^{(x)} dx^1 \wedge \dots \wedge dx^n := \int_{x(M)} (f^{(x)} \circ x^{-1})(\alpha) d^n \alpha.$$

This definition of the integral is independent of the chart chosen. It is straightforward to check that, under a change of chart, $dx^1 \wedge \cdots \wedge dx^n$ picks up a Jacabian determinant and the weight-one density $f^{(x)}$ picks up an inverse Jacobian determinant. The factors picked up from the change of chart thus exactly cancel each other. We will often write the integral of the top-degree form $\omega = f^{(x)} dx^1 \wedge \cdots \wedge dx^n$ in a shorthand form as

$$\int_{x(M)} (f^{(x)} \circ x^{-1})(\alpha) d^n \alpha = \int d^n x f(x).$$

To integrate a scalar function, which is a 0-form, one must first turn it into to a topform. In general, the Hodge star

$$\star: \Omega^k(M) \to \Omega^{n-k}(M)$$

is a map that assigns a (n-k)-form to a k-form. On a manifold with Riemannian metric h, the Hodge star maps the k-form σ to an (n-k)-form $(\star \sigma)$ with components

$$\sigma_{a_1\dots a_k} \mapsto (\star\sigma)_{b_1\dots b_{n-k}} = \frac{\sqrt{|\det h|}}{(n-k)!} \epsilon_{b_1\dots b_{n-k}a_1\dots a_k} h^{a_1m_1} \cdots h^{a_km_k} \sigma_{m_1\dots m_k}$$

where ϵ_{\dots} is the Levi-Civita symbol. The Hodge star of a scalar function $\phi \in C^{\infty}(M)$ produces a top-form. In coordinates, taking the Hodge star of a scalar amounts to multiplying the scalar function with $\sqrt{\det h}$ such that we have

$$\int_M \star \phi = \int_M \sqrt{|\det h|} \, \phi \, dx^1 \wedge \dots \wedge dx^n = \int_{x(M)} (\sqrt{|\det h|} \circ x^{-1})(\alpha) (\phi \circ x^{-1})(\alpha) \, d^n \alpha.$$

A useful theorem for computing integrals of differentials of forms is Stokes' theorem. Suppose we are given $\sigma \in \Omega^{n-1}(M)$, then Stokes' theorem states

$$\int_M d\sigma = \int_{\partial \Sigma} i^*(\sigma),$$

where $i : \partial \Sigma \hookrightarrow \Sigma$ is the canonical inclusion map. Stokes' theorem and the fact that the exterior derivative commutes with the wedge product, gives rise to integration by parts. In particular, given $\sigma \in \Omega^k(M)$ and $\eta \in \Omega^{n-k-1}(M)$ we have

$$\int_M d\sigma \wedge \eta = (-1)^{k-1} \int_M \sigma \wedge d\eta + \int_{\partial M} i^*(\sigma) \wedge i^*(\eta),$$

see for example [1].

Stokes' theorem, the Hodge star and the integration by parts formula are the tools needed to properly treat the boundary terms that come up when taking variational derivatives, which will be treated in appendix B. In particular, we will encounter integrals with coordinate forms

1.

$$\int_{y(\Sigma)} (\sqrt{-h} V^{\mu}) \circ y^{-1})(\alpha) \partial_{\mu} (F \circ y^{-1})(\alpha) d^{3}\alpha,$$

for a vector field (really a vector field and not a density) V with components V^{μ} and a function F,

2.

$$\int_{y(\Sigma)} (\sqrt{-h} T^{\mu\nu} \circ y^{-1})(\alpha) \partial_{\mu} (W_{\nu} \circ y^{-1})(\alpha) d^{3}\alpha,$$

for an anti-symmetric tensor T with components $T^{\mu\nu}$ and a covector field W,

where Σ is a 3-dimensional manifold that can be covered by the chart (Σ, y) and that has a Riemannian metric h with negative signature. These integrals are the coordinate versions of

- 1. $\int_{\Sigma} \star V^{\flat} \wedge dF$,
- 2. $\int_{\Sigma} \star T^{\flat} \wedge dW$, where T^{\flat} has components $T_{\mu\nu}$ and is hence a 2-form.

To the coordinate free versions we can apply the integration by parts formula. Let us first treat $\int_{\Sigma} \star V^{\flat} \wedge dF$. Integration by parts yields

$$\int_{\Sigma} \star V^{\flat} \wedge dF = -\int_{\Sigma} d \star V^{\flat} \wedge F + \int_{\partial \Sigma} i^* (\star V^{\flat}) \wedge i^*(F).$$

Now, $\star d \star V^{\flat}$ is equal to the divergence div V of the vector field V. For the boundary integral, the pullback along the inclusion of the function F amounts simply to restricting F to $\partial \Sigma$. The term $i^*(\star V^{\flat})$ deserves some special attention.

Note that $i^*(\star V^{\flat})$ is a 2-form on $\partial \Sigma$. We can, in fact, compute this term in coordinates explicitly. To this end, take a point $s \in \partial \Sigma$ and consider u and w in $T_s \partial \Sigma$. We compute

$$i^{*}(\star V^{\flat})_{s}(u,w) = (\star V^{\flat})_{s}(di_{s}u, di_{s}w)$$

$$= \frac{1}{2} \left(\sqrt{-h} V^{\nu}(s) \epsilon_{\alpha\beta\nu} dy^{\alpha}_{s} \wedge dy^{\beta}_{s} \right) (di_{s}u, di_{s}w)$$

$$= \frac{1}{2} \left(\sqrt{-h} V^{\nu}(s) \epsilon_{\alpha\beta\nu} d(y^{\alpha} \circ i)_{s} \wedge d(y^{\beta} \circ i)_{s} \right) (u,w)$$

Suppose that we have chosen the coordinates θ on the manifold $\partial \Sigma$ such that $\theta^A = y^A \circ i$ for A = 1, 2, then $d(y^A \circ i) = d\theta^A$. Now, we must decompose dy^3 in a tangential and a normal part, with respect to the metric. Take a covector $r_s \in T_s \Sigma$ such that the following hold:

1.
$$h_s^{-1}(r_s, r_s) = 0,$$

2. $r_s \left(\frac{\partial}{\partial y^A}\right)_s = 0$ for $A = 1, 2$

In other words, r_s^{\sharp} is the unit normal vector to the surface $\partial \Sigma$ at the point s. Introduce a covector field with components M_A and s scalar field M on $\partial \Sigma$ defined such that

$$dy_s^3 = M_A(s)dy_s^A + M(s)r_s.$$

Appropriate sign-bookkeeping ultimately yields that,

$$i^*(\star V^{\flat})_s = \left(V^3(s) - M_A(s)V^A(s)\right) d\theta_s^1 \wedge d\theta_s^2.$$

We thus subtract the part of V tangential to the boundary from the third component of V. In that way, we construct the component of V normal to the boundary with respect to the metric. This is the appropriate form of what is called in vector calculus the "projection on the normal surface element". Note that when we take F = 1, then we precisely obtain Gauss' theorem

$$"\int_{\Sigma} \operatorname{div} V \, d^3 y " = \int_{\Sigma} d \star V^{\flat} = \int_{\partial \Sigma} i^* (\star V^{\flat}) = " \int_{\partial \Sigma} V \cdot d\boldsymbol{a}."$$

We can play the same game for the integral of the anti-symmetric tensor. However, we have to decompose both W and T using the M_A . The resulting boundary integral is

$$\int_{\partial \Sigma} i^* (\star T^{\flat} \wedge W) = \int_{\partial \Sigma} \sqrt{-h} T^{\mu\nu} \left(\epsilon_{A\mu\nu} (W_B + W_3 M_B) + \epsilon_{3\mu\nu} M_A W_B \right) d\theta^A \wedge d\theta^B.$$

The integrals 1 and 2 have now been properly established. We now know what boundary terms come up and we can safely talk about assumptions under which these boundary terms vanish. A very trivial condition for the vanishing of the boundary integrals is that V and T themselves vanish on the boundary.

B Functional derivatives and the Poisson bracket

The Poisson bracket formulation of the dynamic equations for field theory of closed systems provides fundamental insights into the gauge symmetries of the system. In this appendix we establish the Poisson bracket on the type of functionals that are needed in field theory.

A functional

$$F:\mathscr{X}\to\mathbb{R}$$

is a map that assigns a real number to an element of a function space \mathscr{X} . If the space \mathscr{X} has a norm, then the Fréchet derivative of the functional $F : \mathscr{X} \to \mathbb{R}$ at f is defined to be the linear map $A : \mathscr{X} \to \mathbb{R}$ such that

$$\lim_{\|\eta\|_{\mathscr{X}} \to 0} \frac{\|F[f+\eta] - F[f] - A(\eta)\|_{\mathbb{R}}}{\|\eta\|_{\mathscr{X}}} = 0,$$

If the Fréchet derivative exists, then it is unique.

For simplicity, assume that \mathscr{X} consists of functions $f : \mathbb{R} \to \mathbb{R}$. Moreover, for our purposes, it is sufficient to consider functionals F of the form

$$F[f] = \int \mathcal{F}(f, \partial_1 f) dx.$$

For functionals F of this form, we can establish the Fréchet derivative of F at f explicitly in terms of partial derivatives of \mathcal{F} . To do this, we approach the limit in the definition as $\lim_{\epsilon \to 0} \epsilon \eta$. Expanding the function $F[f + \epsilon \eta]$ in powers of ϵ , we have

$$F[f + \epsilon \eta] = F[f] + \frac{dF[f + \epsilon \eta]}{d\epsilon} \bigg|_{\epsilon=0} \epsilon + O(\epsilon^2).$$

The functional $A: \mathscr{X} \to \mathbb{R}$ defined by

$$A(\eta) = \frac{dF[f + \epsilon\eta]}{d\epsilon} \bigg|_{\epsilon=0}$$

is linear. We take A as a candidate for the Fréchet derivative of F and compute that, indeed,

$$\lim_{\epsilon \to 0} \frac{\|F[f + \epsilon\eta] - F[f] - A(\epsilon\eta)\|_{\mathbb{R}}}{\|\epsilon\eta\|_{\mathscr{X}}} = \lim_{\epsilon \to 0} \frac{\|O(\epsilon^2)\|_{\mathbb{R}}}{\epsilon\|\eta\|_{\mathscr{X}}} = 0.$$

It follows by the uniqueness property that A is the Fréchet derivative of F. The Fréchet derivative of the functional F evaluated at f will be denoted $\frac{\delta F}{\delta f}[f]$. It is a functional that maps a function η to the derivative in the direction of η , i.e.

$$\left(\frac{\delta F}{\delta f}[f]\right)[\eta] = \frac{dF[f+\epsilon\eta]}{d\epsilon}\bigg|_{\epsilon=0}$$

Given an arbitrary function η , we can compute

$$\frac{dF[f+\epsilon\eta]}{d\epsilon}\Big|_{\epsilon=0} = \int dx \left[\frac{\partial \mathcal{F}}{\partial f}((x))\eta(x) + \frac{\partial \mathcal{F}}{\partial(\partial_1 f)}((x))\partial_1\eta(x)\right],$$

where the notation $((x)) := (f, \partial_1 f)(x)$ is used to indicate that the dependence on x is through the functions f and $\partial_1 f$. Integrating the last term by parts under the assumption that the boundary term vanishes gives us

$$\frac{dF[f+\epsilon\eta]}{d\epsilon}\Big|_{\epsilon=0} = \int dx \,\eta(x) \left[\frac{\partial \mathcal{F}}{\partial f}(x) - \partial_1 \frac{\partial \mathcal{F}}{\partial(\partial_1 f)}(x)\right].$$

The quantity in square brackets will be called $\frac{\delta F}{\delta f(x)}$. With this definition, the Fréchet derivative may be expressed as

$$\left(\frac{\delta F}{\delta f}[f]\right)[\eta] = \int dx \frac{\delta F}{\delta f(x)} \eta(x)$$

Having established the Fréchet derivatives, which will often be referred to as variational or functional derivatives, we can define the Poisson bracket operation for functionals. For two functionals F and G of functions ϕ and π given in the form

$$F[\phi,\pi] = \int dx \,\mathcal{F}(\phi,\partial_1\phi,\pi,\partial_1\pi) \quad \text{and} \quad G[\phi,\pi] = \int dx \,\mathcal{G}(\phi,\partial_1\phi,\pi,\partial_1\pi)$$

we define the Poisson bracket $\{F, G\}$ as

$$\{F,G\} = \int dx \left[\frac{\delta F}{\delta \phi(x)} \frac{\delta G}{\delta \pi(x)} - \frac{\delta G}{\delta \phi(x)} \frac{\delta F}{\delta \pi(x)} \right]$$

C Equations of motion for Klein-Gordon-Maxwell

Below, the equations of motion for the Klein-Gordon field coupled to the electromagnetic field are presented. Some of the equations are discussed in section 4.3.

$$\begin{split} \dot{E}^{0} &= \partial_{\nu}E^{\nu} - iQ\left(\phi\pi - \phi^{*}\pi^{*}\right) .\\ \\ \dot{E}^{\mu} &= -N_{t}^{\mu}iQ\left(\pi^{*}\phi^{*} - \pi\phi\right) + iQh^{\mu\nu}N_{t}\sqrt{-h}\left(\phi^{*}D_{\nu}\phi - \phi D_{\nu}^{*}\phi^{*}\right) \\ &+ E^{\mu}\partial_{\rho}N_{t}^{\rho} + N_{t}^{\rho}\partial_{\rho}E^{\mu} - N_{t}^{\mu}\partial_{\rho}E^{\rho} - E^{\rho}\partial_{\rho}N_{t}^{\mu} + \partial_{\rho}(h^{\kappa\rho}h^{\mu\nu}F_{\kappa\nu}N_{t}\sqrt{-h}) \\ \\ \\ \dot{\pi} &= \partial_{\rho}(N_{t}^{\rho}\pi) - \partial_{\rho}(h^{\mu\rho}N_{t}\sqrt{-h}(\partial_{\mu}\phi^{*} + iQA_{\mu}\phi^{*})) - iQA_{0}\pi + N_{t}^{\mu}iQA_{\mu}\pi \\ &- iQA_{\nu}h^{\mu\nu}N_{t}\sqrt{-h}(\partial_{\mu}\phi^{*} + iQA_{\mu}\phi^{*}) - M^{2}\phi^{*}N_{t}\sqrt{-h} \\ \\ \\ \\ \dot{\pi}^{*} &= (\dot{\pi})^{*} \\ \\ \\ \\ \dot{\Phi}^{*} &= \frac{\pi^{*}N_{t}}{\sqrt{-h}} + iQA_{0}\phi + N_{t}^{\mu}(\partial_{\mu}\phi - iQA_{\mu}\phi) \\ \\ \\ \\ \\ \\ \\ \dot{\phi}^{*} &= \frac{\pi N_{t}}{\sqrt{-h}} - iQA_{0}\phi^{*} + N_{t}^{\mu}(\partial_{\mu}\phi^{*} + iQA_{\mu}\phi^{*}) \\ \end{array}$$

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