Multisymplectic Geometry on the Three Dimensional General Schrödinger Equation

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Course: CDS 205

June 1, 2007

Abstract

A multisymplectic structure is imposed on the 3-d (three dimensional) general Schrödinger equation. From the multisymplectic form formula, a multisymplectic conservation law is extracted for the 3-d general Schrödinger equation. For the case of infinite spatial domain, the multisymplectic form formula is shown to reduce to a form that coincides with the quantum-mechanical symplectic form, which is defined in terms of the imaginary part of the quantum mechanical Hermitian inner product on the complex Hilbert space of square integrable wavefunctions. Furthermore, the interpretation of the multisymplectic form formula in application to the 3-d general Schrödinger equation with infinite spatial domain and bounded time domain, is that the integrals over the two boundaries at each temporal endpoint are equal in magnitude, and yet opposite in orientation.

Contents

1 Introduction

In 1925, Erwin Schrödinger suggested that the Schrödinger equation would govern the behavior of very small particles. The Schrödinger equation provided the link between the motion of particles and their dependence on time and spatial position, subject to forces external to the system. The time dependent and the time independent Schrödinger equation comes in various forms depending on the system of application.

The part that differentiates one form of the Schrödinger equation from another can be seen in the quantum mechanical Hamiltonian operator. The type of system under study, and the type of information that is desired to attain, is what determines the form of the system's Hamiltonian operator that will be employed by the Schrödinger equation. The *free* Hamiltonian operator in its most basic sense comprises of a kinetic energy operator and some type of potential energy operator. The potential energy function is dependent on the number of particles in the system of study, as well as the type of particles under study, and what type of interaction these particles have with one another. In addition, to the free Hamiltonian operator, a perturbation Hamiltonian is often added. For example, a magnetic field imposed onto a system of particles with intrinsic spin will introduce a perturbation Hamiltonian to be added to the free Hamiltonian.

The goal of this paper is to set up the geometric structure in a mathematical sense, for the general three dimensional Schrödinger equation. The term "general" in used in this paper in the sense that arbitary perturbation Hamiltonians may be added to the free Hamiltonian, as long as perturbations depend only on space, time, and the wavefunction itself.

2 The General Schrödinger Equation

For the purposes of this paper, the general Schrödinger equation is defined in this paper in the following manner. Let $\Psi \in \mathbb{C}$ be the wavefunction, where $\mathbb{C}$ denotes a complex Hilbert space with the well known Hermitian inner product

$$\langle\langle \Psi, \Phi \rangle\rangle = \int \Psi^* \Phi \, d\tau.$$

The well known general Schrödinger equation is

$$\mathbf{i}\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \mathbf{H}_{op} \Psi(\mathbf{r}, t).$$

where $\mathbf{r}$ is a position vector. Let $\mathbf{H}_{op}$ be defined as a possibly perturbed Hamiltoninan operator

$$\mathbf{H}_{op} = \mathbf{H^0} + \mathbf{H^1}$$

where $\mathbf{H^0}$ is the unperturbed Hamiltonian operator, and $\mathbf{H^1}$ is the perturbation to the Hamiltonian operator. Recall that $\mathbf{H^0}$ itself comprises of the sum of a kinetic energy operator and a potential energy operator

$$\mathbf{H^0} = \mathbf{T}_{op} + \mathbf{V}_{op}.$$

where the kinetic energy operator is the real operator $\mathbf{T}_{op} = -\frac{\hbar^2}{2m} \triangle_{\mathbf{r}}$, and the potential energy operator is a complex valued function. The general Schrödinger equation can be written then as

$$\mathbf{i}\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \triangle_{\mathbf{r}} + \mathbf{V}_{op}(\mathbf{r}, t) + \mathbf{H^1}(\mathbf{r}, t, \Psi(\mathbf{r}, t)) \right) \Psi(\mathbf{r}, t).$$

Letting $\bar{\mathbf{V}}_{op}(\bar{\mathbf{r}}, \bar{t}) = \frac{T}{\hbar} \mathbf{V}_{op}(\mathbf{r}, t)$, $\bar{\mathbf{H}}^{\mathbf{1}}{}_{op}(\bar{\mathbf{r}}, \bar{t}, \Psi(\bar{\mathbf{r}}, \bar{t})) = \frac{T}{\hbar} \mathbf{H^1}{}_{op}(\mathbf{r}, t, \Psi(\mathbf{r}, t))$, $\bar{\mathbf{r}} = \sqrt{\frac{2m}{T\hbar}} \mathbf{r}$, and $\bar{t} = \frac{t}{T}$, for some time period T, the general Schrödinger equation is recast as

$$\mathbf{i} \frac{\partial \Psi(\bar{\mathbf{r}}, \bar{t})}{\partial \bar{t}} = \left(-\triangle_{\bar{\mathbf{r}}} + \bar{\mathbf{V}}_{op}(\mathbf{r}, t) + \bar{\mathbf{H}}^{\mathbf{1}}(\bar{\mathbf{r}}, \bar{t}, \Psi(\bar{\mathbf{r}}, \bar{t})) \right) \Psi(\bar{\mathbf{r}}, \bar{t}).$$

Letting $\bar{\mathbf{Z}}(\bar{\mathbf{r}}, \bar{t}, \Psi(\bar{\mathbf{r}}, \bar{t})) = \left(\bar{\mathbf{V}}_{op}(\bar{\mathbf{r}}, \bar{t}) + \bar{\mathbf{H}}^{\mathbf{1}}(\bar{\mathbf{r}}, \bar{t}, \Psi(\bar{\mathbf{r}}, \bar{t})) \right) \Psi(\bar{\mathbf{r}}, \bar{t})$, and then dropping the bar notation yields the dimensionless general Schrödinger equation

$$\mathbf{i} \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -\triangle_{\mathbf{r}} \Psi(\mathbf{r}, t) + \mathbf{Z}(\mathbf{r}, t, \Psi(\mathbf{r}, t)). \tag{1}$$

Note that $\mathbf{Z}(\mathbf{r}, t, \Psi(\mathbf{r}, t))$ takes values in the complex set of numbers, and is a function of time and spatial coordinates, as well as the wavefunction itself.

To facilitate geometrizing of the general Schródinger equation, the imaginary number $\mathbf{i}$ is eliminated from the equation by separating out the imaginary and real part of the wavefunction. This is accomplished by letting $\Psi(\mathbf{r}, t) = p(\mathbf{r}, t) + \mathbf{i}q(\mathbf{r}, t)$. Therefore equation 1 may be rewritten as

$$\begin{aligned} p_t + \triangle q - \mathbf{Im}\{\mathbf{Z}(\mathbf{r}, t, p(\mathbf{r}, t), q(\mathbf{r}, t))\} &= 0 \\ q_t - \triangle p + \mathbf{Re}\{\mathbf{Z}(\mathbf{r}, t, p(\mathbf{r}, t), q(\mathbf{r}, t))\} &= 0. \end{aligned} \tag{2}$$

Please pay special attention to the fact that in general

$$\begin{aligned} \mathbf{Re}\{\mathbf{Z}(\mathbf{r}, t, p(\mathbf{r}, t), q(\mathbf{r}, t))\} &\neq \mathbf{Re}\{\mathbf{Z}(\mathbf{r}, t, \Psi(\mathbf{r}, t))\} \\ \mathbf{Im}\{\mathbf{Z}(\mathbf{r}, t, p(\mathbf{r}, t), q(\mathbf{r}, t))\} &\neq \mathbf{Im}\{\mathbf{Z}(\mathbf{r}, t, \Psi(\mathbf{r}, t))\} \end{aligned}$$

Now suppose there exists a function C such that

$$\begin{aligned} \tfrac{\partial C}{\partial p} &= \mathbf{Re}\{\mathbf{Z}(\mathbf{r}, t, p(\mathbf{r}, t), q(\mathbf{r}, t))\} \\ \tfrac{\partial C}{\partial q} &= \mathbf{Im}\{\mathbf{Z}(\mathbf{r}, t, p(\mathbf{r}, t), q(\mathbf{r}, t))\}. \end{aligned}$$

Consequently the equations in 2 become

$$\begin{aligned} p_t + \triangle q - \tfrac{\partial C}{\partial q} &= 0 \\ q_t - \triangle p + \tfrac{\partial C}{\partial p} &= 0. \end{aligned} \tag{3}$$

Throughout this paper Cartesian coordinates will be utilized, and thus $\triangle = \frac{\partial^2}{\partial x} + \frac{\partial^2}{\partial y} + \frac{\partial^2}{\partial z}$ for $\mathbf{r} = (x, y, z)$.

3 Geometrizing the General Schrödinger Equation

3.1 A Fiber Bundle Structure Imposed on the General Schrödinger Equation

Let $\pi_{XY} : Y \to X$ be a fiber bundle over the oriented manifold X, and let $\phi : U \subset X \to Y$ be a section of π_{XY}. For the three dimensional time dependent Schrödinger equation, the base space X of the fiber bundle is the spatial and time domain, and therefore is coordinated by $\{x_\mu\} = (x, y, z, t)$, where $\mu \in \{1, \ldots, (n+1) = 4\}$, and thus the dimesion of X is four. The fibers over X are elements of Y, where Y is coordinated by the set $\{y^A\}$ ($A \in \{1, \ldots, N\}$), where for the general Schrödinger equation, these coordinates are $\phi(x, y, z, t) = (p, q)$, and the dimension of Y is $N = 2$. The tangent map of ϕ at $k \in X$, $T_k\phi$, is an element of $J^1(Y)_{\phi(k)}$, where $J^1(Y)$ is the first jet bundle over Y. Elements of $J^1(Y)$, can be thought of as fibers over both X and Y, and are defined to be the maps from TY to TX. The first jet bundle $J^1(Y)$ is coordinated by the set $\{v^A_\mu\}$, and thus the dimension of $J^1(Y)$ is $N*(n+1)$. For the case of the general Schrödinger equation, $J^1(Y)$ is coordinated by $(p_t, q_t, p_x, q_x, p_y, q_y, p_z, q_z)$, and the dimension of $J^1(Y)$ is $N*(N+1) = 2*4 = 8$.

The *first jet*, or *first prolongation* of ϕ, denoted by $j^1\phi$, is the map from the base space X to the first jet bundle $J^1(Y)$. Note that $j^1(\phi) \in \Gamma(\pi_{X,J^1(Y)})$ is a section of $J^1(Y)$. The coordinates of $j^1(\phi)$ at a point $k = \{x^\mu\} \in X$ are

$$j^1_k(\phi) = \left(x^\mu, \phi^A(x^\mu), \frac{\partial \phi^A(x^\mu)}{\partial x^\nu}\right)$$

For the 3-d (three dimensional) general Schrödinger equation, $j^1(\phi)$ at a point $k = (x, y, z, t) \in X$ is

$$j^1_k(\phi) = ((x, y, z, t), (p, q), (p_t, q_t, p_x, q_x, p_y, q_y, p_z, q_z)).$$

3.2 Multisymplectic Manifold / Covariant Phase Space

The *dual jet bundle* is denoted by $J^1(Y)^\star$. The *dual jet bundle* consists of the set of affine maps from $J^1(Y)$ to $\Lambda^{(n+1)}(X)$, where $\Lambda^{(n+1)}(X)$ is the set of (n+1)-forms on X (Recall that $(n+1)$ is the dimension of the base space X). To define a multisymplectic manifold, first define the bundle of $(n+1)$ forms on Y, denoted by $\Lambda := \Lambda^{(n+1)}(Y)$, with projection map $\pi_{Y\Lambda} : \Lambda \to Y$. A noteworthy subbundle of Λ is denoted by $Z \subset \Lambda$, and this subbundle consists of the fibers

$$Z_y = \{z \in \Lambda_y | \, \mathbf{i}_v(\mathbf{i}_w z) = 0, \, \forall v, w \in V_y Y\}. \tag{4}$$

Interestingly, the spaces Z and $J^1(Y)^\star$ are isormophic. This fact becomes important later when defining canonical forms on $J^1(Y)^\star$. Denote the canonical $(n+1)$ and $(n+2)$ forms on $\Lambda^{(n+1)}(Y)$ as Θ_Λ and Ω_Λ. By employing the inclusion map, $i_{\Lambda Z} : Z \to \Lambda$, the canonical $(n+1)$ and $(n+2)$ forms on Z are

$$\Theta = i^*_{\Lambda Z}\Theta_\Lambda$$

and

$$\Omega = -d\Theta = i^*_{\Lambda Z}\Omega_\Lambda.$$

Now that all of the necessary structures have been described, it is proper to define the *multisymplectic manifold*, *multiphase space*, or *covariant phase space*, as the pair (Z, Ω), or rather, in words, the subbundle of Λ described in 4, together with the canonical $(n+2)$ form on Z.

Due to the fact that the spaces Z and $J^1(Y)^\star$ are isomorphic, for every form on Z there exists a corresponding form on $J^1(Y)^\star$. Because these spaces are isormorphic, denote the $(n+1)$ and $(n+2)$ form on $J^1(Y)^\star$ with the same notation, as Θ and Ω. These forms are needed to define forms on $J^1(Y)$.

The *Lagrangian density* $\mathcal{L} \in J^1(Y)^\star$ is a smooth bundle map $\mathcal{L} : J^1(Y) \to \Lambda^{n+1}(X)$. For a point $\gamma \in J^1(Y)$, coordinated by $\gamma = (x^\mu, y^A, v^A_\mu)$, $\mathcal{L}$ in coordinates is given by

$$\mathcal{L}(\gamma) = L(x^\mu, y^A, v^A_\mu)d^{n+1}x.$$

Correspondingly, the fiber preserving map over Y associated with $\mathcal{L}$ is $\mathbb{F}\mathcal{L} : J^1(Y) \to J^1(Y)^\star$, and is called the *covariant Legendre transformation*. Let $\gamma, \gamma' \in J^1(Y)_y$, then $\mathbb{F}\mathcal{L}$ is defined as

$$\mathbb{F}\mathcal{L} \cdot \gamma' = \mathcal{L}(\gamma) + \frac{d}{d\varepsilon} |_{\varepsilon=0} \mathcal{L}(\gamma + \varepsilon(\gamma' - \gamma)).$$

The coordinates of the covariant Legendre transformation are

$$f^\mu_A = \frac{\partial L}{\partial v^A_\mu}, \;\; f = L - \frac{\partial L}{\partial v^A_\mu} v^A_\mu.$$

Finally, the *Cartan form* is the canonical $(n+1)$ form on $J^1(Y)$, defined to be the pullback of Θ by $\mathbb{F}\mathcal{L}$ onto $J^1(Y)$

$$\Theta_\mathcal{L} = (\mathbb{F}\mathcal{L})^*\Theta.$$

The canonical $(n+2)$ form is similarly defined by

$$\Omega_\mathcal{L} = -d\Omega_\mathcal{L} = (\mathbb{F}\mathcal{L})^*\Omega.$$

In coordinates, these forms are

$$\Theta_\mathcal{L} = \frac{\partial L}{\partial v^A_\mu} dy^A \wedge d^n x_\mu + L - \frac{\partial L}{\partial v^A_\mu} v^A_\mu d^{n+1}x$$

$$\Omega_{\mathcal{L}} = dy^A \wedge d\left(\frac{\partial L}{\partial v^A_\mu}\right) \wedge d^n x_\mu - d\left(L - \frac{\partial L}{\partial v^A_\mu} v^A_\mu\right) \wedge d^{n+1}x.$$

Recall that for the 3-d general Schrödinger equation, the coordinates of X are (x, y, z, t), the coordinates of Y are (p, q), and the coordinates of $J^1(Y)$ are $(p_t, q_t, p_x, q_x, p_y, q_y, p_z, q_z)$. Then the Lagrangian density for the 3-d general Schrödinger equation is

$$\mathcal{L}(j^1(\phi)) = \frac{1}{2}\left[q_t p - p_t q + p_x^2 + p_y^2 + p_z^2 + q_x^2 + q_y^2 + q_z^2 + 2C\right] dx \wedge dy \wedge dz \wedge dt. \tag{5}$$

Consequently the canonical 4-form on $J^1(Y)$ is

$$\begin{aligned}
\Theta_{\mathcal{L}} \;=\;& \tfrac{q}{2} dp \wedge dx \wedge dy \wedge dz \;-\; \tfrac{p}{2} dq \wedge dx \wedge dy \wedge dz \;+\; p_x dp \wedge dy \wedge dz \wedge dt \\
& + q_x dq \wedge dy \wedge dz \wedge dt \;+\; p_y dp \wedge dz \wedge dx \wedge dt \;+\; q_y dq \wedge dz \wedge dx \wedge dt \\
& + p_z dp \wedge dx \wedge dy \wedge dt \;+\; q_z dq \wedge dx \wedge dy \wedge dt \\
& - \tfrac{1}{2}\left(p_x^2 + p_y^2 + p_z^2 + q_x^2 + q_y^2 + q_z^2 - 2C\right) dx \wedge dy \wedge dz \wedge dt,
\end{aligned}$$

and the canonical 5-form on $J^1(Y)$, is

$$\begin{aligned}
\Omega_{\mathcal{L}} \;=\;& dp \wedge dq \wedge dx \wedge dy \wedge dz \;+\; dp \wedge dp_x \wedge dy \wedge dz \wedge dt \\
& + dq \wedge dq_x \wedge dy \wedge dz \wedge dt \;+\; dp \wedge dp_y \wedge dz \wedge dx \wedge dt \\
& + dq \wedge dq_y \wedge dz \wedge dx \wedge dt \;+\; dp \wedge dp_z \wedge dx \wedge dy \wedge dt \\
& + dq \wedge dq_z \wedge dx \wedge dy \wedge dt \;+\; dp_x \wedge dx \wedge dy \wedge dz \wedge dt \\
& + dq_x \wedge dx \wedge dy \wedge dz \wedge dt \;+\; dp_y \wedge dx \wedge dy \wedge dz \wedge dt \\
& + dq_y \wedge dx \wedge dy \wedge dz \wedge dt \;+\; dp_z \wedge dx \wedge dy \wedge dz \wedge dt \\
& + dq_z \wedge dx \wedge dy \wedge dz \wedge dt \;-\; \tfrac{\partial C}{\partial p} dp \wedge dx \wedge dy \wedge dz \wedge dt \\
& - \tfrac{\partial C}{\partial q} dq \wedge dx \wedge dy \wedge dz \wedge dt.
\end{aligned}$$

3.3 The Euler-Lagrange Equations

To derive the Euler-Lagrange equations of motion, one takes finite variations of the action function with respect to $\phi \in \Gamma(\pi_{XY})$. The *action function* is defined to be

$$\mathcal{S}(\phi) = \int_U \mathcal{L}(j^1(\phi_\lambda))$$

where $\phi : U \to Y$, and $U \in X$ is a submanifold of X with piecewise smooth closed boundary. For a vertical vector field, V on Y, with compact support in U, let η_Y be the flow of V. Then the curve $\phi_\lambda = \eta_\lambda \circ \phi$ is a *finite variation* of ϕ. The map, ϕ, is called a *stationary point*, *extremum*, or *critical point* of the action, if for all variations ϕ_λ of ϕ,

$$d\mathcal{S} \cdot V = \frac{d}{d\lambda}|_{\lambda=0} \int\limits_U \mathcal{L}(j^1(\phi_\lambda)) = 0. \tag{6}$$

From equation 6, the Euler Lagrange equations are extracted after the following manipulations. Using the fact that for all holonomic sections $z \in J^1(Y)$, $\mathcal{L}(z) = z^*\Theta_\mathcal{L}$, equation 6 becomes

$$d\mathcal{S} \cdot V = \frac{d}{d\lambda}|_{\lambda=0} \int\limits_U j^1(\phi_\lambda)^*\Theta_\mathcal{L}.$$

Then because $\phi_\lambda = \eta_\lambda \circ \phi$ as defined above,

$$d\mathcal{S} \cdot V = \frac{d}{d\lambda}|_{\lambda=0} \int\limits_U j^1(\eta_\lambda \circ \phi)^*\Theta_\mathcal{L}.$$

Note that $j^1(\eta_\lambda \circ \phi)$ is the same things as

$$j^1(\eta_\lambda \circ \phi) = j^1(\eta_\lambda) \circ j^1(\phi),$$

and therefore,

$$j^1(\eta_\lambda \circ \phi)^* = j^1(\phi)^* \circ j^1(\eta_\lambda)^*.$$

Consequently, equation 6 can be written as

$$d\mathcal{S} \cdot V = \frac{d}{d\lambda}|_{\lambda=0} \int\limits_U j^1(\phi)^* j^1(\eta_Y^\lambda)^*\Theta_\mathcal{L}.$$

Now because n_λ is the flow of V, by definition

$$\frac{d}{d\lambda}|_{\lambda=0} j^1(\eta_\lambda) = \mathfrak{L}_{j^1(V)}.$$

Thus, equation 6 may be written

$$d\mathcal{S} \cdot V = \int\limits_U j^1(\phi)^* \mathfrak{L}_{j^1(V)}\Theta_\mathcal{L}.$$

Recall that Cartan's magic formula says $\mathfrak{L}_{j^1(V)}\Theta_{\mathcal{L}} = \mathbf{i}_{j^1(V)}\mathbf{d}\Theta_{\mathcal{L}} + \mathbf{d}\,\mathbf{i}_{j^1(V)}\Theta_{\mathcal{L}}$. Also, by definition, $\mathbf{d}\Theta_{\mathcal{L}} = -\Omega_{\mathcal{L}}$. Accordingly, equation 6 becomes

$$\begin{aligned} d\mathcal{S}\cdot V = &\int\limits_U j^1(\phi)^* \left(\mathbf{i}_{j^1(V)}\mathbf{d}\Theta_{\mathcal{L}} + \mathbf{d}\,\mathbf{i}_{j^1(V)}\Theta_{\mathcal{L}}\right) \\ = &\int\limits_U j^1(\phi)^* \left(\mathbf{i}_{j^1(V)}\Omega_{\mathcal{L}} + \mathbf{d}\,\mathbf{i}_{j^1(V)}\Theta_{\mathcal{L}}\right) \\ = &\int\limits_U j^1(\phi)^*\mathbf{i}_{j^1(V)}\Omega_{\mathcal{L}} + \int\limits_U j^1(\phi)^*\mathbf{d}\,\mathbf{i}_{j^1(V)}\Theta_{\mathcal{L}}. \end{aligned}$$

Employing Stokes theorem

$$d\mathcal{S}\cdot V = \int\limits_U j^1(\phi)^*\mathbf{i}_{j^1(V)}\Omega_{\mathcal{L}} + \int\limits_{\partial U} j^1(\phi)^*\mathbf{i}_{j^1(V)}\Theta_{\mathcal{L}}. \tag{7}$$

In order for ϕ to an extremum of $\mathcal{S}$, both terms in 7 must disappear. The multisymplectic form formula, (stated later), employs in its proof the second term of 7, which is

$$\int\limits_{\partial U} j^1(\phi)^*\mathbf{i}_{j^1(V)}\Theta_{\mathcal{L}} = 0.$$

This is to be discussed later. However, the first term in equation 7,

$$\int\limits_U j^1(\phi)^*\mathbf{i}_{j^1(V)}\Omega_{\mathcal{L}} = 0,$$

is to be discussed here, because it is from this term that the Euler Lagrange equations are extracted. The above condition is true, whenever $j^1(V) = W \in TJ^1(Y)$, where $TJ^1(Y)$ consists of vector fields on $J^1(Y)$ that are $\pi_{Y,J^1(Y)}$ vertical, or tangent to $j^1(\phi)$. Thus, ϕ is said to be a solution to the Euler-Lagrange equations whenever

$$j^1(\phi)^*\mathbf{i}_W\Omega_{\mathcal{L}} = 0 \tag{8}$$

for some $W \in TJ^1(Y)$. This very expression, in equation 8, written in coordinates, is the set of Euler-Lagrange equations

$$\frac{\partial L}{\partial y^A}(j^1(\phi)) - \frac{\partial}{\partial x^\mu}\left(\frac{\partial L}{\partial v^A_\mu}(j^1(\phi))\right) = 0.$$

Note that as mentioned before, $\{x^\mu\}$ are coordinates of the base manifold X, $\{y^A\}$ are coordinates Y, which is the fiber bundle over X, and $\{v^A_\mu\}$ are coordinates of $J^1(Y)$, which is the first jet bundle over Y.

3.4 The Lagrangian Formulation Applied to the General Schrödinger Equation

Recall that for the 3-d general Schrödinger equation, $\phi : U \subset X \to Y$, where $\phi(x, y, z, t) = (p, q)$, and $j^1(\phi)$ in coordinates is

$$j^1(\phi) = ((x, y, z, t), (p, q), (p_t, q_t, p_x, q_x, p_y, q_y, p_z, q_z)).$$

Then set of Euler-Lagrange equations for the 3-d general Schrödinger equation, expounded in coordinates is

$$\frac{\partial L}{\partial q} - \frac{\partial}{\partial t}\frac{\partial L}{\partial q_t} - \frac{\partial}{\partial x}\frac{\partial L}{\partial q_x} - \frac{\partial}{\partial y}\frac{\partial L}{\partial q_y} - \frac{\partial}{\partial z}\frac{\partial L}{\partial q_z} = 0, \tag{9}$$

which is equivalent to the original equation of motion

$$p_t + \triangle q - \frac{\partial C}{\partial q} = 0,$$

and

$$\frac{\partial L}{\partial p} - \frac{\partial}{\partial t}\frac{\partial L}{\partial p_t} - \frac{\partial}{\partial x}\frac{\partial L}{\partial p_x} - \frac{\partial}{\partial y}\frac{\partial L}{\partial p_y} - \frac{\partial}{\partial z}\frac{\partial L}{\partial p_z} = 0 \tag{10}$$

which is equivalent to the original equation of motion

$$q_t - \triangle p + \frac{\partial C}{\partial p} = 0.$$

Since $\phi(x, y, z, t) = (p, q)$ is an extremum of the action principle, it is a solution to the Euler-Lagrange equations.

3.5 The Hamiltonian Formulation

The Hamiltonian Formulation is a way of exploring the equations from the perspective of the covariant spaces of the imposed geometric structure, for example, $J^1(Y)^\star$. However, a few more spaces should be described before proceeding, so that a deeper understanding of these structures and their implications may be attained.

The *primary constraint manifold*, denoted $P_{\mathcal{L}}$, is defined to be the image of the covariant Legendre transformation of the first jet bundle $P_{\mathcal{L}} = \mathbb{F}\mathcal{L}(J^1(Y))$, with the necessity that $\mathbb{F}\mathcal{L}$ is a diffeomorphism onto $P_{\mathcal{L}}$, and

$P_{\mathcal{L}} = \mathbb{F}\mathcal{L}(J^1(Y))$ is a smooth submanifold of $J^1(Y)^\star$. In this case, the Lagrangian density, $\mathcal{L}$ is called *regular*.

Define the connection on Y, as $\mathfrak{U} : TY \to VY$, such that $\mathfrak{U} : T_yY \to V_yY$ satisfies

$$\mathfrak{U} = Identity\ on\ VY.$$

The space VY is the *vertical subbundle* of TY, whose fibers are

$$V_yY = \{v \in T_yY | T\pi_{XY} \cdot v = 0\}.$$

Note that T_yY =image$(\gamma) \oplus V_yY$, where $\gamma \in J^1(Y)_y$. Also, the *horizontal space* is defined as $hor_y = ker(\mathfrak{U}_y)$, so that $T_yY = hor_y \oplus V_yY$. Thus, for an element $\gamma \in J^1(Y)_y$, the image(γ) is isomorphic to $ker(\mathfrak{U}_y)$. The *covariant Hamiltonian* $\mathcal{H} : P_{\mathcal{L}} \to \Lambda^{n+1}(X)$ may then be defined by

$$\mathcal{H}(\mathbb{F}\mathcal{L}(\gamma)) = D_{\mathfrak{U}}\mathcal{L}(\gamma) \cdot \gamma - \mathcal{L}(\gamma).$$

Thus, written in coordinates, $\mathcal{H}$ is

$$\mathcal{H} = Hd^{n+1}x_\mu = \left(\frac{\partial L}{\partial v_A}(v_\mu^A + \mathfrak{U}_\mu^A) - L\right) d^{n+1}x_\mu.$$

By defining the inclusion map $i^*_{J^1(Y)}, P_{\mathcal{L}} : P_{\mathcal{L}} \to J^1(Y)^\star$, the canonical $(n+1)$ form, and the $(n+2)$ form on $J^1(Y)^\star$, can be pulled back to the primary constraint manifold $P_{\mathcal{L}}$ as

$$\Theta_{\mathcal{H}} = i^*_{J^1(Y)^\star, P_{\mathcal{L}}}\Theta$$
$$\Omega_{\mathcal{H}} = i^*_{J^1(Y)^\star, P_{\mathcal{L}}}\Omega.$$

These canonical forms on $P\mathcal{L}$ are important in explaining the equivalence between the Lagrangian formulation and the Hamiltonian formulation. A few more additional notions should be defined before attempting to explain this equivalence.

If $j^1(\phi)$ is the first jet of the section $\phi \in \Gamma(\pi_{XY})$, then the *conjugate* to $j^1(\phi)$ is defined by

$$\tilde{j}^1(\phi) = \mathbb{F}\mathcal{L} \circ j^1(\phi).$$

Note that $\tilde{j}^1(\phi) \in \Gamma(\pi_{X,P_{\mathcal{L}}})$ is also a *holonomic* section of $\pi_{X,P_{\mathcal{L}}}$. Furthermore, $z = j^1(\phi)$, is said to be *Hamiltonian* if

$$z^*(\mathbf{i}_F\Omega_{\mathcal{H}}) = 0 \tag{11}$$

for all $F \in T(P_{\mathcal{L}})$. Equation 11 is the set of *multihamiltonian* equations. The set of multihamiltonian equations and the set of Euler-Lagrange equations are said to be implicative of each other. This implication is stated in the following Lemma that was extracted from Marsden, and Shkoller [1].

Lemma 1. *If $\mathbb{F}\mathcal{L} : J^1(Y) \to P\mathcal{L}$ is a fiber bundle diffeomorphism over Y, and $\phi \in \Gamma(\pi_{XY})$, then the following are equivalent*

$$\begin{array}{ll} (i) & \tilde{j}^1(\phi)^* \mathbf{i}_U \Omega_{\mathcal{H}} = 0, \quad \forall U \in T(P_{\mathcal{L}}); \\ (ii) & j^1(\phi)^* \mathbf{i}_W \Omega_{\mathcal{L}} = 0, \quad \forall W \in T(J^1(Y)). \end{array}$$

Note that (i) is the set of multihamiltonian equations, and (ii) is the set of Euler-Lagrange equations.

The proof of Lemma 1 can be found in Marsden, and Shkoller [1]. The following theorem was also extracted from Marsden, and Shkoller [1], explains the equivalence of the solution of the Euler-Lagrange equations to the solution of multihamiltonian equations.

Theorem 1. *If $\mathbb{F}\mathcal{L} : J^1(Y) \to P_{\mathcal{L}}$ is a fiber bundle diffeomorphism over Y, and $\phi \in \Gamma\pi_{XY}$, then the following are equivalent:*

$$\begin{array}{ll} (i) & \phi \text{ is a stationary point of } \int_X \mathcal{L}(j^1(\phi)); \\ (ii) & \tilde{j}^1(\phi) \text{ is a Hamiltonian section for } \mathcal{H}. \end{array}$$

Note that ϕ is a solution to the Euler-Lagrange equations, and $\tilde{j}^1(\phi)$ solves the set of multihamiltonian equations. Thus, solving the Euler-Lagrange equations is equivalent to solving the multihamiltonian equations.

The following proposition is also taken from Marsden, and Shkoller [1].

Proposition 1. *If $\mathbb{F}\mathcal{L} : J^1(Y) \to P\mathcal{L}$ is a fiber diffeomorphism and $\phi \in \Gamma(\pi_{XY}$, then $\tilde{j}^1(\phi)$ is a Hamiltonian system for $\mathcal{H}$ if and only if*

$$\mathbf{i}_{\frac{\partial}{\partial x^\mu}} \tilde{j}^1(\phi)(df^\mu \wedge d\phi) = -dH(\tilde{j}^1(\phi)). \tag{12}$$

where $\mu \in \{1, \ldots, (n+1)\}$.

It is noteworthy that 12 *is equivalent to the equation in Bridges*[3].

$$\mathbf{M}^\mu \frac{\partial \mathbf{n}}{\partial x^\mu} = -\nabla_{\mathbf{n}} H(\mathbf{n}),$$

where the index μ denotes a sum over all coordinates in the base space, and $\mathbf{n}$ is the vector $\mathbf{n} = (y^A, v^A_\nu)$, where ν denotes the ν^{th} spatial coordinate in the base space. If the dimension of $\mathbf{n}$ is $(m \times 1)$, then each $\mathbf{M}^\mu$ is a $m \times m$ matrix, $\mathbf{M}^\mu \in \mathbb{R}^{m \times m}$.

3.6 The Hamiltonian Formulation Applied to Schödinger Equation

Recall that the Hamiltonian density of the 3-d general Schrödinger equation, written in coordinates, is

$$\mathcal{H} = H d^{n+1} x_\mu = \left(\frac{\partial L}{\partial v_A} (v^A_\mu + \mathfrak{U}^A_\mu) - L \right) d^{n+1} x_\mu .$$

Thus, a connection, $\mathfrak{U}$, must be employed before proceeding. In this case, the trivial connection is selected. The trivial connection is merely the natural projection, where the action is coordinated by $(0, v^A)$, and thus, $\mathfrak{U}^A_\mu = 0$. Consequently, the covariant Hamiltonian for the 3-d general Schrödinger equation is regarded as $\mathcal{H} = H dx \wedge dy \wedge dz \wedge dt$, where

$$H = \frac{\partial L}{\partial p_t} p_t + \frac{\partial L}{\partial q_t} q_t + \frac{\partial L}{\partial p_x} p_x + \frac{\partial L}{\partial q_x} q_x + \frac{\partial L}{\partial p_y} p_y + \frac{\partial L}{\partial q_y} q_y + \frac{\partial L}{\partial p_z} p_z + \frac{\partial L}{\partial q_z} q_z - L$$

and thusly,

$$H = \frac{1}{2} \left(p_x^2 \; + \; p_y^2 \; + \; p_z^2 \; + \; q_x^2 \; + \; q_y^2 \; + \; q_z^2 \; - \; 2C \right) . \tag{13}$$

To case the equations of motion in a hamiltonian formulation, the following change of coordinates is utilized

$$\begin{array}{ll} v_1 = \frac{\partial L}{\partial p_x} = p_x & w_1 = \frac{\partial L}{\partial q_x} = q_x \\ v_2 = \frac{\partial L}{\partial p_y} = p_y & w_2 = \frac{\partial L}{\partial q_y} = q_y \\ v_3 = \frac{\partial L}{\partial p_z} = p_z & w_3 = \frac{\partial L}{\partial q_z} = q_z . \end{array}$$

Recasting equation 3 using these coordinates yields the first order equations

$$\begin{array}{l} q_t - v_{1x} - v_{2y} - v_{3y} = -\frac{\partial C}{\partial p} \\ -p_t - w_{1x} - w_{2y} - w_{3y} = -\frac{\partial C}{\partial q} \\ p_x = v_1 \\ q_x = w_1 \\ p_y = v_2 \\ q_y = w_2 \\ p_z = v_3 \\ q_z = w_3 . \end{array} \tag{14}$$

Also, H in the new coordinates becomes

$$H = \frac{1}{2}\left(v_1^2 + v_2^2 + v_3^2 + w_1^2 + w_2^2 + w_3^2 - 2C\right). \tag{15}$$

Then by letting $\mathbf{n} = (p, q, v_1, w_1, v_2, w_2, v_3, w_3)^T$, the equations in 14 are written in compact notation as

$$\mathbf{M}\frac{\partial \mathbf{n}}{\partial t} + \mathbf{K_x}\frac{\partial \mathbf{n}}{\partial x} + \mathbf{K_y}\frac{\partial \mathbf{n}}{\partial y} + \mathbf{K_z}\frac{\partial \mathbf{n}}{\partial z} = -\nabla_{\mathbf{n}} H(\mathbf{n}), \tag{16}$$

where the matrices in the above equation are defined by

$$\mathbf{M} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \mathbf{K_x} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\mathbf{K_y} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \mathbf{K_z} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

These matrices, $\mathbf{M}$, $\mathbf{K_x}$, $\mathbf{K_y}$, and $\mathbf{K_z}$, will be useful in the development of the multisymplectic structure, and the multisymplectic conservation law, in the next section.

It is easy to see that equation 16 is Bridges equation defined in Proposition 1. Thus, by a combination of Theorem 1 and Proposition 1, solving equation 16 is equivalent to solving the Euler-Lagrange equations.

4 The Multisymplectic Structure

To define a multisymplectic structure, the notion of a presymplectic form must be defined. A presymplectic form is a bilinear 2-form that is closed, skew-symmetric, but not necessarily nondegenerate. A set of presymplectic forms together with a manifold comprise a *multisymplectic structure*. For the matrices $\mathbf{M}$, $\mathbf{K_x}$, $\mathbf{K_y}$, and $\mathbf{K_z}$, in the previous section, define the presymplectic forms:

$$\begin{aligned}\omega(a,b) &= \langle Ma, b\rangle \\ \kappa_x(a,b) &= \langle K_x a, b\rangle \\ \kappa_y(a,b) &= \langle K_y a, b\rangle \\ \kappa_z(a,b) &= \langle K_z a, b\rangle\end{aligned}$$

where the matrix representation of these forms is defined by

$$g(a,b) = \langle Ga, b\rangle = a^T G^T b,$$

where $G \in \mathbb{R}^{8\times 8}$. Then $(TJ^1(Y), \omega, \kappa_x, \kappa_y, \kappa_z)$ is a multisymplectic structure of the general Schrödinger equation.

5 The Multisymplectic Form Formula

Before stating the multisymplectic form formula, it is necessary to classify the types of sections and vector fields that are employed in theorem, so that it will hold true.

Suppose $U \subset X$ is a smooth submanifold, with piecewise smooth closed boundary. Then $\mathcal{C}^\infty$ is the set of smooth maps

$$\mathcal{C}^\infty = \{\phi : U \to Y\} | \pi_{XY} \circ \phi : U \to X \texttt{ is an embedding}\}.$$

Define $\mathcal{C}$ as the infinite dimensional manifold that is the closure of $\mathcal{C}^\infty$ in the Hilbert space. Next, define the set of solutions to the Euler-Lagrange equations

$$\mathcal{P} = \{\phi \in \mathcal{C} | j^1(\phi)^* \mathbf{i}_W \Omega_{\mathcal{L}} = 0,\ \forall W \in TJ^1(Y)\}.$$

Lastly, define the set of vector fields that solve the first variation equation to the Euler-Lagrange equations (in equation 6)

$$\mathcal{F} = \{V \in T_\phi \mathcal{C} | j^1(\phi)^* \mathfrak{L}_{j^1(V)} \mathbf{i}_B \Omega_{\mathcal{L}} = 0,\ \forall B \in TJ^1(Y)\}.$$

Now that all of the necessary components have been stated, the multisymplectic form formula may be introduced.

Theorem 2. ***The Multisymplectic Form Formula***
If $\phi \in \mathcal{P}$ (ϕ is a solution to the Euler-Lagrange equations), then $\forall V, W \in \mathcal{F}$ (for all V and W that solve the first variation equations (equation 6) of the Euler-Lagrange equations),

$$\int_{\partial U} j^1(\phi)^* \mathbf{i}_{j^1(V)} \mathbf{i}_{j^1(W)} \Omega_{\mathcal{L}} = 0$$

where $j^1(V), j^1(W) \in J^1(Y)$.

The proof of this theorem can be found in Marsden, Patrick, and Shkoller[2]. It is noteworthy that several implicating theorems can be extracted from the multisymplectic structure and the multisymplectic form formula. A few of these implicating theorems will be discussed in what follows.

Theorem 3. *The multisymplectic form formula implies the multisymplectic conservation law.*

$$\frac{\partial \omega}{\partial t} + \frac{\partial \kappa_x}{\partial x} + \frac{\partial \kappa_y}{\partial y} + \frac{\partial \kappa_z}{\partial z} = 0$$

Proof. Let $V, W \in \mathcal{F}$, and $j^1(V), j^1(W) \in \mathfrak{X}(J^1(Y))$ be $\pi_{X,J^1(Y)}$ vertical vector fields. The vector fields $j^1(V), j^1(W)$ on $J^1(Y)$ are coordinated by the expressions

$$\begin{aligned} j^1(V) \;\; = \;\; & V^p \tfrac{\partial}{\partial p} + V^q \tfrac{\partial}{\partial q} + V^{p_t} \tfrac{\partial}{\partial p_t} + V^{q_t} \tfrac{\partial}{\partial q_t} + V^{p_x} \tfrac{\partial}{\partial p_x} + \\ & V^{q_x} \tfrac{\partial}{\partial q_x} + V^{p_y} \tfrac{\partial}{\partial p_y} + V^{q_y} \tfrac{\partial}{\partial q_y} + V^{p_z} \tfrac{\partial}{\partial p_z} + V^{q_z} \tfrac{\partial}{\partial q_z}, \end{aligned}$$

and

$$\begin{aligned} j^1(W) \;\; = \;\; & W^p \tfrac{\partial}{\partial p} + W^q \tfrac{\partial}{\partial q} + W^{p_t} \tfrac{\partial}{\partial p_t} + W^{q_t} \tfrac{\partial}{\partial q_t} + W^{p_x} \tfrac{\partial}{\partial p_x} + \\ & W^{q_x} \tfrac{\partial}{\partial q_x} + W^{p_y} \tfrac{\partial}{\partial p_y} + W^{q_y} \tfrac{\partial}{\partial q_y} + W^{p_z} \tfrac{\partial}{\partial p_z} + W^{q_z} \tfrac{\partial}{\partial q_z}. \end{aligned}$$

The expression $\mathbf{i}_{j^1(V)} \mathbf{i}_{j^1(W)} \Omega_{\mathcal{L}}$ is the 3 form

$$\begin{aligned} \mathbf{i}_{j^1(V)} \mathbf{i}_{j^1(W)} \Omega_{\mathcal{L}} \;\; = \;\; & (V^q W^p - V^p W^q)\, dx \wedge dy \wedge dz \\ & + (V^{p_x} W^p + V^{q_x} W^q - V^p W^{p_x} - V^q W^{q_x})\, dy \wedge dz \wedge dt \\ & + (V^{p_y} W^p + V^{q_y} W^q - V^p W^{p_y} - V^q W^{q_y})\, dz \wedge dx \wedge dt \\ & + (V^{p_z} W^p + V^{q_z} W^q - V^p W^{p_z} - V^q W^{q_z})\, dx \wedge dy \wedge dt \end{aligned} \tag{17}$$

However, it is also the case that

$$\omega(j^1(V), j^1(W)) = V^p W^q - V^q W^p$$

$$\begin{aligned}
\kappa_x(j^1(V), j^1(W)) &= V^{p_x} W^p + V^{q_x} W^q - V^p W^{p_x} - V^q W^{q_x} \\
\kappa_y(j^1(V), j^1(W)) &= V^{p_y} W^p + V^{q_y} W^q - V^p W^{p_y} - V^q W^{q_y} \\
\kappa_z(j^1(V), j^1(W)) &= V^{p_z} W^p + V^{q_z} W^q - V^p W^{p_z} - V^q W^{q_z}.
\end{aligned}$$

As a result, $\mathbf{i}_{j^1(V)}\mathbf{i}_{j^1(W)}\Omega_{\mathcal{L}}$ can be expressed in terms of the presymplectic forms

$$\begin{aligned}
\mathbf{i}_{j^1(V)}\mathbf{i}_{j^1(W)}\Omega_{\mathcal{L}} \;\; = \;\; & -\omega(j^1(V), j^1(W))dx \wedge dy \wedge dz + \kappa_x(j^1(V), j^1(W))dy \wedge dz \wedge dt \\
& +\kappa_y(j^1(V), j^1(W))dz \wedge dx \wedge dt + \kappa_z(j^1(V), j^1(W))dx \wedge dy \wedge dt.
\end{aligned} \tag{18}$$

Recall that the multisymplectic form formula states

$$\int_{\partial U} j^1(\phi)^* \mathbf{i}_{j^1(V)}\mathbf{i}_{j^1(W)}\Omega_{\mathcal{L}} = 0.$$

Thus

$$\int_{\partial U} -\omega(\star)dx \wedge dy \wedge dz + \kappa_x(\star)dy \wedge dz \wedge dt + \kappa_y(\star)dz \wedge dx \wedge dt + \kappa_z(\star)dx \wedge dy \wedge dt = 0 \tag{19}$$

where $(\star) = (j^1(V), j^1(W))$. As defined previously, U is a smooth four dimensional submanifold of X with piecewise smooth closed boundary. Therefore after applying Stokes' Theorem to equation 19, it becomes

$$\int_{U} \left(\frac{\partial}{\partial t}\omega(\star) + \frac{\partial}{\partial x}\kappa_x(\star) + \frac{\partial}{\partial y}\kappa_y(\star) + \frac{\partial}{\partial z}\kappa_z(\star)\right) dx \wedge dy \wedge dz \wedge dt = 0. \tag{20}$$

Now, because $j^1(V)$ and $j^1(W)$ are *arbitrary* vector fields on $J^1(Y)$, and U is an *arbitrary* smooth submanifold of X,

$$\frac{\partial \omega}{\partial t} + \frac{\partial \kappa_x}{\partial x} + \frac{\partial \kappa_y}{\partial y} + \frac{\partial \kappa_z}{\partial z} = 0,$$

which is the multisymplectic conservation law. $\square$

Theorem 4. *For the case where the base space $U \subset X$ is coordinated with infinite spatial domain, in other words, if*

$$U = \{(x, y, z, t) \in \mathbb{R}^3 \times \mathbb{R} \,|\, x \in (-\infty, \infty),\ y \in (-\infty, \infty), \&\ z \in (-\infty, \infty)\},$$

then the relationship between the quantum mechanical symplectic form, $\Omega(\Psi, \Phi)$, and the presymplectic form, $\omega\left(j^1(V), j^1(W)\right)$, is

$$\Omega(\Psi, \Phi) = -2 \int\limits_{\partial U} \omega\left(j^1(V), j^1(W)\right) dx \wedge dy \wedge dz.$$

Please note that in this case, $j^1(V)$ is associated with the wavefunction Ψ, and $j^1(W)$ is associated with the wavefunction Φ, in the following manner

$$\begin{aligned} j^1(V) \;\; &= \;\; p^\Psi \tfrac{\partial}{\partial p} + q^\Psi \tfrac{\partial}{\partial q} + V^{p_t} \tfrac{\partial}{\partial p_t} + V^{q_t} \tfrac{\partial}{\partial q_t} + V^{p_x} \tfrac{\partial}{\partial p_x} + \\ &\quad\;\; V^{q_x} \tfrac{\partial}{\partial q_x} + V^{p_y} \tfrac{\partial}{\partial p_y} + V^{q_y} \tfrac{\partial}{\partial q_y} + V^{p_z} \tfrac{\partial}{\partial p_z} + V^{q_z} \tfrac{\partial}{\partial q_z} \end{aligned}$$

and

$$\begin{aligned} j^1(W) \;\; &= \;\; p^\Phi \tfrac{\partial}{\partial p} + q^\Phi \tfrac{\partial}{\partial q} + W^{p_t} \tfrac{\partial}{\partial p_t} + W^{q_t} \tfrac{\partial}{\partial q_t} + W^{p_x} \tfrac{\partial}{\partial p_x} + \\ &\quad\;\; W^{q_x} \tfrac{\partial}{\partial q_x} + W^{p_y} \tfrac{\partial}{\partial p_y} + W^{q_y} \tfrac{\partial}{\partial q_y} + W^{p_z} \tfrac{\partial}{\partial p_z} + W^{q_z} \tfrac{\partial}{\partial q_z}. \end{aligned}$$

where $p^\Psi = \mathbf{Re}\{\Psi\}$, $q^\Psi = \mathbf{Im}\{\Psi\}$, and $p^\Phi = \mathbf{Re}\{\Phi\}$, $q^\Psi = \mathbf{Im}\{\Phi\}$.

Note that the quantum mechanical symplectic form is defined in terms of the ordinary quantum mechancial Hermitian inner product on the complex Hilbert space of L^2 wavefunctions[4]*, $\langle\langle\Psi, \Phi\rangle\rangle$, as*

$$\Omega(\Psi, \Phi) = -2\mathbf{Im}\langle\langle\Psi, \Phi\rangle\rangle.$$

Proof. The presymplectic form, $\omega(\cdot, \cdot)$, acting on the vector fields, $j^1(V), j^1(W) \in TJ^1(Y)$, as defined above, is

$$\omega\left(j^1(V), j^1(W)\right) = p^\Psi q^\Phi - q^\Psi p^\Phi.$$

Thus

$$\int\limits_{\partial U} \omega\left(j^1(V), j^1(W)\right) dx \wedge dy \wedge dz = \int\limits_{\partial U} \left(p^\Psi q^\Phi - q^\Psi p^\Phi\right) dx \wedge dy \wedge dz. \quad (21)$$

As stated in the theorem, the quantum mechanical symplectic form is defined in terms of the ordinary quantum mechancial Hermitian inner product on the complex Hilbert space of L^2 wavefunctions, $\langle\langle\Psi, \Phi\rangle\rangle$, as

$$\Omega(\Psi, \Phi) = -2\mathbf{Im}\langle\langle\Psi, \Phi\rangle\rangle,$$

where

$$\langle\langle\Psi, \Phi\rangle\rangle = \int \Psi^{\star}\Phi \, d\tau$$

which in Cartesian coordinates is

$$\langle\langle\Psi, \Phi\rangle\rangle = \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \Psi^{\star}\Phi \, dx \wedge dy \wedge dz.$$

Let $\Psi = \mathbf{Re}\{\Psi\} + \mathbf{iIm}\{\Psi\}$, and $\Phi = \mathbf{Re}\{\Phi\} + \mathbf{iIm}\{\Phi\}$. Then the Hermitian inner product of Ψ and Φ is

$$\langle\langle\Psi, \Phi\rangle\rangle = \int \Psi^{\star}\Phi \, d\tau = \int \left(\mathbf{Re}\{\Psi\} - \mathbf{iIm}\{\Psi\}\right)\left(\mathbf{Re}\{\Phi\} + \mathbf{iIm}\{\Phi\}\right) \, d\tau.$$

Expanding the above product yields,

$$\langle\langle\Psi, \Phi\rangle\rangle = \int \left(\mathbf{Re}\{\Psi\}\mathbf{Re}\{\Phi\} + \mathbf{Im}\{\Psi\}\mathbf{Im}\{\Phi\}\right) d\tau + \mathbf{i}\int \left(\mathbf{Re}\{\Psi\}\mathbf{Im}\{\Phi\} - \mathbf{Im}\{\Psi\}\mathbf{Re}\{\Phi\}\right) d\tau.$$

Now let $\mathbf{Re}\{\Psi\} = p^{\Psi}$, $\mathbf{Im}\{\Psi\} = q^{\Psi}$, $\mathbf{Re}\{\Phi\} = p^{\Phi}$, $\mathbf{Im}\{\Phi\} = q^{\Phi}$. Then the Hermitian inner product of Ψ and Φ becomes

$$\langle\langle\Psi, \Phi\rangle\rangle = \int \left(p^{\Psi}p^{\Phi} + q^{\Psi}q^{\Phi}\right) \, d\tau + \mathbf{i}\int \left(p^{\Psi}q^{\Phi} - q^{\Psi}p^{\Phi}\right) \, d\tau$$

The symplectic form for quantum mechanics is

$$\Omega(\Psi, \Phi) = -2\mathbf{Im}\langle\langle\Psi, \Phi\rangle\rangle = -2\int \left(p^{\Psi}q^{\Phi} - q^{\Psi}p^{\Phi}\right) \, d\tau.$$

In Cartesian coordinates this is

$$\Omega(\Psi, \Phi) = -2\mathbf{Im}\langle\langle\Psi, \Phi\rangle\rangle = -2\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \left(p^{\Psi}q^{\Phi} - q^{\Psi}p^{\Phi}\right) \, dx \wedge dy \wedge dz.$$

But because

$$U = \{(x, y, z, t) \in \mathbb{R}^3 \times \mathbb{R} \mid x \in (-\infty, \infty),\ y \in (-\infty, \infty), \&\ z \in (-\infty, \infty)\},$$

then

$$\int_{\partial U} \omega\left(j^1(V), j^1(W)\right) dx \wedge dy \wedge dz = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \omega\left(j^1(V), j^1(W)\right) dx \wedge dy \wedge dz = \mathbf{Im}\langle\langle \Psi, \Phi\rangle\rangle.$$

and consequently

$$\Omega(\Psi, \Phi) = -2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \omega\left(j^1(V), j^1(W)\right)\ dx \wedge dy \wedge dz.$$

Therefore, it is proven that:

$$\Omega(\Psi, \Phi) = -2 \int_{\partial U} \omega\left(j^1(V), j^1(W)\right)\ dx \wedge dy \wedge dz.$$

□

Theorem 5. *For the 3-d general Schrodinger equation with infinite spatial domain, and bounded time domain, $t \in [T_1, T_2]$, the integrals along the boundaries at $t = T_1$ and $t = T_2$ are equal in magnitude but opposite in orientation. In other words*

$$\int_{\partial U_{T_1}} \omega(j^1(V), j^1(W)) dx \wedge dy \wedge dz = -\int_{\partial U_{T_2}} \omega(j^1(V), j^1(W)) dx \wedge dy \wedge dz.$$

Proof. From the proof of 5, the multisymplectic form formula implies that

$$\int_{\partial U} -\omega(\star) dx \wedge dy \wedge dz + \kappa_x(\star) dy \wedge dz \wedge dt + \kappa_y(\star) dz \wedge dx \wedge dt + \kappa_z(\star) dx \wedge dy \wedge dt = 0. \tag{22}$$

Now, for reasons explained after the following statement, the multisymplectic form formula applied to a system with an infinite spatial domain but bounded time domain reduces to

$$\int_{\partial U} \omega(j^1(V), j^1(W)) dx \wedge dy \wedge dz = 0. \tag{23}$$

This phenomena occurs due to the fact that in the multisymplectic form formula, the integration takes place along the *boundary* of the domain U. Yet, for the case that the system possesses bounded time domain, and unbounded, or infinite spatial domain, there does not exist a boundary that *proceeds along* the temporal domain, upon which to integrate. Thus, each form in 22 that includes the term dt, simply disappears.

Now because the time coordinate is bounded, this means that there is an upper limit in time, and a lower limit in time. Thus, for each integration in the triple integral, there are two boundaries to integrate along in equation 23. Denote the lower boundary by ∂U_{T_1}, and the upper boundary by ∂U_{T_2}. Then equation 23 becomes

$$\int\limits_{\partial U_{T_1}} \omega(j^1(V), j^1(W)) dx \wedge dy \wedge dz + \int\limits_{\partial U_{T_2}} \omega(j^1(V), j^1(W)) dx \wedge dy \wedge dz = 0.$$

As a result,

$$\int\limits_{\partial U_{T_1}} \omega(j^1(V), j^1(W)) dx \wedge dy \wedge dz = - \int\limits_{\partial U_{T_2}} \omega(j^1(V), j^1(W)) dx \wedge dy \wedge dz.$$

Thus, the integrals along the boundaries at time $t = T_1$ and time $t = T_2$, that is, the integrals along ∂U_{T_1} and ∂U_{T_2}, are equal in magnitude, but opposite in orientation. $\square$

6 Conclusion

The methodology in this paper can certainly be easily extended to higher dimensional systems. For example, for a system with N particles, the $3N$-dimensional Schrödinger equation can be geometrized in an analogous fashion, with the base space being coordinated by $3N$ spatial coordinates instead of 3. Additionally, the base space may be coordinated by any other dependent variable that one may wish to consider, that the wavefunction is related to.

The geometric framework presented in this paper can be utilized to derive integrators for various partial differential equations. For example, the Veselov-type discretization, normally applied to the regular Lagrangian formulation, may be applied to multisymplectic field theory for the purpose of deriving variational integrators[1]. This method was applied in Chen[5] to the nonlinear Schrödinger equation. It is hoped that the work presented here has laid the groundwork for Veselov-type discretization techniques to be applied to the general Schrödinger equation.

Optimistically, the geometric structure imposed on the Schrödinger equation will lead to greater insight in one's study of theoretical physics and chemistry. The trick is to relate the mathematical objects in this framework to an object or idea that corresponds to reality in the physical world. For example, what does the multisymplectic conservation law correspond to in the "real world"? Most likely this idea has already been explored. However, asking such types of question will lead to either 1) a higher level of knowledge that is already known, 2) a higher level of discovery in quantum mechanics, or 3) a wider area of application. All three areas are well worth the effort that will take to pose and answer such questions.

7 References

1. J.E. Marsden, S. Shkoller, *Math. Proc. Camb. Phil. Soc.*, **125**, 553-575, (1999).

2. J.E. Marsden, G.W. Patrick, S. Shkoller, *Comm. Math. Phys.*, **199**, 351-395, (1998).

3. T.J. Bridges, *Math. Proc. Phil. Soc.*, **121**, 147-190, (1997).

4. J.E. Marsden, T.S. Ratiu, *Introduction to Mechanics and Symmetry*, Springer-Verlag, (1999).

5. J.B. Chen, M.Z. Qin, *Numer. Math. Partial Differential Equations*, **18**, 523-536, (2002).