Quantization of Contact Manifolds and Thermodynamics

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Abstract

The physical variables of classical thermodynamics occur in conjugate pairs such as pressure/volume, entropy/temperature, chemical potential/particle number. Nevertheless, and unlike in classical mechanics, there are an odd number of such thermodynamic co-ordinates. We review the formulation of thermodynamics and geometrical optics in terms of contact geometry. The Lagrange bracket provides a generalization of canonical commutation relations. Then we explore the quantization of this algebra by analogy to the quantization of mechanics. The quantum contact algebra is associative, but the constant functions are not represented by multiples of the identity: a reflection of the classical fact that Lagrange brackets satisfy the Jacobi identity but not the Leibnitz identity for derivations. We verify that this ‘quantization’ describes correctly the passage from geometrical to wave optics as well. As an example, we work out the quantum contact geometry of odd-dimensional spheres.
“A theory is the more impressive the greater the simplicity of its premises, the more different kinds of things it relates, and the more extended its area of applicability. Therefore the deep impression that classical thermodynamics made upon me. It is the only physical theory of universal content which I am convinced will never be overthrown, within the framework of applicability of its basic concepts.” – A. Einstein

1 Introduction

In classical thermodynamics, as in classical mechanics, observables come in canonically conjugate pairs: pressure is conjugate to volume, temperature to entropy, magnetic field to magnetization, chemical potential to the number of particles etc. An important difference is that the thermodynamic state space is odd dimensional. Instead of the phase space forming a symplectic manifold ( necessarily even dimensional) the thermodynamic state space is a contact manifold, its odd dimensional analogue[1].

Upon passing to the quantum theory, observables of mechanics become operators; canonically conjugate observables cannot be simultaneously measured and satisfy the uncertainty principle

$$\Delta p \Delta q \geq \hbar.$$  \hspace{1cm} (1)

Is there is an analogue to this uncertainty principle[1] for thermodynamically conjugate variables? Is there such a thing as ‘quantum thermodynamics’ where pressure or volume are represented as operators?

The product of thermodynamic conjugates such as $\Delta P \Delta V$ has the units of energy rather than action. So if there is an uncertainty relation $\Delta P \Delta V \geq h_1$, it is clear that $h_1$ cannot be Plank’s constant as in quantum mechanics.

In principle, there could be macroscopic systems for which the thermal fluctuations in aggregate quantities such as pressure or volume are small, yet the quantum fluctuations are not small. For example[2], a gas of cold atoms confined by a potential has an uncertain position for the ‘wall’ containing it: the uncertainty in the position of the wall is of the order of the wavelength $\lambda$ of the atoms. An uncertainty in the position of the wall by $\Delta x$ leads to an uncertainty in the volume of $\Delta V = A \Delta x$, where $A$ is the area of the wall.

Similarly, the pressure of the gas is also uncertain, since pressure is the change of momentum per unit area per unit time of the particles reflected by the potential: the uncertainty of momentum is of order $\frac{\hbar}{\Delta x}$. The number of collisions per unit time is $\rho v A$ where, $v$ the typical velocity and $\rho$ the number density. Thus we should expect $\Delta P = \frac{\hbar}{\Delta x} \rho v A$.

$$\Delta P \Delta V \geq h_1 = \hbar \nu, \hspace{0.5cm} \nu \approx \rho v A.$$ \hspace{1cm} (2)

As the system becomes very large, the $PV$ scales like the volume while the r.h.s. of the uncertainty relation scales as the area; in this sense it becomes small in many familiar systems.

[1]There is already an uncertainty relation[2] for statistical rather than quantum fluctuations of thermodynamica quantities, where the analogue of $\hbar$ is $kT$.

[2] I thank Anosh Joseph for discussions on this topic.
This justifies the usual practice in quantum statistical mechanics textbooks, of calculating the internal energy of a quantum system such as a Bose gas or a Fermi gas by averaging over states and then using it in thermodynamics as if it is a classical system to derive the equation of state.

But there should be systems large enough for thermodynamics to be applicable but small enough that the uncertainty cannot be ignored, of the order of surface effects. It would be exciting to test this prediction experimentally. The appearance of area here is reminiscent of the ‘holographic principle’ in quantum gravity. Our argument suggests that the quantum thermodynamic effects are particularly important in systems where the Area and Volume scale the same way, as in hyperbolic spaces.

Another possible application of quantum thermodynamics is to blackholes. Classical general relativity predicts that blackholes obey the rules of classical thermodynamics, with the entropy being proportional to the area of the horizon. Although we don’t yet have a quantum theory of gravity (string theory being the main, but not the only, candidate) we can expect that the quantity with the dimensions of energy that appear in the quantum thermodynamic uncertainty relations is Plank mass. For a black hole that is small enough, it could be important to describe thermodynamic observables such as mass and area as operators, thus significantly affecting the debate on the final state of black hole evaporation.

In this paper we will explore the mathematical problem of quantizing contact geometry. This is of interest for other reasons than thermodynamics in any case. Quantum or non-commutative notions of geometry are playing an increasing role in many areas of physics and mathematics \[3\]. Deformations of classical notions of Riemannian geometry are central to quantum theories of gravity such as string theory, M-theory and loop quantum gravity. Quantum analogues of symplectic geometry arise as soon one considers the geometry of the phase space in quantum theory. As the odd dimensional sibling of symplectic geometry, contact geometry should also have a quantum analogue, with applications as varied as for contact geometry: in constructing knot invariants, or in quantizing systems with a constraint. Our own original motivation was to understand the possible quantum deformations of the $S^5$ that appear in the Maldacena correspondence between gauge and string theories. But we will present the results in a broader context.

We begin with a review of how contact geometry arises in classical physics, because much of this material does not seem to be widely accessible in the modern literature in physics. We follow closely the approach of Arnold and Givental \[1\] for the classical theory, as a starting point for our quantization. See also the books by Buchdahl \[4\] and the influential review articles by Lieb and Yngvason \[6\] that revive this classical subject.

### 2 Thermodynamics

Consider a material in an enclosure of volume $V$, pressure $P$, temperature $T$, entropy $S$ and internal energy $U$. The first law of thermodynamics says that infinitesimal changes of these thermodynamic variables must satisfy

\[
\alpha \equiv dU + PdV - TdS = 0
\]
Although there appears to be only one condition among the variations of the five co-ordinates, there is no solution with four independent variables; i.e., there is no four-dimensional submanifold all of whose tangent vectors $v$ satisfy the condition $i_v \alpha = 0$. Of course, this is because the condition above is not a scalar, but a ‘Pfaffian system’ of equations. The number of independent variables of such a system can only be determined by a subtler analysis using the language of differential forms. In fact the theory of differential forms was originally developed in part to understand thermodynamics.

If there were four out of five independent variables, there would have been a function $f$ that vanished on the hypersurface of solutions. Also there would be another function $g$ such that $\alpha = f dg$. The integrability condition (of Frobenius) for that to be the case is $\alpha \wedge da = 0$, which is not satisfied in our case. Indeed, even $\alpha \wedge (da)^2 \sim dU dP dV dT dS \neq 0$ everywhere, so there is not even a three dimensional submanifold that solves $\alpha = 0$.

A submanifold of maximal dimension all of whose tangent vectors are annihilated by $\alpha$ is called a Lagrangian submanifold. In our example, the dimension of a Legendre submanifold is two, which therefore is the number of independent thermodynamic degrees of freedom.

In other words, the first law of thermodynamics implies that only two out of the five variables $U, P, V, T, S$ are independent: the remaining variables are given by the equations of state. The particular two dimensional submanifold chosen as solution will depend on the material since it depends on the equations of state. This key insight is due to J. W. Gibbs\[7\], in his first paper.

So far, the internal energy $U$ appears to have a special status as the ‘unpaired’ variable. However, this is illusory: the first law of thermodynamics can also be expressed as $dS - \beta dU + \tilde{P} dV = 0$ where $\beta = \frac{1}{T}, \tilde{P} = \frac{P}{T}$. This can be viewed as the condition for maximizing $S$ subject to the constraint that internal energy $U$ and volume are held fixed: then $\beta, \tilde{P}$ are the Lagrange multipliers for these constraints.

Giving $S$ as a function of $U, V$ (The Fundamental Relation) is a way of determining the Legendre submanifold of a substance: the remaining variables are then given as derivatives $\beta = \left[ \frac{\partial S}{\partial U} \right]_V, \tilde{P} = -\left[ \frac{\partial S}{\partial V} \right]_U$.

For the monatomic ideal gas for example, the gas law and equipartition of energy give

$$PV = nRT, \quad U = \frac{3}{2} nRT.$$ (4)

Here $n$ is the number of atoms in the gas divided by the Avogadro number. The condition $dS - \beta dU + \tilde{P} dV = 0$ then determines entropy:

$$S = nR \log \left[ \frac{U \frac{3}{2}}{V} \right]$$ (5)

up to a constant.

Conversely, this Fundamental Relation determines all the other relations among the thermodynamical quantities. The intensive variables $\beta, \tilde{P}$, are given by derivatives w.r.t. their conjugate variables:

$$\frac{1}{T} = \left( \frac{\partial S}{\partial U} \right)_V = \frac{3nR}{2U}, \quad \frac{P}{T} = -\left( \frac{\partial S}{\partial V} \right)_U = \frac{nR}{V}.$$ (6)
We can also describe the Legendre submanifold using co-ordinates $S, P$ or $T, V$ by rewriting the condition $\alpha = 0$ in the forms
\[ d[U - PV] + VdP + TdS = 0, \quad \text{or} \quad d[U + TS] - PdV - SdT = 0. \] (7)

We can chose any pair as the fundamental variables as long as they are not conjugate to each other. Each choice provides a co-ordinate system on the Legendre submanifold.

In each picture there is a Thermodynamical Potential $u$, fundamental variables $q^i$ and their conjugate variables $p_i$ such that
\[ du - p_i dq^i = 0. \] (8)

This is the condition for minimizing (or maximizing) $u$ subject to the condition that $q^i$ are held fixed; the conjugate variables $p_i$ are the Lagrange multipliers for these constraints. The different equivalent choices of fundamental variables are related by Legendre transformations.

Given a function $F$ of the five variables and the condition $\alpha \equiv du - p_i dq^i = 0$, there is a one-parameter family of transformations, given as the solutions of the ordinary differential equations
\[ \dot{q}^i = \frac{\partial F}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial F}{\partial q^i} - p_i \frac{\partial F}{\partial u}, \quad \dot{u} = p_i \frac{\partial F}{\partial p_i} - F. \] (9)

The tangent to these curves are in the kernel of $\alpha$; i.e., any solution to the above ODEs will be consistent with the first law of thermodynamics. We can use these transformations to interchange fundamental variables.

For example, the choice $F = \frac{1}{2}(p_1^2 + q_1^2)$ interchanges $q_1 \rightarrow p_1, p_1 \rightarrow -q_1$ and $u \rightarrow u - p_1 q_1$ after a ‘time’ $\pi/2$. As another example, $p$ generates a scaling of $u$ and $q$.

If the generating function is independent of $u$, the transformation of $p, q$ are the canonical transformations familiar from classical mechanics. But in general they are not. Another, important difference is that there are here an odd number of variables in the thermodynamic phase space.

3 Characteristic Curves

The same mathematical structures occur other branches of physics, such as classical mechanics and geometrical optics. More generally, in the theory of characteristics of partial differential equations\textsuperscript{8}.

Suppose we have a first order quasi-linear PDE
\[ a^i(q, u) \frac{\partial u}{\partial q^i} = b(q, u). \] (10)

This is the problem of finding a surface tangential to the vector field $a^i \frac{\partial}{\partial q^i} + b \frac{\partial}{\partial u}$ at all points. That is, changing $q^i$ by $a^i dt$ has the effect of changing $u$ by $b dt$. In other words, the surface that solves the PDE is ruled by the integral curves (‘characteristic curves’) of this vector field. Hence, solving the PDE is equivalent to finding the general solution of the system of ODEs,
\[ \frac{dq^i}{dt} = a^i(q(t), u(t)), \quad \frac{du}{dt} = b(q(t), u(t)). \] (11)
This idea in fact generalizes even to a nonlinear first order PDE

\[ F(u, \frac{\partial u}{\partial q}, q) = 0, \]  

(12)

if we allow \( p_i = \frac{\partial u}{\partial q_i} \) as extra variables. To the function \( F(u, p, q) \) is associated the ordinary differential equations for characteristic curves

\[ \dot{q} = \frac{\partial F}{\partial p}, \quad \dot{p} = -\frac{\partial F}{\partial q} - p \frac{\partial F}{\partial u}, \quad \dot{u} = \frac{\partial F}{\partial p} - F. \]  

(13)

In other words given the condition \( \alpha \equiv du - pdq = 0 \) on the infinitesimals, and a function \( F \) we can construct the vector field

\[ V_F = \left[ p \frac{\partial F}{\partial p} - F \right] \frac{\partial}{\partial u} - \left[ \frac{\partial F}{\partial q} + p \frac{\partial F}{\partial u} \right] \frac{\partial}{\partial p} + \frac{\partial F}{\partial p} \frac{\partial}{\partial q} \]  

(14)

whose integrals are the characteristic curves.

If we impose the condition

\[ du - p_i dq^i = 0 \]  

(15)

on infinitesimal variations, each function \( u(q) \) defines a Lagrangean submanifold. The problem of solving the PDE \( F(u, \frac{\partial u}{\partial q}, q) = 0 \) becomes that of finding an intersection of a Lagrangean submanifold with the hypersurface defined by \( F(u, p, q) = 0 \). So every hypersurface on a contact manifold must be ‘ruled’ by curves, the characteristic curves of the corresponding PDE.

In a medium whose refractive index depends on position and direction, the eikonal equation of geometrical optics takes the form

\[ g^{ij}(x) \frac{\partial u}{\partial x^i} \frac{\partial u}{\partial x^j} = k^2 \]  

(16)

where \( k \) is the wave number. Thus,

\[ F(u, p, x) = g^{ij}(x)p_ip_j - k^2. \]  

(17)

The characteristic curves are the light rays; they are the solutions of the ODE above with this choice of \( F \).

### 4 Classical Mechanics

Although it has become fashionable to formulate classical mechanical in terms of symplectic geometry, the Hamilton-Jacobi formulation is best understood in terms of an odd-dimensional phase space of co-ordinates \((u, q, p)\) where \( u \) is the eikonal or Hamilton’s principal function. The condition \( du - p_i dq^i = 0 \) is satisfied if

\[ p_i = \frac{\partial u}{\partial q^i}. \]  

(18)
The constancy of energy

\[ F(q, p) = H(q, p) - E = 0 \tag{19} \]

defines a hypersurface on this odd-dimensional phase space which is ruled by the characteristic curves generated by this function

\[ \dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}, \quad \dot{u} = p \frac{\partial H}{\partial p} - H + E. \tag{20} \]

The first pair are the Hamilton’s equations; the last equation gives the variation of the eikonal along a classical trajectory.

This larger phase space allows as symmetries the Legendre transformations whose generator can depend on the eikonal \( u \) in addition to \( p \) and \( q \). As we saw, these are more general than the above canonical transformations whose generators only depend on \( p \) and \( q \). Thus they can accommodate the general first order partial differential equation rather than just the Hamilton-Jacobi equations above.

The first order PDE of mechanics and optics are in fact, the approximation to the wave equation in the limit of small wavelength. Thus it becomes interesting to develop a unifying framework for quantizing contact structures that include mechanics, optics and thermodynamics. There are also interesting applications to fluid mechanics [5].

5 Legendrian Knots

We digress briefly to make contact with a fashionable topic of mathematics [9]. An embedding of \( S^1 \) in \( R^3 = \{(u, q, p)\} \) is a Legendrian knot if all its tangent vectors are in the kernel of the contact form \( du - pdq \). Any closed curve in the plane with \( \oint pdq = 0 \) will give a knot, simply by choosing \( u \) to be integral of \( pdq \) along the curve. Conversely, every Legendrian knot is determined by its projection to the \((p, q)\) plane. A continuous one parameter family of contact transformations that does not make the curve intersect itself is a contact isotopy. Invariants of Legendrian knots under such contact isotopies are of interest in topology of three manifolds [9]. Since the condition of being a contact isotopy is stronger than an isotopy, it is knots that are equivalent in the usual sense might be distinct as Legendrian knots: there are more invariants in Legendrian knot theory. Ideas from quantum theory have re-invigorated conventional knot theory [10]: perhaps a theory of quantum contact manifolds can do the same for Legendrian knots.

6 Contact Structure

It is time to reformulate the above nineteenth century physics in the language of twentieth century mathematics.

**Defn.**

A contact form on a manifold of dimension \( 2n + 1 \) is a one-form that satisfies

\[ \alpha \wedge (d\alpha)^n \neq 0 \tag{21} \]
at each point. Two such forms are considered equivalent if they only differ by multiplication by a positive function (a ‘gauge transformation’):

\[ \alpha \sim f \alpha. \]  

(22)

A contact manifold has a contact form in each co-ordinate patch, with such positive functions relating overlapping patches.

A contact structure should be thought of as the equation \( \alpha = 0 \) which picks out a subspace of the tangent space at each point of the manifold. However, the Frobenius integrability condition for these to fit together as tangent spaces of some submanifold is maximally violated.

A submanifold all of whose the tangent vectors will satisfy \( \alpha = 0 \) is said to be ‘integral’. If the contact manifold is of dimension \( 2n + 1 \), the largest dimension for an integral submanifold will be \( n \). Such a maximal integral submanifold is called a Legendre submanifold.

An analogue of Darboux’s theorem says that there is a local co-ordinate system (and choice of gauge) in which contact form is

\[ \alpha = du - \sum_{i=1}^{n} p_i dq^i. \]  

(23)

Thus \( \mathbb{R}^{2n+1} \) with this choice is the basic example of a contact manifold. A Legendre submanifold is given by the \( n \) dimensional subspace with co-ordinates \( p^i \), holding \( u, q^i \) constant. Another Legendre submanifold is given by \( (u(q), \frac{\partial u}{\partial q}, q) \) for some generic function \( u(q) \).

The condition for a vector field \( V \) to preserve a contact structure is that there exist a function \( g_V \) such that

\[ \mathcal{L}_V \alpha = g_V \alpha. \]  

(24)

The commutator of two such functions will still satisfy this condition.

If we choose local co-ordinates such that \( \alpha = du - p dq^i \), such a vector field is always of the form

\[ V = \left[ \frac{\partial F}{\partial p} - F \right] \frac{\partial}{\partial u} - \left[ \frac{\partial F}{\partial q} + p \frac{\partial F}{\partial u} \right] \frac{\partial}{\partial p} + \frac{\partial F}{\partial q} \frac{\partial}{\partial q} \]  

(25)

where the Hamiltonian of \( V \) is \( F = -i_V \alpha \) and \( g_V = -\frac{\partial F}{\partial u} \).

There is thus a one-one correspondence between contact vector fields and their Hamiltonians. Unlike for symplectic vector fields, a constant added to \( F \) will change \( V_F \). Note that the integral curves of the contact vector field are precisely the characteristic curves of \( F \) we obtained earlier. Since \( V_F(F) = -F \frac{\partial F}{\partial u} \), if the initial value of \( F \) is zero it will remain zero for ever. Thus the solution to \( F(u, \frac{\partial u}{\partial q}, q) = 0 \), given the value of \( u \) on a boundary curve in the \( q \)-space, can be obtained by starting at each point on the boundary and evolving along the integral curves of \( V_F \).

If we replace \( F \) by a function \( \phi(F) \) (where \( \phi : R \rightarrow R \) has non-zero derivative everywhere) the vector field changes as \( V_F \mapsto \phi(F)V_F \): the integral curves are unchanged except for their parametrization. Thus each hypersurface in a contact manifold determines a family of characteristic curves that lie on them. Through
each point on the hypersurface passes exactly one such curve: these curves rule the hypersurface.

It will be of interest to look at the special case $\mathcal{L}_V \alpha = 0$. Such vector fields preserve the volume form $\alpha (d\alpha)^n$ and so might also be called incompressible contact vector fields. Clearly they are determined by a generating function that is independent of $u$, basically canonical transformations.

### 6.1 Digression: Reeb Dynamics

A contact form by itself also defines a family of curves. The two-form $d\alpha$ is of maximal rank; so there is a vector field, unique up to multiplication by a non-zero function, such that $i_V d\alpha = 0$. Its integral curves are then well defined: a change $V \to fV$ only affects the parametrization of the curves. This is the Reeb dynamics of a contact form [11]. A contact manifold does not however determine a contact form: the choice of a particular contact form representing a contact structure is analogous to the choice of a generating function $F$ in the last section. We have to choose here a section of a line bundle; i.e., make a choice of gauge representing the contact form. We can see that these Reeb curves extremize the action $\int \alpha$.

This dynamics is not invariant under the transformation $\alpha \to f\alpha$ but is instead invariant under the addition of an exact form $\alpha \to \alpha + d\lambda$. If $\alpha = H dt - pdq$ with $H$ depending on $t, p, q$ describes a time dependent hamiltonian system. The action principles states that the dynamics consist of curves that extremize the action $\int [pdq - H dt]$; i.e., satisfy the Hamilton-Jacobi equations. Thus time dependent hamiltonian mechanics is exactly the Reeb dynamics for the above contact form. This is a different point of view on mechanics from the one using contact structures. Important unsolved problems in this subject include the Weinstein conjecture on the existence of a periodic orbit for the dynamics on any compact contact manifold[12].

### 7 Canonical Quantization in Contact Geometry

The standard example of a symplectic manifold is a co-tangent bundle; the analogous example for a contact manifold is the projective co-tangent bundle. In co-ordinates $x^\mu$ on a space $X$, the co-tangent bundle $T^*X$ has a one-form $\theta = k_\mu dx^\mu$ and symplectic form $dk_\mu dx^\mu$. On the fibers we have an action of the group $R^\times$ of non-zero real numbers, $k_\mu \mapsto \lambda k_\mu$. The quotient of $T^*X - X$ under this action of $R^\times$ is the projective co-tangent bundle $PT^*X$.

Under this action, $\theta \mapsto \lambda \theta$, so it becomes a one-form $\alpha$ (defined only up to multiplication by a non-zero scalar function) on the quotient. This is the contact structure on $PT^*X$.

If $\dim X = n + 1$ the contact manifold is of dimension $2n + 1$. The real projective spaces which are the fibers over each point of $X$ are Legendre submanifolds. A hypersurface in this contact manifold can be given by an equation

$$F(x, k) = 0$$

where $F : T^*X \to R$ is a homogenous function on the cotangent space:

$$F(x, \lambda k) = \lambda^n F(x, k).$$
These curves will rule the hypersurface \( F(u,q,p) = 0 \). Such a hypersurface will define a family of characteristic curves that rule it. It will be convenient to make a choice of this function that has as simple a dependence on \( k \) as possible (e.g., polynomial if possible) because this will simplify the quantization.

This point of view is particularly appropriate for null geodesics on a pseudo-Riemannian manifold \( X \). The phase space for these geodesics is the projective cotangent space. There is a natural hypersurface \( g^{\mu\nu} k_{\mu} k_{\nu} = 0 \) on this contact manifold. The characteristic curves of this hypersurface are the null geodesics. A ‘quantization’ should recover the wave equation on \( X \).

Whenever a classical dynamical system can be formulated in terms of the characteristic curves of a hypersurface \( F(x,k) = 0 \) on a projective cotangent bundle \( PT^*X \), we have a quantization in the ‘Schrodinger picture’. The wave functions of the system are then complex valued functions \( \psi : X \to C \) satisfying the wave equation

\[
\left[ F\left(x, \frac{\partial}{\partial x}\right) + \cdots \right] \psi = 0.
\]  

(28)

The \( \cdots \) denotes lower derivative terms that represent the ordering ambiguities: the rule of canonical quantization can only give the highest order piece as only the principal symbol is known in the classical theory. Remember that for the equation \( F(x,k) = 0 \) to be well-defined on the projective space, \( F(x,k) \) must be homogenous in \( k \). Thus the constant \( -i\hbar \) in the usual rule for canonical quantization \( k \mapsto -i\hbar \frac{\partial}{\partial x} \) drops out of the wave equation.

In the eikonal approximation \( \psi(x) = e^{\frac{i}{\hbar} u(x)} \) with small \( \hbar \) we will get back the equation for the Legendre submanifold determined by \( F \):

\[
F\left(x, \frac{\partial u}{\partial x}\right) = 0.
\]  

(29)

Applied to the case of null geodesics this gives the wave equation

\[
\left[ g^{\mu\nu} \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x^\nu} + \cdots \right] \psi = 0.
\]  

(30)

Physically, this is not quantization as such, but the passage from geometrical optics to wave optics.

If we determine the lower order terms by the requirement of invariance under co-ordinate transformations, we get the d’Alembertian operator

\[
\frac{\partial}{\partial x^\mu} \left( \sqrt{|g|} g^{\mu\nu} \frac{\partial \psi}{\partial x^\nu} \right) = 0
\]  

(31)

When there is no natural identification of the contact manifold as a projective cotangent space, we need a more abstract approach.

8 The Lagrange Bracket

Let us recall again familiar notions from classical mechanics.

A symplectic form is a closed two-form that is non-degenerate:

\[
d\omega = 0, \quad i_{\omega} = 0 \Rightarrow v = 0.
\]  

(32)
This of course requires the manifold carrying \( \omega \) to be even dimensional.

A symplectomorphism (‘canonical transformation’) is a diffeomorphism that preserves the sympletic form, \( \phi^* \omega = \omega \). Infinitesimally, a symplectic vector field satisfies \( \mathcal{L}_v \omega = 0 \). Since \( \mathcal{L}_v \omega = d(i_v \omega) \), this implies that locally there is a function (‘generating function’) such that

\[
i_v \omega = dg_v.
\]

(33)

The commutator of two symplectic vector fields is also symplectic. This defines a commutator (‘Poisson bracket’) on the generating functions:

\[
\{g_1, g_2\} = r(dg_1, dg_2)
\]

(34)

where \( r \) is the inverse tensor of \( \omega \). These brackets satisfy the axioms of a Poisson Algebra.

**Defn.**

A **Poisson Algebra** is a commutative algebra \( A \) with identity along with a bilinear \( \{,\} : A \otimes A \to A \) that satisfies

1. \( \{g_1, g_2\} = -\{g_2, g_2\} \)
2. \( \{\{g_1, g_2\}, g_3\} + \{\{g_2, g_3\}, g_1\} + \{\{g_3, g_1\}, g_2\} = 0 \)  Jacobi identity
3. \( \{g_1, g_2 g_3\} = \{g_1, g_2\} g_3 + g_2 \{g_1, g_3\} \)  Leibnitz Rule

The last property implies that the Poisson bracket of a constant with any function is zero.

The basic example is the algebra of functions on the plane:

\[
\{g_1, g_2\} = \partial_x g_1 \partial_y g_2 - \partial_y g_1 \partial_x g_2.
\]

(35)

More generally the set of function on a symplectic manifold form a Poisson algebra, with bracket we gave earlier. Conversely, if the Poisson algebra is non-degenerate (the only elements that have zero Poisson bracket with everything are constants) it arises from a symplectic manifold this way.

Also, the set of functions on the dual of a Lie algebra is a Poisson algebra (Kirillov):

\[
\{F, G\}(\xi) = i_\xi [dF, dG]
\]

(36)

The commutator of two contact vector fields is again a contact vector field. This induces a bracket on functions, called the **Lagrange bracket**:

\[
(F, G) = FG_u - F_u G + p (F_p G_u - F_u G_p) + F_p G_q - F_q G_p
\]

(37)

with the summations over indices implied.

This satisfies the Jacobi identity but not the Leibnitz rule: even the bracket of the constant with a function may not be zero:

\[
(1, G) = G_u.
\]

(38)

**Defn**

A commutative algebra \( A \) with identity and a bilinear \( (,) : A \times A \to A \) is a **Generalized Poisson Algebra** if

\[\text{We follow the terminology of Arnold}\]. There are also some other unrelated things called Lagrange brackets in for example, the textbook by Goldstein.
1. \((g_1, g_2) = -(g_2, g_2)\)
2. \(((g_1, g_2), g_3) + ((g_2, g_3), g_1) + ((g_3, g_1), g_2) = 0\)
3. \((g_1, g_2 g_3) = (g_1 g_2) g_3 + g_2 (g_1, g_3) + (1, g_1) g_2 g_3.\) The Generalized Leibnitz Rule

The main point is that the constant function is no longer in the center. The commutant of the constant function is a Poisson algebra.

With the choice \(\alpha = du - pdq\) on the simplest case of \(R^3\), the analogue of the canonical commutation relations can now be worked out:

\[
\begin{align*}
(p, q) &= w, & (w, q) &= 0, & (w, p) &= 0 \\
(u, q) &= 0, & (u, p) &= p, & (u, w) &= w
\end{align*}
\]

The element \(w\) (which is simply the constant function 1) is not central anymore. \(w, p, q\) span a Heisenberg sub-algebra. \(u\) generates the automorphism of the Heisenberg algebra which scales \(w, p\). Since the Leibnitz rule is replaced by the new identity, we have to be careful about using these commutation relations to derive brackets for more general functions. e.g., \((u, pq) = 0\).

9 Deformation Quantization of Contact Structures

Recall that given a constant Poisson tensor \(\tau^{ij}\) on a vector space, we can quantize it by defining the star product on functions

\[
f \star g(\xi) = \left[ e^\frac{-i}{\hbar} \frac{\partial}{\partial \xi^i} \sigma_{ij} \frac{\partial}{\partial \xi^j} f(\xi) \right]_{\xi = \xi'}
\]

If we expand in powers of \(\hbar\), to zeroth order we get just the pointwise product, then the Poisson bracket then various higher order derivatives that fit amazingly into an associative product when all terms are taken into account.

We will now present a similar way of turning the space of functions on a contact vector space into an associative algebra: the zeroth order will be the pointwise product, the first order the Lagrange bracket and so on.

The key idea is to note that a contact vector space \(V\) is always the ‘projectivization’ of some symplectic vector space \(\tilde{V}\): the functions on \(V\) lift uniquely to homogenous functions of degree one on \(\tilde{V}\). Contact vector fields lift to vector fields on \(\tilde{V}\) that commute with the scaling. So we can lift them up, multiply them and then project to get the star product on the contact vector space.

Given a function on \(V\), we define a function on \(\tilde{V}\),

\[
\tilde{F}(w, u, q, p) = wF(u, q, wp).
\]

Then

\[
\left[ \frac{\partial \tilde{F}}{\partial w} \right]_{w=1} = F(u, q, p) + p \frac{\partial F}{\partial p}
\]

so that

\[
\{\tilde{F}, \tilde{G}\}_{w=1} = (F, G).
\]
We use this idea to extend the $\ast$-product as well:

$$F \ast G = \left[ e^{-\frac{i\bar{\hbar}}{2} \left( \frac{\partial^2}{\partial w \partial u'} + \frac{\partial^2}{\partial q \partial p'} \right)} w F(u, q, wp) u' G(u', q', w' p') \right]_{w=w'=1, u=0, p=0, q=q'} . \quad (43)$$

It is clear that this multiplication is associative as it is a special case of the usual $\ast$-product of Moyal. Moreover, to leading order in $\bar{\hbar}$, it is the commutative product plus the Lagrange bracket:

$$F \ast G = FG - \frac{i\bar{\hbar}}{2} (F,G) + \cdots \quad (44)$$

This non-commutative multiplication now contains all the quantum effects. By expanding the exponential in a power series we can get a more explicit form of the $\ast$-product.

It is convenient to think of this algebra as represented on wave functions that depend on $u, q$. The correspondence principle is

$$F(u, q, p) \mapsto \hat{F} = F(u, q, \frac{\partial^2}{\partial q \partial u}) - i\bar{\hbar} \frac{\partial}{\partial u} \psi(q, u) + \cdots \quad (45)$$

the dots being terms that needed to be added to make the operator hermitean. The precise formula is

$$\hat{F}\psi(q, u) = \int w F\left(\frac{u + u'}{2}, \frac{q + q'}{2}, wp\right) e^{i\bar{\hbar}\left(p(q-q') + w(q-q')\right)} \psi(q', u') \frac{dp dq' du'}{(2\pi)^{n+1}}$$

Even the constant function is represented by an operator: $1 \mapsto -i\bar{\hbar} \frac{\partial}{\partial u}$. For example, the hypersurface $p^2 + V(q) - E = 0$, corresponding to a hamiltonian that is independent of $u$, leads to the Schrödinger-like equation

$$\left(\frac{(-i\bar{\hbar})^2}{\partial q} + V(q) - E\right) \psi(q, u) = 0 \quad (46)$$

The ansatz $\psi(q, u) = e^{iu\chi(q)} \psi(q)$ then yields the usual Schrödinger equation

$$\left(\frac{(-i\bar{\hbar})}{\partial q} \right)^2 + V(q) - E \psi(q) = 0 \quad (47)$$

for $\psi(q)$.

More generally, given a function $F(u, q, p)$ that does depend on $u$, classically we have first order PDE

$$F\left(\chi(q), q, \frac{\partial \chi}{\partial q}\right) = 0 \quad (48)$$

which defines a Legendre submanifold. Upon quantization we get the linear differential equation $\hat{F}\psi(q, u) = 0$ where $\hat{F}$ is given by the integral formula above. Up to ordering ambiguities

$$F\left(u, q, \frac{(-i\bar{\hbar})^2}{\partial u\partial q} \right) \left(\frac{(-i\bar{\hbar})}{\partial u}\right) \psi(q, u) = 0 \quad (49)$$
In the semi-classical approximation the solution of the above wave equation is
\[ \psi(q, u) \approx e^{i\bar{\hbar}[u + \chi(q)]} \tag{50} \]
with \( \chi(q) \) satisfying the first order PDE
\[ F \left( \chi(q), q, \frac{\partial \chi}{\partial q} \right) = 0 \tag{51} \]

### 10 Odd-dimensional Quantum Spheres

There are several examples of quantum spheres known in the literature \cite{13}. They are quantum deformations of the sphere thought of as the set of unit vectors in Euclidean space. If this vector space is even dimensional, it can carry a symplectic structure and then the odd dimensional sphere embedded in it inherits a contact structure. We will study the quantum deformation of these ‘contact spheres’ as an example.

Let us begin with a constant symplectic structure \( \omega_{ij} \) on a vector space of dimension \( 2n \) and a sphere \( n^i n^i = 1 \) in it. This is just the energy surface of a harmonic oscillator; there is a vector field on the surface of the sphere which defines the time evolution of the hamiltonian function \( x^i x^i \) on the ambient vector space containing the sphere. If the characteristic values of the anti-symmetric matrix (which are proportional to the periods of the normal modes of the harmonic oscillator) are all equal, this co-ordinate will be periodic, the ‘angle’ variable conjugate to the hamiltonian \( x^i x^i \).

Given a function on the sphere we can expand it in ‘spherical harmonics’:
\[ F(n) = F_0 + F_i n^i + F_{ij} \frac{n^i n^j}{2!} + \cdots \tag{52} \]

The coefficients are symmetric traceless tensors. We can lift this function on the sphere to the ambient vector space
\[ \tilde{F} = x^2 \left[ F_0 + F_i x^i + F_{ij} \frac{x^i x^j}{2!} + \cdots \right] \tag{53} \]

The factor \( x^2 \) in front ensures that the Poisson bracket on the ambient space restricts to the Lagrange bracket on the sphere:
\[ \{ \tilde{F}, \tilde{G} \}_{x^2=1} = (F, G). \tag{54} \]

Quantization of the algebra of functions on the contact manifolds is now just the quantization of the lift of these functions. More precisely we already have the usual Moyal \( \ast \)-product on the function on the symplectic vector space. We define the star product of functions on the sphere to be
\[ F \ast G = \left[ \tilde{F} \ast \tilde{G} \right]_{x^2=1} \tag{55} \]

Thus even the constant function goes over to an operator that is not the multiple of the identity.
We can also represent this algebra on the Hilbert space of the harmonic oscillator. The metric $\delta_{ij}$ and the symplectic structure together define a complex structure on the vector space. The quadratic function $x^2$ being the hamiltonian is then the function

$$H(z) = \sum_{a=1}^{n} \omega_a z^a \bar{z}^a. \quad (56)$$

Here $\omega_i$ are the frequencies of the normal modes of the harmonic oscillator. Or, $\omega_a$ are equal to half the reciprocal of the characteristic values of the symplectic tensor. Every polynomial on the vector space can be written as a polynomial in $z^a, z\bar{a}$:

$$\Phi = \Phi_0 + \Phi_a z^a + \Phi_{ab} \frac{1}{2!} z^a z^b + \Phi_{aa} z^a \bar{z}^a + \Phi_{ab} \frac{1}{2!} z^a \bar{z}^b + \cdots \quad (57)$$

The Hilbert space of the harmonic oscillator is the space of polynomials in the $z^a$. The inner product is defined by declaring the monomials

$$z_1^{N_1} \cdots z_n^{N_n} \quad (58)$$
to be orthonormal. The above polynomial becomes the operator

$$\hat{\Phi} = \Phi_0 + \Phi_a A^a + \Phi_{ab} \frac{1}{2!} A^a A^b + \Phi_{aa} \frac{1}{2!} (A^a A^a + A^a A^\dagger a) + \Phi_{ab} \frac{1}{2!} A^a A^{\dagger b} + \cdots \quad (59)$$

We have chosen the symmetric ordering of operators.

Now we can see how each function on the sphere goes over to an operator on this quantum Hilbert space. The constant function 1 goes over to the hamiltonian operator:

$$\hat{H} = \sum_{a} \omega_a [A^\dagger a A^a + \frac{1}{2}]. \quad (60)$$

More generally the function $F(n) = F_0 + F_i n^i + F_{ij} \frac{n^i n^j}{2} + \cdots$ on the sphere becomes

$$\hat{F} = F_0 \hat{H} + F_a \frac{1}{2} [\hat{H}, A^a] + \cdots \quad (61)$$

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