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2007 J. Phys. A: Math. Theor. 40 9883

(http://iopscience.iop.org/1751-8121/40/32/013)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **40** (2007) 9883–9904 doi:10.1088/1751-8113/40/32/013

# $\mathcal{PT}$ and $\mathcal{CPT}$ quantum mechanics embedded in symplectic quantum mechanics

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Received 23 February 2007, in final form 13 June 2007
Published 24 July 2007
Online at stacks.iop.org/JPhysA/40/9883

**Abstract**
A real-valued symplectic group underlies the dynamics of quantum-mechanical systems. Exploring the embedding of unitary groups clarifies the relation of non-Hermitian $\mathcal{PT}$- and $\mathcal{CPT}$-symmetric quantum theories of recent interest. Symmetries of the full dynamical framework are quite rich and reveal new viewpoints on many topics in quantum theory. Transformations mixing 'upper' and 'lower' components of certain symplectic multiplets are indistinguishable from coupling antimatter degrees of freedom. Quantities long identified with *physical observables* are valid canonical coordinates of the theory, without needing support from measurement doctrine. Dirac's canonical quantization is derived from consistency, and would be redundant as a new postulate. A second-order dynamical framework exists in which observables are just the same as the underlying degrees of freedom.

PACS number: 03.65.Ge

## 1. What is quantum dynamics?

The meaning of quantum theory is still evolving. A few years ago Bender *et al* [1] contradicted the esteemed postulate that quantum Hamiltonian operators must be Hermitian. A broader criterion of $\mathcal{PT}$-symmetric theories was proposed. The work has had such impact that we can safely call the field '$\mathcal{PT}$ theories' or '$\mathcal{PT}$ ($\mathcal{CPT}$) quantum mechanics' without confusion.

The work opened new opportunities to rethink what is meant by quantum mechanics. History bypassed the most general coordinate transformations, and replaced them with a misleading notion that 'Hermiticity' in ordinary form would be an invariant concept. Although Hermiticity guarantees unitary time evolution and real eigenvalues, the invariant fact of unitary evolution does not imply Hermiticity in the usual sense of transpose-conjugate operations on matrix elements [1–3]. The more general concept of pseudo-Hermitian operators [3] as a class with real eigenvalues is invariant under similarity transformations. Whether physical Hamiltonians can then be characterized by $\mathcal{PT}$ or $\mathcal{CPT}$ symmetries is an interesting debate. In some cases the $\mathcal{PT}$–$\mathcal{CPT}$ extensions are found equivalent to ordinary quantum mechanics in transformed coordinates, but debate is not over. It is interesting to break the mold with counterexamples of invariantly distinct type, as we shall do.

For physical meaning, rules of quantum theory must also be related to the meaning obtained from measurements. Without engaging a philosophical morass of measurement theory, there remain gaps in how quantum coordinates are set up and interpreted. This cannot be separated from the symmetries of the dynamical framework. The purpose of this paper is to extend quantum mechanics further. We may as well enlarge the symmetry group of the dynamics to the largest possible, the symplectic ($\mathcal{S}p$) group. This is a genuine extension that subsumes the usual rules, while allowing novel possibilities which are genuinely and invariantly 'new'. It is also a pleasure to see old results emerge in refreshing form and without the need to make new postulates traditionally thought necessary for their justification.

### *1.1. Developing a different point of view*

In the standard approach to quantum theory a finite number of classical degrees of freedom $q_i(t)$ are 'promoted' by postulate to Hermitian operators $\hat{\mathcal{Q}}_i$. The operators are said to play the role of 'observables' although they cannot be directly measured. It can be non-trivial simply to test whether or not an operator is 'Hermitian', because common definitions are tied to interlocked conventions between the operator and the state space, and the conventions are not themselves observable.

Let operators have a hat () and symbol $\langle\rangle$ denote the usual expectation. Consider what information lies in the time evolution of $\langle\hat{x}_i\rangle(t)$ and $\langle\hat{p}_i\rangle(t)$ and all other possible expectations $\langle\hat{\mathcal{Q}}_i\rangle$. There is a consensus that such expectation values can be measured. In full view of statistical fluctuations, the *numerical value* of each $\langle\hat{\mathcal{Q}}_i\rangle$ is a perfectly definite thing. We ask if it is manifestly impossible for a group of determined engineers to develop a theory of the observables based on the observables. Symbolically there should exist an invertible map of a suitable set of operators into generalized coordinates $Q_i$,

$$\langle\hat{\mathcal{Q}}_i\rangle \rightleftarrows Q_i. \tag{1}$$

Existence of such an 'engineering theory' is tantamount to existence of sets of coupled differential equations $D_t Q_i = f(Q_i)$ that determine the coordinate time evolution, where $D_t$ would be appropriate time-derivative operators.

While appealing for its deterministic flavor, it is by no means obvious that any such relations could possibly be consistent with quantum theory. The usual Ehrenfest relations show that time evolution of $\langle\hat{\mathcal{Q}}_i\rangle$ is definitely *not* those of the classical theory from which canonical quantization starts. Quantum dynamics also uses unobservable variables that are lost when projecting to observables. Despite these difficulties working with observable coordinates $Q_i$ is a central point. It permits separation of those transformations which are mere notation compared to those with physical consequences. The power comes from *compensating coordinate changes of operators and states that cancel in forming observables*. It is then surprising that when the map is constructed, there exist generalized coordinates $Q_i(t)$ for which the time evolution is *Hamiltonian* (section 4.1.1).

Here symplectic transformations and symmetries enter in the most fundamental way. Hamiltonian structure implies a conjugacy of coordinate ($q$) and momentum ($p$) variables arranged in pairs. We must discover from the map itself whether the Hamiltonian generalized coordinate $Q_i$ is momentum-like or coordinate-like. Then each observable $Q_i(t)$ turns out to be paired with a particular conjugate-phase variable long identified as 'unobservable'. This structure is developed independently from measurement theory, and does not need it for justification, yet dovetails remarkably with it. Exactly half the variables used in a first-order description cannot be observed. However autonomous *second-order* differential equations exist relating $Q$'s in terms of $Q$'s, completing the task of relating observables to dynamics. This task is close to the program expressed by 't Hooft [4] although in unexpected form.

While these 'good coordinates' are a focus, there always remain the usual linear coordinate transformations among degrees of freedom carried out by representation theory

$$|\psi\rangle \to |\psi\rangle' = V|\psi\rangle;$$
$$\langle\psi|\mathcal{Q}_i|\psi\rangle \to \langle\psi|V^\dagger \mathcal{Q}_i V|\psi\rangle = \Lambda_{ij}\langle\psi|\mathcal{Q}_j|\psi\rangle;$$
$$Q_i \to Q_i' = \Lambda_{ij} Q_j;$$

Such transformations are agreements to rename *invariant* observables in terms of one other, a freedom necessary to retain. Intricate canonical transformations that mix $q$'s and $p$'s on a hidden phase space are dual to the complex unitary transformations of conventional quantum theory. There is great variation on how dynamical degrees of freedom are defined and counted. It would be absurd to mistake the position operator $\hat{x}$ with a single expectation $\langle\hat{x}\rangle$. Under canonical quantization a single classical degree of freedom is replaced by an infinite number of complex dynamical components, whether represented by a wave, a ket vector or a Hilbert space operator. Because much of our approach is new, the paper develops everything independently, and in the most elementary manner possible.

In section 2, there is a review and a brief summary of complex similarity transformations developed in $\mathcal{PT}$ theories. The complex components are then broken down to more general real-valued canonical coordinates in the following section. Definitions and counting of degrees of freedom are given here. Unitary versus non-unitary transformations are classified in section 2.2.4. Special topics of time reversal, hidden gauge symmetries and 'faster than Hermitian' quantum mechanics are developed as other special symplectic transformations. The symplectic group has two disconnected components which naturally map into classical antimatter and $\mathcal{CPT}$ symmetry in section 3. The role of Poisson brackets is viewed afresh in section 4. From the precedence of dynamical symmetries the bracket structure becomes a derived notation, as in classical physics, without any need to be postulated separately. Lie algebra relations are then developed, with a novel discussion of canonical quantization. Generalized Ehrenfest relations are developed as exact dynamical equations in section 4.1.1. A simple example of dynamics which is not unitarily equivalent to the usual quantum theory is given in section 4.2. A brief summary is given in section 5.

## 2. Symplectic dynamical symmetry

For completeness we first review the elementary symmetries of the quantum dynamical framework.

In Schroedinger picture the usual state vector $|\psi\rangle$ obeys the equation

$$\mathrm{i}|\dot{\psi}\rangle = \hat{H}|\psi\rangle \tag{2}$$

called 'the equation of motion in Schroedinger coordinates'. Let $U(t)$ be an arbitrary time-dependent unitary operator acting on the space of $|\psi\rangle$

$$|\psi\rangle \to |\psi\rangle_U = U(t)|\psi\rangle; \qquad U(t)U(t)^\dagger = U(t)^\dagger U(t) = 1.$$

Then the equation for the transformed state is

$$\mathrm{i}|\dot{\psi}\rangle_U = \hat{H}_U|\psi\rangle_U; \qquad \hat{H}_U = U\hat{H}_U U^\dagger + \mathrm{i}\dot{U}U^\dagger. \tag{3}$$

The statement that $\hat{H} = \hat{H}^\dagger$ is transformed into the rule $\hat{H}_U = \hat{H}_U^\dagger$ under which Hermiticity is a unitary invariant. Conversely, all the solutions of equation (2) are given by

$|\psi(t)\rangle = V(t)|\psi(0)\rangle$, where $V(t)$ is directly related to $H$. The generator of the transformation comes by differentiation

$$\hat{H} = \mathrm{i}\dot{V}V^{\dagger}(t) \tag{4}$$

with $\hat{H}$ Hermitian. It follows that a feature of unitary evolution and invariance of the equation of motion under unitary transformations are one and the same. It is a very basic result that has traditionally led to *restricting* transformations to the unitary group by reasoning that has come to be challenged. Measurement theory also plays a role in highlighting unitary evolution, but it is a role we consistently separate from dynamics.

### *2.1. Complex similarity transformations*

Extension of ordinary quantum mechanics to a complex $\mathcal{PT}$-related framework comes by introducing a complex similarity transformation $S$. The view of Mostafazadeh [3] is reviewed here with certain additions for later use.

Let

$$\begin{aligned} &|\psi\rangle \to |\psi\rangle_S = S|\psi\rangle, \\ &\hat{H} \to \hat{H}(S) = S\hat{H}S^{-1}, \\ &\mathrm{i}|\dot{\psi}\rangle_S = \hat{H}(S)|\psi\rangle_S, \end{aligned} \tag{5}$$

where in the last line we restricted $\dot{S} = 0$.

Simultaneously we revise the rules for inner products to include a *metric*. The invariant inner product is the sandwich

$$\langle\psi|g|\psi\rangle, \tag{6}$$

retaining the usual meaning for brackets. Invariance requires

$$\langle\psi|g|\psi\rangle \to \langle\psi'|g'|\psi'\rangle = \langle\psi|g|\psi\rangle, \tag{7}$$

requiring the transformation rule

$$g' = S^{\dagger-1}gS^{-1}. \tag{8}$$

That is, each index of $g$ transforms covariantly. If norms are positive and real, then $g$ is a positive matrix and can be transformed to '1'. Alternatively $g' = (SS^{\dagger})^{-1}$ is the transformation from $g = 1$ to $g'$.

It is convenient to define

$$\begin{aligned} &\psi_\mu = \langle\mu|\psi\rangle; \\ &\psi^{*\mu} = \langle\psi|g|\mu\rangle; \\ &\langle\psi|g|\psi\rangle = \psi^{*\mu}\psi_\mu. \end{aligned} \tag{9}$$

In the same notation the equation of motion is

$$\mathrm{i}\dot{\psi}_\mu = H_\mu^\nu(S)\psi_\nu,$$

where $H_\mu^\nu(S)$ is a matrix of no particular symmetry. This equation can also be written with a covariant derivative

$$\begin{aligned} \mathrm{i}\dot{\psi}_\mu &= \frac{\partial\mathcal{H}}{\partial\psi^{\mu*}}; \\ \mathcal{H} &= \psi^{\mu*}H_\mu^\nu(S)\psi_\nu \\ &= \psi_\mu^*H^{\mu\nu}(S)\psi_\nu. \end{aligned} \tag{10}$$

The last expression shows $H^{\mu\nu}(S)$ is necessarily Hermitian if $\mathcal{H}$ is real for all $\psi$. In matrix language

$$(gH(S))^\dagger = H^\dagger(S)g^\dagger = gH(S), \qquad H^\dagger(S) = gH(S)g^{-1}, \tag{11}$$

with $g = g^\dagger$. This is the transformation of Hermiticity 'in the Dirac sense' into new coordinates [3].

The unitary group itself is transformed: each element $U \to U_S = SUS^{-1}$. The unitary operators no longer obey the matrix-element conditions of unitary, but obey a new relation

$$U_S^\dagger g_S U_S = g_S. \tag{12}$$

That is, the unitary transformations become the isometry group.

The invariant features define what is important. The spectrum of eigenvalues of Hermitian operators is real and invariant under similarity. Unfortunately this requires finding the eigenvalues as a test. Alternately, given $g_S$ one can test and identify all $U_S$. After this classification one can reverse all the arguments: given a theory with metric $g_S$ for inner products, nobody can stop us from diagonalizing $g_S$, constructing $S^{-1}$ and going to coordinates where $g_S = 1$. If theory had not started with unit metric and Hermiticity, we would *obtain* the unit metric by a sequence of coordinate transformations. With deference to measurement, 'there is no observable distinction' in complicating the theory with a non-trivial metric destined to cancel out. It is absolutely a matter of convenience which set of coordinates might be preferred.

Conventional motivation for Hermitian Hamiltonians and ordinary unitary transformations is obvious. Yet it is not realistic to dismiss debate over $\mathcal{PT}$–$\mathcal{CPT}$-symmetric theories by formal statements of their spectrum. We maintain that increasing the coordinate freedom should be viewed as a positive development. As a matter of fact, practical physics as a whole is exactly the art of manipulating coordinate systems. Bender *et al* [5] show a case where perturbation theory is much more stable for a system in a non-Hermitian form. For this reason use of new coordinates is hardly an insignificant affair.

There is plenty of motivation for exploring even more general forms.

### *2.2. Real extension*

Here we discuss a real-valued extension which yields some remarkable results. First note that a real-valued extension of quantum theory stands to be *more general* than complex ones. Counting the components $\psi_i = \langle i|\psi\rangle$ as if on a finite-dimensional space, there are $2N$ real degrees of freedom on $N$ complex dimensions. The most general complex unitary transformation preserving $\langle\psi|\psi\rangle$ is called $U(N)$ with $N^2$ freedoms. The most general real transformation preserving $\langle\psi|\psi\rangle$ is called $O(2N)$ with $N(2N-1)$ freedoms. Complex transformations are restricted by operating exclusively on matched pairs of real numbers.

Nothing can stop us from mixing real and imaginary parts more imaginatively. Rather than considering linear combinations of $|\psi\rangle$, we may consider combinations of $|\psi\rangle$ and $\langle\psi|$.

We separate real and imaginary parts

$$\eta_i = \mathrm{Re}\,\psi_i, \qquad \zeta_i = \mathrm{Im}\,\psi_i.$$

(Writing 'kets' and 'bras' adds little and is suppressed.) To generalize the dynamics we postulate a real-valued functional $\mathcal{H}(\eta_i, \zeta_i)$ with few *a prior* restrictions. Start by re-writing equation (10) in the new variables,

$$\begin{aligned} &\mathrm{i}(\dot\eta_i + \mathrm{i}\dot\zeta_i) = \frac{\partial\mathcal{H}(\eta_i,\zeta_i)}{\partial(\eta_i - \mathrm{i}\zeta_i)}; \\ &\mathcal{H}(\eta_i,\zeta_i) \to \langle\psi|\hat{H}|\psi\rangle \qquad \text{(linear theory).} \end{aligned} \tag{13}$$

Take the real and imaginary parts to find

$$\dot{\eta}_i = \frac{1}{2}\frac{\partial\mathcal{H}(\eta_i, \zeta_i)}{\partial\zeta_i}; \qquad \dot{\zeta}_i = -\frac{1}{2}\frac{\partial\mathcal{H}(\eta_i, \zeta_i)}{\partial\eta_i}. \tag{14}$$

We recognize this as Hamilton's equations, up to factors

$$\dot{q}_i = \frac{\partial\mathcal{H}}{\partial p_i}; \qquad \dot{p}_i = -\frac{\partial\mathcal{H}}{\partial q_i};$$
$$q_i = \eta_i/\sqrt{2}; \qquad p_i = \zeta_i/\sqrt{2}.$$

Then

$$\psi_i = \frac{q_i + \mathrm{i}p_i}{\sqrt{2}}. \tag{15}$$

In the last lines we made the projections onto an orthogonal basis explicit with index $i$. Othogonality will not be an invariant concept, and more general meaning will soon be explored. Symbols $q$ and $p$ are not to be confused with operators, which have 'hats'[1].

The symmetry group of Hamilton's equations is well known [6]. It is developed by combining $(\eta_i, \zeta_i)$ or $(q_i, p_i)$ into a long multiplet $\Phi = (q_1 \cdots q_N, p_1 \cdots p_N)$ in which form the equation appears as

$$\dot{\Phi} = J\frac{\partial\mathcal{H}}{\partial\Phi}. \tag{16}$$

Here $J$ is a matrix with block representation

$$J = \begin{pmatrix} 0 & 1_{N\times N} \\ -1_{N\times N} & 0 \end{pmatrix}. \tag{17}$$

Under a real-valued $2N \times 2N$ transformation $S$, the equation transforms

$$\Phi \to \Phi_S = S\Phi; \qquad \dot{\Phi}_S = SJS^T\frac{\partial\mathcal{H}}{\partial\Phi}. \tag{18}$$

Superscript $T$ denotes the *transpose*. The *symplectic group* of $2N$ dimensions is the set of matrices such that

$$SJS^T = J. \tag{19}$$

The transformations preserve the *symplectic metric* $J$. Arvind *et al* [7] give a useful review of the $\mathcal{S}p$ group.

*Objectivity of the real-valued phase space.* We have shown that extending ordinary complex quantum dynamics to more general real coordinates yields a classical underlying dynamical system. The Hamiltonian structure of $q$'s and $p$'s will be maintained under all $\mathcal{S}p$ transformations, and it cannot be wiped out except by non-$\mathcal{S}p$ transformations. For dynamical purposes one may objectively view the phase space of $q$'s and $p$'s as being as 'real as any other'.

Yet by developing a constructive procedure, the particular $q$ and $p$ coordinates are tied to the conventions from which they have been constructed. For one thing, the quadratic appearance of a Hamiltonian in particular coordinates (fiducial form $\mathcal{H}(\eta_i, \zeta_i) = \langle\psi|\hat{H}|\psi\rangle$) is not a symplectic invariant. Myriad seemingly *nonlinear* classical systems may actually represent quantum systems in new coordinates, and vice versa. Indeed the 'canonical quantization' by which the usual Schroedinger operators can be motivated is not $\mathcal{S}p$ invariant. We will revisit

[1] Joining $q$'s and $p$'s into one object in equation (15), when they generally have different dimensions, requires introduction of a scale with the dimensions of action set to unity. The same action scale will relate units of energy to those of time: without an external definition of either it is meaningless to quibble.

it in section 4.2. In section 4.1.1, we will explore more general coordinate transformations, including the general relation of the canonical coordinates to observables.

*Upper and lower components.* We may also complexify the multiplet $\Phi$ with the map

$$\Phi = \begin{pmatrix} q_1 \\ q_2 \\ \cdots \\ p_1 \\ p_2 \\ \cdots \end{pmatrix} \to \Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \cdots \\ \psi_1^* \\ \psi_2^* \\ \cdots \end{pmatrix}. \tag{20}$$

The map is a unitary transformation

$$\Psi = \Omega\Phi; \qquad \Omega = \frac{1}{\sqrt{2}} \begin{pmatrix} 1_{N\times N} & \mathrm{i}1_{N\times N} \\ 1_{N\times N} & -\mathrm{i}1_{N\times N} \end{pmatrix},$$

with

$$\Omega\Omega^\dagger = 1_{2N\times 2N}. \tag{21}$$

The invariant meaning of the transformation $\Omega$ is found in its diagonalization of the $\mathcal{S}p$ metric $J$,

$$\Omega J \Omega^\dagger = -\begin{pmatrix} \mathrm{i}1_{N\times N} & 0 \\ 0 & -\mathrm{i}1_{N\times N} \end{pmatrix}. \tag{22}$$

On the basis $\Psi$ $\mathcal{S}p$ transformations become $S \to S_\Psi = \Omega S \Omega^\dagger$. For some purposes the complex symplectic form is very convenient. We will shortly discuss the interpretation of the 'upper' and 'lower' components of $\Psi$.

*Finite versus continuous freedoms.* We used finite-dimensional notation for illustration and simplicity. One may describe a state vector $|\psi\rangle$ on a space with a continuous basis label $|x\rangle$ via its matrix elements $\langle x|\psi\rangle$. As in quantum field theory, the continuous label can be treated as an index, $\psi_x = \langle x|\psi\rangle$. Restricting $x$ to discrete values labeled by integer-valued index $i$ recovers the finite-dimensional notation. There are then three types of underlying canonical systems under the map $\psi_x \to (q_x + \mathrm{i}p_x)/\sqrt{2}$. There are finite-dimensional systems, as typified by spin models, countably infinite-dimensional systems, as for mass points on an infinite line, and continuously infinite systems, assumed with Schroedinger differential operators.

The basic dynamical equation of motion for continuously infinite systems becomes

$$\mathrm{i}\dot{\psi}(x) = \frac{\delta}{\delta\psi^*(x)}\mathcal{H}(\psi(x), \psi(x)^*),$$

where $\delta/\delta\psi(x)$ is the functional derivative. In conventional coordinates $\mathcal{H}$ is a functional of the type

$$\mathcal{H}(\psi(x), \psi(x)^*) = \int \mathrm{d}^3x\, \psi(x)^* \hat{H} \psi(x)^*,$$

where in Schroedinger's theory $\hat{H} \to -NN^2/2m + V(x)$ uses differential operators. We are not concerned with motivating the Schroedinger operator via semi-classical correspondence. We treat Hamiltonians as 'given' by outside information.

Subtleties of the continuum limit are important, and it is impossible to list all possible variations of physical consequence. Truncating to particular finite or infinite subsets of the Hilbert space is very common and perfectly compatible with finite-dimensional notation. A workman-like attitude towards the continuum limit is developed in lattice methods of quantum mechanics and quantum field theory. In these areas it is recognized that problematic features of straightforward truncation are usually either trivial or irrelevant. If the physical limit becomes a research problem there is usually a good reason.

Returning to our discussion of $\mathcal{PT}$-symmetric systems: the construction generalizes quantum dynamics to an entirely classical form regardless of the Hamiltonian or its dimensionality. Symplectic transformations permit 'the largest possible' symmetry group of the equation of motion, and are *not all* equivalent to unitary transformations in new coordinates.

*2.2.1. The largest coordinate transformation group.* Nothing in our procedure depends on orthonormal labeling, and we may use 'generalized coordinates' freely.

The largest group on the coordinates $q_i$ is $GL(N)$, the general linear group of $N$ dimensions. *Non-linear* transformations[2] are treated as linear in differentials, $\mathrm{d}q' = \mathcal{G}\,\mathrm{d}q$, where $\mathcal{G} \in GL(N)$.

The fact that $GL(N)$ is a subgroup of $\mathcal{S}p(2N)$ is clear from the generator relations developed below, (equation (34)). We can short circuit the argument with an elementary physical one. In Lagrangian mechanics, any $GL(N)$ transformation on generalized coordinates $q \rightarrow q'$ is allowed. Since our $q$'s and $p$'s are $c$-numbers (not operators), the Lagrangian $\mathcal{L}$ exists with the formula

$$\mathcal{L}(q, \dot{q}) = p\dot{q} - \mathcal{H}(q, p). \tag{23}$$

(Indices and sums implied.) The point transformation $\mathcal{L}(q, \dot{q}) \rightarrow \mathcal{L}(q', \dot{q}')$ develops the conjugate $p' = \partial\mathcal{L}/\partial\dot{q}'$, completing the $\mathcal{S}p(2N)$ transformation.

In this physical fashion, we expand the transformation group *on the coordinates* to be the largest one possible covariant on equations of motion. $GL(N)$ is also the largest group *on the momenta* if this is desired. Finally, the full group of canonical transformations mixing $p$'s and $q$'s contains many more generators. There is a certain logic that *either* a set of coordinates *or* a set of momenta can be observed, but not necessarily both. This is very clear with gauge-coupled theories we discuss. 'Autonomous formulations' come from eliminating $q$'s or $p$'s, as developed shortly in section 2.2.3.

*2.2.2. Time reversal.* Under time reversal we have

$$q_i(t) \rightarrow q_i(-t), \qquad p_i(t) \rightarrow -p_i(-t),$$

so that naturally

$$\psi(t) \rightarrow \psi^*(-t). \tag{24}$$

Linear theories, with Hamiltonians as quadratic forms, have

$$\mathcal{H}(q, p) = \Phi^T \hat{H}_\Phi \Phi; \qquad \hat{H}_\Phi = \begin{pmatrix} h_{qq} & h_{qp} \\ h_{pq} & h_{pp} \end{pmatrix}. \tag{25}$$

The terms $h_{qq}$ and $H_{pp}$ are even, and $h_{qp} = h_{pq}^T$ are odd under time reversal. When complexified by our rule of equation (15), 'mixed forms' containing $h_{qp}$ and $h_{qp}$ will become proportional to $i$. From the canonical transformation theory we reproduce the operator replacement rule $i \rightarrow -i$ for time reversal developed earlier [1, 8].

[2] Throughout the paper the methods using linear transformations are readily extended to nonlinear transformations which are locally linear in the differentials.

*2.2.3. Autonomous gauge-coupled theories.* It is interesting that the mixed-form Hamiltonians are *gauge-coupled theories* of unlimited dimension. The demonstration is quite entertaining. Replace symbols in equation (25) using

$$h_{qq} = K; \qquad h_{pp} = M^{-1}; \qquad h_{qp} = -\Gamma^T M. \tag{26}$$

Complete the square

$$\mathcal{H}(q,p) = \tfrac{1}{2}pM^{-1}p + \tfrac{1}{2}qKq + qM\Gamma p + p\Gamma^T Mq,$$

$$= \tfrac{1}{2}(p - \mathcal{A}(q))M^{-1}(p - \mathcal{A}(q)) + \mathcal{V}; \tag{27}$$

$$\mathcal{A}(q) = \Gamma q; \qquad \mathcal{V} = \tfrac{1}{2}q(K - \Gamma^T M^{-1}\Gamma)q. \tag{28}$$

Observe that $\mathcal{A}(q)$ serves as vector potential with associated curvature

$$\mathcal{F}_{ij} = \frac{\partial \mathcal{A}_i}{\partial q_j} - \frac{\partial \mathcal{A}_j}{\partial q_i} = \Gamma_{ij} - \Gamma_{ji}.$$

Gauge transformations leave $F_{ij}$ unchanged while changing $\mathcal{A}(q)$. A gauge transformation respecting quadratic $\mathcal{H}$ is the rule $\mathcal{A}(q) \to \mathcal{A}(q) + \Sigma q$, where $\Sigma = \Sigma^T$. These canonical $p$'s are not gauge invariant.

Eliminating $p$'s produces an autonomous equation for $q$ which is gauge invariant, involving only an invariant curvature. From Hamilton's equations

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} = (M^{-1}(p - \mathcal{A}))_i; \qquad \dot{q}_i = -\frac{\partial \mathcal{H}}{\partial p_i} = -\dot{q}_j \frac{\partial \mathcal{A}}{\partial q_i}.$$

After substitution find the *generalized Lorentz force*

$$M\ddot{q}_i = \dot{q}_i \mathcal{F}_{ij} + \mathcal{E}_i. \tag{29}$$

The quantity $\mathcal{E}_i = -\partial \mathcal{V}/\partial q_i - \partial \mathcal{A}_i(q)/\partial t$ is invariant under time-dependent gauge transformations.

The coordinate $p$ was eliminated above, revealing the gauge invariant coupling of $q$'s. Curiously we can also eliminate $q$'s and discover a gauge invariant coupling of $p$'s. The algebra is given in an appendix. The Lorentz $p$-force equation is

$$K^{-1}\ddot{p}_i = \dot{p}_j \left( \frac{\partial \mathcal{A}_i(p)}{\partial p_j} - \frac{\partial \mathcal{A}_j(p)}{\partial p_i} \right) + \frac{\partial \mathcal{A}_j(p)}{\partial t} - \frac{\partial \mathcal{U}(p)}{\partial p_i}. \tag{30}$$

Here $\mathcal{A}(p) = \Gamma_p p$ in the quadratic theory with $\Gamma_p = K h_{qp}$. A symmetric part of $\Gamma_p$ produces no curvature and has no effect on the autonomous equations for $p$. In this case the coordinates $q$ are not gauge invariant (see the appendix, equation (A.2)).

There are several reasons for highlighting this peculiar duality. First, gauge transformations enlarge the notion of 'equivalent Hamiltonians'. Certain $\mathcal{PT}$-symmetric theories are complex, representing a generalized magnetic coupling in particular coordinates. Classifying those which are equivalent depends on the decision, 'what is the physical phase space?' Second, Hamiltonian dynamics is deeply configured with equal treatment of $q$'s and $p$'s, while physics as a whole seems to treat them differently. The equation shows the duality is restored at the bottom.

Finally, we will reopen the old and basic issue whether the $2N$-dimensional phase space and $p$'s might be mere mathematical constructs invented to manage equations. When $p$'s can be eliminated then second-order time evolution for $q$'s and a phase space of half the usual dimension is perfectly valid. There is clear motivation for preferring this when $p$'s are not gauge invariant. When $q$'s are not gauge invariant there is motivation for reduction to half-dimension using autonomous equations for $p$'s. Without dwelling too much on this obvious fact, reduction to half the dimensions seems important and we return to it in section 4.1.1.

$$\begin{tikzcd}
\Phi \arrow[rr, "Sp"] & & \Phi \arrow[dd, "\Omega^{-1}"] \\
& & \\
\Psi, \Psi^* \arrow[uu, "\Omega"] \arrow[rr, "\cancel{U}"] & & \Psi, \Psi^*
\end{tikzcd}$$

**Figure 1.** Transforming from Hermitian to non-Hermitian systems: the complex non-unitary transformations are equivalent to going to real-valued phase-space coordinates, making $\mathcal{S}p$ transformations, and returning to complex coordinates.

*2.2.4. Hermitian and non-Hermitian forms.* Quadratic forms are coordinate dependent, having inherited their matrix elements from the coordinates chosen in equation (25). A basic question, then, is how $\mathcal{PT}$ theories transform one convention to another.

Under a linear transformation we have two expressions for the same concept,

$$\Phi \to \Phi_S = S\phi; \qquad \Psi \to \Psi_S = S_\Psi \Psi. \tag{31}$$

Selecting the upper components of $\Psi$ we have

$$\psi'_S = V(S)\psi + W(S)\psi^*. \tag{32}$$

Let us explore the special transformations that do not mix upper and lower components of $\Psi$, namely $\psi$ and $\psi^*$ (figure 1).

Proceed with an infinitesimal transformation, writing

$$S = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{33}$$

The $\mathcal{S}p$ condition of equation (19) yields

$$d = -a^T; \qquad b = b^T; \qquad c = c^T. \tag{34}$$

Thus matrix $d$ is eliminated, while matrix $a$ is unrestricted. It has $N^2$ parameters, the $GL(N)$ generator. The two symmetric matrices $b, c$ have $N(N+1)$ parameters, making a total of $N(2N+1)$ parameters, the known dimension of the $\mathcal{S}p$ group [7].

Compute the infinitesimal change

$$\delta q = aq + bp; \qquad \delta p = cq - a^T p, \tag{35}$$

and substitute $q$ and $p$ from equation (15). We obtain

$$V(S) = \tfrac{1}{2}(a - a^T + \mathrm{i}(b - c)); \qquad W(S) = \tfrac{1}{2}(a + a^T + \mathrm{i}(b + c)). \tag{36}$$

The condition that $W = 0$ so that $S$ not mix $\psi$ and $\psi^*$ is

$$a = -a^T; \qquad c = -b = -b^T. \tag{37}$$

The transformation becomes

$$\delta \begin{pmatrix} q \cdots \\ p \cdots \end{pmatrix} = \begin{pmatrix} a & b \\ b & -a \end{pmatrix} \begin{pmatrix} q \cdots \\ p \cdots \end{pmatrix}; \qquad \delta\psi = \frac{\delta q + \mathrm{i}\delta p}{\sqrt{2}} \to \mathrm{i}(b - \mathrm{i}a)\psi.$$

The result is expressed more simply as

$$\delta\psi = \mathrm{i}G\psi; \qquad G = b - \mathrm{i}a = G^\dagger.$$

The $\mathcal{S}p$ transformations *not mixing* $\psi$ with $\psi^*$ are precisely the unitary group acting on $\psi$.

As consistent the matrices $a, b$ make $N(N+1)/2+N(N-1)/2 = N^2$ independent Hermitian generators.

Conversely the remaining $N^2 + N$ transformations that *do mix* $\psi$ with $\psi^*$ are *not unitary*. Unless specially contrived to commute they will *not* preserve the Hermiticity of an operator. Suppose we start with a Hermitian quantum system. Consulting figure 1: to make a non-Hermitian system of general kind, transform from $\psi \to \Phi$, then transform $\Phi$ under $\mathcal{S}p$ elements which violate equation (37) and transform back to $\psi_S$. One may also transform directly. The point is to identify the subgroup preserving $\langle\psi|\psi\rangle$ as the intersection $O(2N)\bigcap Sp(2N)$, which is simply $U(N)$ expressed in real coordinates.

We have accomplished a primary goal of expressing the relation of $\mathcal{PT}$ theories to ordinary ones in invariant terms. The transformations that revise Hermiticity are the *coset* $SP(2N)/U(N)$, and they do not form a group.

*2.2.5. Diagonal re-scalings.* The $\mathcal{S}p$ group preserves areas on the phase space, and in a definite sense consists of the maximal compact subgroup (unitary) transformations plus diagonal re-scalings $\Lambda$. A unique representation[3] is

$$S = U_1 \Lambda U_2^T; \qquad U_1 U_1^T = U_2 U_2^T = 1_{2N\times 2N}, \tag{38}$$

with

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \lambda_{N-1}^{-1} & 0 \\ 0 & 0 & 0 & 0 & \lambda_N^{-1} \end{pmatrix}.$$

The proof is straightforward. First show that $SS^T$ is in the group. By construction $SS^T = U_1\Lambda^2 U_1^T$ is symmetric, and by diagonalizing it we can construct orthogonal $U_1$ and eigenvalues $\Lambda$. Choose the signs of $U_1$ to make them positive. Similarly get $U_2$ from $S^T S$. With $U_1$ and $U_2$ necessarily in the group we use $2N^2$ parameters, leaving $N$ parameters for the $2N \times 2N$ diagonal $\Lambda$. Each singular value must come with its inverse, due to area-preservation pair by pair of the $\mathcal{S}p$ transformations.

Thus all transformations that revise Hermiticity are classified as products of discrete 'row-swappings', 'ordinary unitaries' so familiar in quantum theory, and diagonal re-scalings. Discrete row swaps with negative determinant define *parity* transformations. We will explore other transformations in section 3.

*2.2.6. Example: faster than Hermitian quantum mechanics.* Let us now work an example of an interesting $\mathcal{S}p$ transformation.

Consider the following simple transformation mixing $\psi$ and $\psi^*$:

$$\begin{pmatrix} \psi_1' \\ \psi_2^{*\prime} \end{pmatrix} = \gamma \begin{pmatrix} 1 & -\mathrm{i}\beta \\ \mathrm{i}\beta & 1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2^* \end{pmatrix}. \tag{39}$$

This is written in $2 \times 2$ form, suppressing the other transformations obvious by complex conjugation. What is needed for this transformation to be $\mathcal{S}p$? Expand it to $4 \times 4$ real form

$$\begin{pmatrix} q_1' \\ q_2' \\ p_1' \\ p_2' \end{pmatrix} = \gamma \begin{pmatrix} 1 & 0 & 0 & \beta \\ 0 & 1 & \beta & 0 \\ 0 & \beta & 1 & 0 \\ \beta & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix}.$$

[3] The representation is unique up to discrete orderings of the diagonal elements.

The transformation is $\mathcal{S}p$ provided

$$\frac{1}{\gamma^2}\begin{pmatrix}1 & \beta\\ \beta & 1\end{pmatrix}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}1 & \beta\\ \beta & 1\end{pmatrix}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$$

with each element a $2\times 2$ block. Solving gives the parameter constraint

$$\gamma^2(1-\beta^2)=1 \tag{40}$$

or

$$\beta=\sin\alpha; \qquad \gamma=\frac{1}{\cos\alpha}. \tag{41}$$

The transformation matrix becomes

$$\gamma\begin{pmatrix}1 & -\mathrm{i}\beta\\ \mathrm{i}\beta & 1\end{pmatrix}\to\frac{1}{\cos\alpha}\begin{pmatrix}1 & -\mathrm{i}\sin\alpha\\ \mathrm{i}\sin\alpha & 1\end{pmatrix}=\mathcal{C}\mathcal{P}; \tag{42}$$

$$\mathcal{C}=\frac{1}{\cos\alpha}\begin{pmatrix}\mathrm{i}\sin\alpha & 0\\ 0 & -\mathrm{i}\sin\alpha\end{pmatrix}; \qquad \mathcal{P}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{43}$$

The identification of matrices $\mathcal{C}$ as representing charge conjugation and parity on a finite-dimensional system has been discussed previously [8]. Equation (42) recovers the 'faster than Hermitian' transformation of Bender, Brody, Jones and Meister [9].

The fact that the unitary distance between points is not invariant is a defining feature of non-unitary transformations. This becomes particularly interesting when we extend the geometry to the $\mathcal{S}p$ transformations. The indefinite $\mathcal{S}p$ metric does not allow a non-zero invariant notion of 'length', as the basic invariant $\Phi^T J\Phi = 0$. In effect, certain points separated by zero distance are a natural $\mathcal{S}p$ concept. The conceptually interesting problem of the *symplectic brachistochrone* problem appears to be this: given two states $|\psi_1\rangle, |\psi_2\rangle$ equivalent to two points $\Phi_1$, $\Phi_2$ on a phase space, what can we say about Hamiltonians that connect them? The *bradystochrone* problem is to find the *slowest* transformation. From Hamilton–Jacobi theory, these are the coordinates in which the Hamiltonian developing states is *zero*, namely the Heisenberg representation.

*2.2.7. All $\mathcal{S}p$ transformations are Hamiltonian.* Hamiltonian time evolution of course preserves Hamilton's equations and is therefore $\mathcal{S}p$. Reversing the question, do all $\mathcal{S}p$ transformations correspond to evolution under some Hamiltonian?

From the generator relation, infinitesimal $\mathcal{S}p$ transformations on the $\Phi$ coordinates take the form

$$S=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}+\begin{pmatrix}a & b_s\\ c_s & -a^T\end{pmatrix},$$

where $b_s$ and $c_s$ are symmetric. To recover the physical interpretation of equation (26), replace symbols

$$b\to M^{-1}; \qquad c\to -K; \qquad a\to -M^{-1}\Gamma.$$

The infinitesimal changes are

$$\mathrm{d}q = M\Gamma p\,\mathrm{d}t + Mq\,\mathrm{d}t; \qquad \mathrm{d}p = Kq-\Gamma^T M^T p. \tag{44}$$

Inserting the metric $J$ this becomes

$$\begin{aligned}\begin{pmatrix}\mathrm{d}q\\ \mathrm{d}p\end{pmatrix} &= J\begin{pmatrix}K & =\Gamma^T M^{-1}\\ -M^{-1}\Gamma & M^{-1}\end{pmatrix}\begin{pmatrix}q\\ p\end{pmatrix}\mathrm{d}t\\ &= J\frac{\partial\mathcal{H}}{\partial\Phi}\,\mathrm{d}t\end{aligned} \tag{45}$$

where the local Hamiltonian is just equation (27). No matter what the $\mathcal{S}p$ transformation it is equivalent to a locally linearized Hamiltonian generator of quadratic type.

Then *locally* on the phase space all possibilities are exhausted by quadratic forms and generators which are either compact or non-compact, either equivalent to the ordinary theory or one generating rescalings. It is important that non-unitary $\mathcal{S}p$ transformations mix $\psi$ with $\psi^*$ and must invariably include conjugation on the complex coordinates. There seems to be a link missing in the literature, however, and that link involves *antimatter.*

## 3. Classical antimatter

Antimatter is invariably associated with special relativity and quantization. Yet any quantum theory induces a classical structure. It follows that antimatter must be realized as a classical dynamical system.

Return to Hamilton's equations,

$$\dot{\Phi} = J\frac{\partial \mathcal{H}}{\partial \Phi}. \tag{46}$$

It is responsible for inducing a symplectic flow of time evolution. But there is an alternative way to set up physics. Suppose we replace $J \to -J$. The $\mathcal{S}p$ group is not changed since $SJS^T \to J$ is not changed. We have shown that $\mathcal{S}p$ transformations are always Hamiltonian theories. But no $\mathcal{S}p$ transformation will change $J \to -J$. It follows that the Hamiltonian world comes in two distinct varieties, $J$ form and anti-$J$ form.

The *anti-Hamilton* equations using $-J$ are

$$\dot{q}_- = -\frac{\partial \mathcal{H}_-}{\partial p_-}; \tag{47}$$

$$\dot{p}_- = \frac{\partial \mathcal{H}_-}{\partial q_-}. \tag{48}$$

Indices have been suppressed. Is this a distinctly different physics or a change of convention?

First, we may convert the new equations to the old ones by reversing the direction of time, $t \to -t$ with $\mathcal{H}$ fixed. This is a feature of antimatter. Second, we may convert the new equations to the old ones by reversing the sign of $\mathcal{H}_-$ with $t$ fixed. This is another feature of antimatter. Third, the coupling to an electromagnetic field is reversed. It is reversed for the formal coupling to $\mathcal{A}$, equation (28) and it is reversed for the 'macroscopic' coupling done in continuum theories with $-\mathrm{i}\vec{\nabla} - e\vec{A}$. Finally, the complex version of the basic transformation $\mathcal{C}$ converts $\psi$ to $\psi^*$ and (up to canonical transformations) is unique. The features listed define antimatter.

Note that if a system consists entirely of matter or antimatter alone, it is mere convention to choose either the usual form of Hamilton's equations or the anti-form. Conversely: if a system consists of a mixture of matter and antimatter, it is not a matter of convention and there are definite physical consequences. The distinction can become observable depending on the symmetries of Hamiltonian. When the upper and lower components are mixed, combinations diagonalize $\mathcal{C}$ to make self-conjugate states with eigenvalues $\pm 1$, just as seen in explicit calculations. We suggest a more general interpretation of the $\mathcal{PT}$ and $CPT$ invariant theories that have been so fascinating in the literature: they permit couplings to antimatter.

It is surprising that neither special relativity nor quantum field theory is needed to justify the interpretation. The question of whether time evolution proceeds unitarily is related but separate. In section 4.2, we return to the question of antimatter and positive definite probabilities of relativistic quantum mechanics.

*3.1. Continuum re-scalings and the* $\mathrm{i}\hat{x}$ *theory*

As noted with equation (38), certain non-unitary $\mathcal{S}p$ transformations are essentially diagonal rescalings,

$$S = U_1 \Lambda U_2; \qquad \Lambda = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{pmatrix}. \tag{49}$$

Here $\lambda$ is an $N \times N$ diagonal matrix. We explore the complex representation of such transformations in order to relate them to operator-based continuum $\mathcal{PT}$ theories seen in the literature. The mixing of upper and lower components is very interesting.

When $\Phi \to \Lambda\Phi$ we have $\Psi \to \Lambda_\Psi \Psi$, with $\Lambda_\Psi = \Omega\Lambda\Omega^\dagger$, so that

$$\Lambda_\Psi = \begin{pmatrix} 1/\sqrt{2} & \mathrm{i}/\sqrt{2} \\ 1/\sqrt{2} & -\mathrm{i}/\sqrt{2} \end{pmatrix} \begin{pmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -\mathrm{i}/\sqrt{2} & \mathrm{i}/\sqrt{2} \end{pmatrix},$$
$$= \begin{pmatrix} \lambda + \lambda^{-1} & \lambda - \lambda^{-1} \\ \lambda - \lambda^{-1} & \lambda + \lambda^{-1} \end{pmatrix}. \tag{50}$$

In terms of mixing upper and lower components, the transformed matrix is the operation

$$\psi' = c_+ \psi + c_- \psi^*; \qquad c_\pm = \tfrac{1}{2}(\lambda \pm \lambda^{-1}).$$

Inverting gives

$$\lambda^{\pm 1} = c_+ \pm c_-; \qquad c_+^2 - c_-^2 = 1. \tag{51}$$

The constraint is solved by $c_+ = \cosh(y)$, $c_- = \sinh(y)$ and finally

$$\Lambda_\Psi = \begin{pmatrix} \cosh(y) & \sinh(y) \\ \sinh(y) & \cosh(y) \end{pmatrix}.$$

Since $\lambda$ was by definition diagonal, we have the Minkowski ('Lorentz') group $O^N(1,1)$ with $N$ generators.

Continuum $\mathcal{PT}$ physics has generally focused on the bound states. Perhaps the simplest case is the Hamiltonian [1]

$$H = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\hat{x}^2 + \mathrm{i}\hat{x}.$$

Attention to boundary conditions and use of continuation in the complex plane has led to explicit solution to large families of theories, as in the elegant work of Ahmed *et al* [10]. We should also mention $-\hat{x}^4$ theory, recently solved by contour deformation and conversion to a non-Hermitian theory by Jones *et al* [11]. The bound eigenstates $\psi_{\mathrm{bound}}$ are real-valued in coordinates where $\hat{H} = \hat{H}^\dagger$. From reality we write $\psi_{\mathrm{bound}} = \psi_+$, where

$$\psi_\pm = \psi \pm \psi^*.$$

The complementary option for mapping $\psi_{\mathrm{bound}}$ is of course $\psi_-$. The Lorentz transformation of $\psi_\pm$ is

$$\psi_\pm^{*\prime} = \mathrm{e}^{\pm y} \psi_\pm. \tag{52}$$

Such states can fairly be called $\mathcal{S}p$*-light-cone coordinates*.

Then from the $O(1,1)^N$ subgroup in light-cone coordinate, diagonal re-scalings of $\hat{H}$ have a representation

$$\hat{H} \to \hat{H}_y = \mathrm{e}^y \hat{H}\, \mathrm{e}^{-y}. \tag{53}$$

Let $y \to p$ be the real eigenvalues of the continuum momentum operator $\hat{p}$. We have recovered

$$\tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\hat{x}^2 + \mathrm{i}\hat{x} = \mathrm{e}^{\hat{p}} \left(\tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\hat{x}^2\right) \mathrm{e}^{-\hat{p}}.$$

Similarly, it was shown [11] that a transformation with $y = c_1 p + c_2 p^3$ reverts the $-x^4$ theory to conventional form. These transformations have previously been obtained by operator methods requiring human observation and cleverness. The group structure is quite simple and systematic. Yet putting an arbitrary $\mathcal{S}p$ into a canonical form such as equation (49) is seldom easy. By starting off with the group properties an infinite number of interesting $\mathcal{S}p$ transformations can be produced: perhaps this might be productive in constructing new $\mathcal{S}p$ theories.

## 4. Brackets from dynamics

Given an induced classical dynamics there exist Poisson brackets. Certain known results of quantum theory, also generalized to $\mathcal{PT}$-symmetric theories [12], then fall into place beautifully.

Let $A, B$ be functions of $q_i, p_i$. We define the Poisson brackets (PB) as

$$\{A, B\}_{\mathrm{PB}} = \sum_i \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}. \tag{54}$$

Let symbols $Q, P$ represent new $\mathcal{S}p$-related canonical coordinates. The PB of an $\mathcal{S}p$ transformation $q_i, p_i \rightarrow Q_i, P_i$ are manifestly invariant, with $\{Q_i, P_j\} = \delta_{ij}$ a test the transformation is $\mathcal{S}p$.

Now consider projective functions that are special quadratic 'sandwiches'

$$A(Q, P) = P\hat{A}Q,$$

with a corresponding expression for $B$. Here $\hat{A}$ is a matrix we call a 'representation' (rep.) of the quantity $A$. Appropriateness of this word usage will become clear. For the moment any particular $\hat{A}$ simply produces a projective rule returning one piece of information per matrix.

The PB algebra of $A$ and $B$ develops an algebra for the matrices

$$\begin{aligned}\{A, B\}_{\mathrm{PB}} &= \sum_i \frac{\partial P\hat{A}Q}{\partial Q_i}\frac{\partial P\hat{B}Q}{\partial P_i} - \frac{\partial P\hat{A}Q}{\partial P_i}\frac{\partial P\hat{B}Q}{\partial Q_i},\\ &= P\hat{A}\hat{B}Q - P\hat{B}\hat{A}Q.\end{aligned}$$

Since the $P \cdots Q$ symbols always remain outside of this sandwich, we can replace them by a 'round projection' symbol using

$$A \rightarrow P\hat{A}Q \equiv (\hat{A}).$$

The PB of $(\hat{A})$ and $(\hat{B})$ map into the commutator of the reps

$$\{(\hat{A}), (\hat{B})\}_{PB} = ([\hat{A}, \hat{B}]).$$

In particular, if $\hat{H}$ is a Hamiltonian rep., then time dependence of any quantity obeys

$$\frac{\mathrm{d}(\hat{A})}{\mathrm{d}t} = ([\hat{H}, \hat{A}]) + \frac{\partial(A)}{\partial t}.$$

The time dependence can then be transferred to the matrices, namely the Heisenberg representation.

By construction the transformation from $q_i, p_i \rightarrow \psi_i, \psi_i^*$ is canonical up to a factor. Calculate the PB to verify

$$\begin{aligned}\{\psi_a, \psi_b^*\}_{PB} &= \sum_i \frac{\partial \psi_a}{\partial q_i}\frac{\partial \psi_b^*}{\partial p_i} - \frac{\partial \psi_a}{\partial p_i}\frac{\partial \psi_b^*}{\partial q_i},\\ &= -\mathrm{i}\delta_{ab}.\end{aligned} \tag{55}$$

This conjugacy motivates quadratic sandwiches using the complex variables. Define the pointy projection

$$(\hat{A}) \rightarrow \langle \hat{A}_\psi \rangle = \langle \psi | \hat{A}_\psi | \psi \rangle,$$

where $\hat{A}_\psi$ is the transformed rep of $\hat{A}$ into complex coordinates. The subscript $\psi$ can then be dropped without confusion. The PB become

$$\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\}_{PB} = \mathrm{i} \sum_k \frac{\partial \langle \hat{A} \rangle}{\partial \psi_k} \frac{\partial \langle \hat{B} \rangle}{\partial \psi_k^*} - \frac{\partial \langle \hat{B} \rangle}{\partial \psi_k} \frac{\partial \langle \hat{A} \rangle}{\partial \psi_k^*}. \tag{56}$$

On continuous infinite dimensions replace $\sum_k \partial/\partial\psi_k \rightarrow \int \mathrm{d}x\, \delta/\delta\psi_x$.

The projective maps are then assessed through their transformation properties. The meaning of each $\langle \hat{A}_k \rangle$ is entirely subsumed by its PB algebra. And by calculation the algebra of the pointy projections is exactly the algebra of the matrix representations, up to $i$

$$\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\}_{PB} = \mathrm{i}\langle [\hat{A}, \hat{B}] \rangle.$$

Since this fact is true for any $|\psi\rangle$, it is a general consistency relation that starts with the Lie algebra of the projections, and predicts the Lie algebra of the commutators

$$\begin{aligned} &\text{given} \quad \{A, B\}_{PB} = C \\ &\text{then} \quad \rightarrow \quad \mathrm{i}[\hat{A}, \hat{B}] = \hat{C}. \end{aligned} \tag{57}$$

The rule of equation (57) is sometimes called 'canonical quantization'. We find it is a derived fact, not a separate postulate.

*Example*. Let the $q$'s and $p$'s be components of irreducible representations of the rotation group. For each irrep. $s$, let the transformation rule under rotations be

$$|\psi^s\rangle \rightarrow (1 + \mathrm{i}\vec{\theta} \cdot \vec{J}^s)|\psi^s\rangle.$$

Here $\hat{J}_i^s$ are the spin-$s$ rotation generators. No quantum mechanics is involved in this entirely geometrical classification. We form the pointy projections $\langle J_i^s \rangle$, and calculate the PB

$$\{\langle \hat{J}_i^s \rangle, \langle \hat{J}_j^s \rangle\}_{PB} = \langle [\hat{J}_i^s, \hat{J}_i^s] \rangle = \mathrm{i}\epsilon_{ijk} \langle \hat{J}_k \rangle.$$

Without any measurement doctrine the $\langle J_i^s \rangle$ are already the classical spin of the dynamical system[4]. Perhaps the most familiar case is spin 1. Then $\langle J_i^{s=1} \rangle = \epsilon_{ijk} q_j p_k$, the Newtonian result. Similarly, a set of $q$'s and $p$'s transforming like spinor components predicts a literal classical spin $\vec{s} = \langle \vec{\sigma} \rangle / 2$ where $\vec{\sigma}$ are the Pauli matrices.

### *4.1. Consistency questions in the relativistic case*

Since $(q, p) \rightarrow (\psi, \mathrm{i}\bar{\psi})$ is canonical up to i, we can express the Schroedinger action $S$ in complex coordinates as

$$S_{\text{Schroed}} = \int \mathrm{d}t\, p_i \dot{q}_i - \mathcal{H} = \int \mathrm{d}t\, \mathrm{i}\langle \psi | \dot{\psi} \rangle - \langle \psi | \hat{H} | \psi \rangle.$$

The bracket $\langle \psi | \dot{\psi} \rangle$ implies an integration over the volume element $\mathrm{d}^3x$ when dealing with Schroedinger operators. Compare the Klein–Gordon (KG) action of relativistic quantum mechanics

$$S_{\text{KG}} = \int \mathrm{d}t\, \mathrm{d}^3x \frac{1}{2} \dot{\varphi}^* \dot{\varphi} - \frac{1}{2} \vec{\nabla} \varphi^* \vec{\nabla} \varphi - \frac{m^2}{2} \varphi^* \varphi.$$

[4] It is generally necessary to verify the full PB algebra of all projections, as developed from transformation properties of $\psi$.

An ancient line of argument holds this is obtained by canonical quantization of $\hat{p} \to -\mathrm{i}\vec{\nabla}$, writing $\hat{H}^2 \to \hat{p}^2 + m^2$, just as the Schroedinger operator was obtained from $\hat{H} \to \hat{p}^2/2m + V$.

Yet relativistic quantum mechanics is known not to be a consistent quantum theory. An inconsistency lies in misapplying the PB rules in the KG theory. From Lagrangian physics the conjugate variables are

$$p_\phi = \frac{\delta \mathcal{L}}{\delta \dot{\varphi}} = \frac{1}{2}\dot{\varphi}^*; \qquad p_\phi^* = \frac{\delta \mathcal{L}}{\delta \dot{\varphi}^*} = \frac{1}{2}\dot{\varphi}.$$

In KG theory the round projections are

$$(\hat{A}) = \int \mathrm{d}x \frac{1}{2}\dot{\varphi}^* \hat{A}\phi + \frac{1}{2}\dot{\varphi}\hat{A}\phi^*. \tag{58}$$

The PB algebra of round projections is again transferred to the commutator algebra of the matrix representations. The kinematically consistent representations of total momentum and position in the KG theory are then

$$(\hat{p}) = \int \mathrm{d}^3x \frac{1}{2}\dot{\varphi}^*(-\mathrm{i}\vec{\nabla})\phi + \frac{1}{2}\dot{\varphi}(-\mathrm{i}\vec{\nabla})\phi^*;$$

$$(\hat{x}) = \int \mathrm{d}^3x \frac{1}{2}\dot{\varphi}^* \vec{x}\phi + \frac{1}{2}\dot{\varphi}\vec{x}\phi^*.$$

It follows by algebra that

$$\{(\hat{p})_i, (\hat{x})_j\}_{PB} = -\mathrm{i}\delta_{ij}. \tag{59}$$

This is just the same algebra that makes use of $-\mathrm{i}\vec{\nabla}$ a consistent momentum operator in the Schroedinger theory, but in that case $p_\psi = \mathrm{i}\bar{\psi}$. It is kinematically inconsistent to use $-\mathrm{i}\phi^*\vec{\nabla}\phi$ as the momentum density in the KG theory. Recognition of equation (59) is very old, with a different development given e.g. in the textbook by Roman [13]. Many textbooks also derive the momentum density from Noether's Theorem [14].

Historically conservation laws were not obtained from Noether's theorem, but by manipulating equations of motion. That approach lacks the connection between conjugacy of a *particular* collective momentum tied to a *particular* conjugate symmetry. The search for a positive-definite conserved probability was particularly influential, and a good example. Every Lie algebra represented by round projections has a 'grand center' that always commutes with everything: it is the operator $\hat{A} \to 1$. Using this in equation (58) the conserved current density is

$$\rho_{\mathrm{KG}} = \tfrac{1}{2}(\dot{\phi}^*\phi - \phi^*\dot{\phi}).$$

In the Schroedinger theory $\hat{A} \to 1$ gives $\bar{\psi}\psi$. Each form is conserved from symmetry under the global $U(1)$ 'gauge transformation' of multiplication of fields by $\exp(\mathrm{i}\delta)$, but only the Schroedinger case is positive definite. The result clarifies the fact that building dynamics under the presumption of operator replacement rules led to inconsistency ultimately reconciled in quantum field theory.

We have come full circle exploring the role of Hermitian operators and their coordinate dependence under traditional usage. The Dirac rule to 'replace every classical quantity $A$ by a Hermitian operator $\hat{A}$ to produce a quantum theory' is kinematic in general. It may be kinematically inconsistent if misapplied. Reiterating this, the importance of 'Hermitian operators' comes from their helpful notation encoding symplectic structure that pre-exists in the dynamical framework.

*4.1.1. Exact Eherenfest.* An interesting consequence may be useful for solving or approximating quantum theories. Our use closes our chain of logic relating observables to coordinates.

The PB relations have no more and no less content than Hamilton's equations. Therefore if we find variables $Q_k = \langle \hat{Q}_k \rangle$ and $P_k = \langle \hat{P}_k \rangle$ which are canonically conjugate, the equation of motion is simply

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{Q}_k \rangle = \frac{\partial \mathcal{H}(Q_k, P_k)}{\partial \langle \hat{P}_k \rangle}; \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{P}_k \rangle = -\frac{\partial \mathcal{H}(Q_k, P_k)}{\partial \langle \hat{Q}_k \rangle}.$$

Conversely, a complete solution to these equations for a complete set of variables predicts $\psi_k, \psi_k^*$. Then every exact Ehrenfest relation is a canonical equation of motion linked to the underlying degrees of freedom. These relations are useful, and a *different* set of equations traditionally developed for purposes of semi-classical approximations should not be confused.

Expressing $\mathcal{H}$ in terms of expectations is unconventional, and it is admittedly difficult to construct a large number of conjugate operators. Progress is made with symmetries. The usual $N \times N$ complex Hamiltonian commutes with $N - 1$-independent mutually commuting operators $\hat{\mathcal{Q}}_J$, $J = 1, \ldots, N$. Make a basis for these operators in their diagonal frame with $\mathcal{Q}_1 = \mathrm{diag}(1, 0, 0\ldots)$, $\mathcal{Q}_2 = \mathrm{diag}(0, 1, 0, 0\ldots)$, etc. Since $\hat{\mathcal{Q}}_J$ commute with $\hat{H}$ from the bracket algebra, they generate symmetries of the Hamiltonian with parameters $\Theta_J$

$$|\psi\rangle \to \exp(\mathrm{i}\Theta_J \mathcal{Q}_J)|\psi\rangle;$$

$$\mathcal{H} \to \mathcal{H};$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathcal{Q}_J \rangle = -\frac{\partial \mathcal{H}}{\partial \Theta_J} = 0.$$

The last line uses $\Theta_j$ as coordinates of $\psi$, and canonical degrees of freedom conjugate to $\langle \mathcal{Q}_J \rangle$.

By this strategy we can express $\mathcal{H}$ using $\mathcal{Q}_J$ as pointy projections. In the mutually commuting frame,

$$\mathcal{H} = \sum_J \langle \mathcal{Q}_J \rangle \omega_J.$$

The $\Theta_J$ equations are

$$\frac{\mathrm{d}\Theta_J}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial \langle \mathcal{Q}_J \rangle} = \omega_J; \qquad \Theta_J(t) = \Theta_J(0) + \omega_J t.$$

Half of the canonical coordinates then reduce to cyclic variables: angles $\Theta_J$ that are classically unobservable. The term 'classically unobservable' is accurate: an ideal cyclic variable cannot be observed while maintaining the symmetry that makes it cyclic.

Symmetry then leaves $\langle \mathcal{Q}_J \rangle$ as candidates for 'observables' in the $\mathcal{S}p$ sense. It is remarkable that exactly the same projections have long been known as observables on experimental grounds. The related questions of how averages are used in $\mathcal{PT}$ theories have been elucidated in the work of Japaridze [15] also re-examining the Ehrenfest relations. Traditionally a strictly literal interpretation of unobservables has been imposed for quantum systems, while measurements of classical systems were long considered ignorable perturbations. The two are not so different, but pursuing the interesting differences would lead to foundations of measurement theory beyond the scope of discussion.

Returning to the goal stated in the introductory passages, we have now built the map of $\langle \mathcal{Q}_J \rangle \to Q_i$, while finding half the Hamiltonian coordinates are absent from observables.

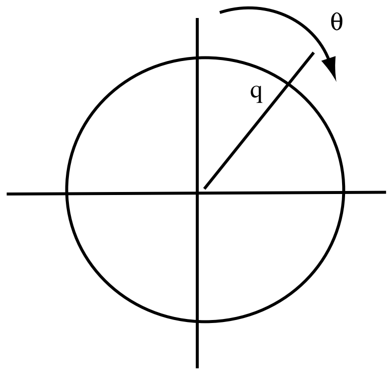


**Figure 2.** Compactification. Coordinate $q \to \cos(\theta/2)$ makes a periodic invertible map.

A first-order formalism cannot proceed from knowing half the canonical variables. However we only need half the Hamiltonian coordinates when we go to the second-order gauge-invariant formalism via equations (29) or (30). It follows that autonomous and complete second-order time evolution relating observables to observables can always be constructed. This is an interesting conceptual development reducing the quantum system to an experimentally direct formulation. At the same time, any gains in practical efficiency would have to come from specific examples and prove themselves against the awesomely effective calculation tools developed within the conventional approach.

### *4.2. A quantum model with imaginary frequencies*

Previous literature on $\mathcal{CP}$-symmetric theories have respected this ordinary meaning of unitarity with time evolution on torii. Yet physical quantum systems are also observed to evolve with imaginary frequencies, for example when particles decay. Such systems are invariably embedded in larger systems with toroidal evolution. Because of its intrinsic interest we explore an alternative system evolving with imaginary frequencies.

Hyperbolic evolution is made by Hamiltonians with 'wrong-sign' oscillators

$$H(q_i, p_i) = \sum_i \frac{\omega_i}{2}\left(p_i^2 - q_i^2\right), \tag{60}$$

where $\omega$ is real. This sort of system can be transcribed into bilinears in $\psi^2, \psi^{*2}$, and transformed further by unlimited $\mathcal{S}p$ transformations. Whatever the coordinates, it appears that little of quantum theory can be salvaged if the coordinates evolve with unlimited range.

To continue let us *compactify* coordinate $q$'s to run on a finite range (figure 2). The case of one canonical pair suffices for illustration. Let $\theta$ be the angle parameter on a closed space, $0 < \theta < 2\pi$. A naive compactication might assign $q \to \theta$, identifying $q \equiv q + 2\pi$. Unfortunately that map is inconsistent with the Hamiltonian equation (60), which is not periodic in $q$.

An invertible periodic transformation (figure 2) is given by

$$q = \cos(\theta/2). \tag{61}$$

Under $\theta \to \theta + 2\pi$ the variable transforms with a sign change $q \to -q$: we have compactifation with a twist. Besides invertibility, the reason for the half-angle map will become clear shortly.

Using the full freedom of $\mathcal{S}p$ symmetries, we transform variables using the Lagrangian

$$L(q,\dot q) = \frac{1}{2\omega}\dot q^2 + \frac{\omega}{2}q^2;$$
$$\rightarrow L(\theta,\dot\theta) = \frac{1}{8\omega}\dot\theta^2\sin^2(\theta/2) + \frac{\omega}{4}\cos(\theta). \tag{62}$$

In its nonlinear form we recognize the physical interpretation. It is the Lagrangian of a Newtonian mass point glued to a rolling wheel and subject to gravity. The solution to time evolution takes the form

$$\theta(t) = 2\cos^{-1}(a\,\mathrm{e}^{-\omega t} + (1-a)\,\mathrm{e}^{\omega t}),$$

where $a$ is a constant of initial conditions. Note that $\mathrm{e}^{\pm\omega t}$ appear in the time evolution without any catastrophic consequences.

The example shows how an autonomous system with exponential time dependence can sometimes be interpreted. Points $\dot\theta \rightarrow \pm\infty$ may occur. However they are coordinate singularities with no physical meaning. If a rolling wheel can cycle between positive and negative exponential growth while being perfectly physical, we may question proscriptions forbidding such behavior, which cannot be so general.

A radical feature of the model system equation (60) is conservation of a 'wrong-sign' quadratic form. If notions of probability itself can sensibly be extended to negative real numbers—and there is a literature[5] on this point [16]—a wrong-sign quadratic form might be converted to a compatible probability theory. Further exploration would take us into unknown territory.

## 5. Summary

The whole of quantum dynamics has a real $\mathcal{S}p$ representation which allows far richer transformations than the usual unitary set. The transformations from Hermitian Hamiltonians to non-Hermitian ones use just those $\mathcal{S}p$ transformations which are non-compact. They mix $\psi$ and $\psi^*$ in the conventional, coordinate-dependent view using $\mathcal{CPT}$ transformations. The Dirac 'quantization postulate' is seen to be a derived consequence of consistency. The Ehrenfest relations are exact equations of motions for certain canonically transformed variables. Quantities recognized as experimental observables are precise canonical coordinates of the theory via a series of coordinate transformations.

These results have been found in an approach leaving open for exploration the most basic decision on the group of time evolution. If the Hamiltonian uses those generators of the $\mathcal{S}p$ group which produce a compact subgroup, it is invariantly the same system as an ordinary one, perhaps including antimatter, and then cast into more general coordinates. Other cases would constitute new physics. It might be dynamically consistent to make $\mathcal{H}$ a function implementing nonlinear time evolution. The simplest possibility to extend the dynamics further would involve Hamiltonians with non-compact generators. Although this is interesting for itself, we caution that quantum rules of measurement and statistical interpretation are deeply contrived to mesh with unitary transformations. Further extension of dynamics and statistical interpretation would seem to need simultaneous development.

[5] 'Negative probability' is invariably associated with the school of this reference. Feynman's contribution is also interesting. See [17].

## Acknowledgments

I thank Carl Bender for highlighting the subject of $\mathcal{PT}$-symmetric theories to me at *Miami '06* and helpful discussions. Mihailo Bakovich has been helpful with references. Work partially supported by DOE grant number DE-FG02-04ER14308.

## Appendix

Let the Hamiltonian be a quadratic form

$$\mathcal{H}(q,p) = \tfrac{1}{2}\Phi^T \hat{H}_\Phi \Phi; \qquad \hat{H}_\Phi = \frac{1}{2}\begin{pmatrix} h_{qq} & h_{qp} \\ h_{qp}^T & h_{pp} \end{pmatrix}. \tag{A.1}$$

Towards developing an autonomous equation for $p$ write

$$h_{qq} = K; \qquad h_{pp} = M^{-1};$$
$$h_{qp} = K\Gamma_p; \qquad \mathcal{A}(p) = \Gamma_p p.$$

The Hamiltonian is

$$\mathcal{H} = \tfrac{1}{2}(q - \mathcal{A}(p))K(q - \mathcal{A}(p)) + \mathcal{U}(p); \qquad \mathcal{U}(p) = \tfrac{1}{2}p\left(M^{-1} - \Gamma_p^T K \Gamma_p\right).$$

From Hamilton's equations,

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} = -K(q_i - \mathcal{A}_i(p)); \qquad q_i = -K^{-1}\dot{p}_i + \mathcal{A}_i(p). \tag{A.2}$$

This eliminates $q$, which in this approach is gauge dependent. Taking the time derivative of the last equation gives

$$-K^{-1}\ddot{p}_i = \dot{q}_i - \frac{\partial \mathcal{A}_i(p)}{\partial p_j}\dot{p}_j - \frac{\partial \mathcal{A}_i(p)}{\partial t}.$$

From the other Hamilton equation

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} = -K(q_j - \mathcal{A}_j(p))\frac{\partial \mathcal{A}_j(p)}{\partial p_i} + \frac{\partial \mathcal{U}(p)}{\partial p_i},$$
$$= \dot{p}_j \frac{\partial \mathcal{A}_j(p)}{\partial p_i} + \frac{\partial \mathcal{U}(p)}{\partial p_i}.$$

Combining terms gives the Lorentz $p$-force equation

$$K^{-1}\ddot{p}_i = \dot{p}_j\left(\frac{\partial \mathcal{A}_i(p)}{\partial p_j} - \frac{\partial \mathcal{A}_j(p)}{\partial p_i}\right) + \frac{\partial \mathcal{A}_j(p)}{\partial t} - \frac{\partial \mathcal{U}(p)}{\partial p_i}. \tag{A.3}$$

The multiplet $\mathcal{A}_\mu(p) = (\mathcal{U}, \mathcal{A}_j(p))$ can be transformed by $\mathcal{A}_\mu(p) \to \mathcal{A}_\mu(p) + (-\partial\theta/\partial t, \partial\theta/\partial p_i)$ without changing the equation of motion.

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