Canonical Quantization

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1 Canonical quantization of a particle

1.1 The Heisenberg picture

One of the most direct ways to quantize a classical system is the method of *canonical quantization* introduced by Dirac. The prescription is remarkably simple, and stems from the close relationship between Hamiltonian mechanics and quantum mechanics.

A *dynamical variable* is any function of the phase space coordinates and time, $f(q_i, p_i, t)$. Given any two dynamical variables, we can compute their Poisson bracket, $\{f, g\}$ as described in our discussion of Hamiltonian mechanics. In particular, the time evolution of any dynamical variable is given by

$$\frac{df}{dt} = \{H, f\} + \frac{\partial f}{\partial t}$$

and for any canonically conjugate pair of variables,

$$\{p_i, q_j\} = \delta_{ij}$$

To quantize the classical system, we let the canonically conjugate variables become operators (denoted by a "hat", $\hat{o}$), let all Poisson brackets be replaced by $\frac{i}{\hbar}$ times the *commutator* of those operators, and let all dynamical variables (including the Hamiltonian) become operators through their dependence on the conjugate variables:

$$\{\ ,\ \} \rightarrow \frac{i}{\hbar}[\ ,\ ] \quad (1)$$

$$(p_i, q_j) \rightarrow (\hat{p}_i, \hat{q}_j) \quad (2)$$

$$f(p_i, q_j, t) \rightarrow \hat{f} = f(\hat{p}_i, \hat{q}_j, t) \quad (3)$$

The operators are taken to act linearly on a vector space, and the vectors are called "states." This is all often summarized, a bit too succinctly, by saying "replace all Poisson brackets by commutators and put hats on everything." This simple set of rules works admirably.

1.2 Example

As a simple example, let's quantize the simple harmonic oscillator. In terms of the canonical variables (p_i, x_j) the Hamiltonian is

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}k\mathbf{x}^2$$

We quantize by making the replacements

$$x_j \Rightarrow \hat{x}_j$$
$$p_i \Rightarrow \hat{p}_i$$

$$
\begin{aligned}
\{p_i, x_j\} &= \delta_{ij} \Rightarrow \frac{i}{\hbar}[\hat{p}_i, \hat{x}_j] = \delta_{ij} \\
\{x_i, x_j\} &= 0 \Rightarrow \frac{i}{\hbar}[\hat{x}_i, \hat{x}_j] = 0 \\
\{p_i, p_j\} &= 0 \Rightarrow \frac{i}{\hbar}[\hat{p}_i, \hat{p}_j] = 0 \\
\hat{H} &= \frac{\hat{\mathbf{p}}^2}{2m} + \frac{1}{2}k\hat{\mathbf{x}}^2
\end{aligned}
$$

We therefore have

$$
\begin{aligned}
[\hat{p}_i, \hat{x}_j] &= -i\hbar\delta_{ij} \\
[\hat{x}_i, \hat{x}_j] &= 0 \\
[\hat{p}_i, \hat{p}_j] &= 0
\end{aligned}
$$

and the Hamiltonian operator, $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \frac{1}{2}k\hat{\mathbf{x}}^2$. The transformed Heisenberg equations of motion are

$$
\begin{aligned}
\frac{d\hat{x}_j}{dt} &= \frac{i}{\hbar}[\hat{H}, \hat{x}_j] \\
&= \frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2m} + \frac{1}{2}k\hat{\mathbf{x}}^2, \hat{x}_j\right] \\
&= \frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2m}, \hat{x}_j\right] \\
&= \frac{i\hat{p}_i}{m\hbar}\left[\hat{p}_i, \hat{x}_j\right] \\
&= -i\hbar\delta_{ij}\frac{i\hat{p}_i}{m\hbar} \\
&= \frac{\hat{p}_j}{m}
\end{aligned}
$$

and similarly

$$
\begin{aligned}
\frac{d\hat{p}_j}{dt} &= \frac{i}{\hbar}[\hat{H}, \hat{p}_j] \\
&= -k\hat{x}_j
\end{aligned}
$$

Quantum operators act on *states*. To define a complete set of states, we find the eigenstates of the Hamiltonian operator. This is simplified if we define new operators,

$$
\begin{aligned}
\hat{a}_i &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q}_i + \frac{i}{m\omega}\hat{p}_i\right) \\
\hat{a}_i^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q}_i - \frac{i}{m\omega}\hat{p}_i\right)
\end{aligned}
$$

Then the Hamiltonian is simply

$$
\hat{H} = \hbar\omega\left(\hat{a}_i^\dagger\hat{a}_i + \frac{1}{2}\right)
$$

and we have commutation relations,

$$
\begin{aligned}
\left[\hat{a}_i, \hat{a}_j^\dagger\right] &= \frac{m\omega}{2\hbar}\left[\left(\hat{q}_i + \frac{i}{m\omega}\hat{p}_i\right), \left(\hat{q}_j - \frac{i}{m\omega}\hat{p}_j\right)\right] \\
&= \frac{m\omega}{2\hbar}\frac{i}{m\omega}\left(-2i\hbar\hat{1}\delta_{ij}\right) \\
&= \hat{1}\delta_{ij} \\
[\hat{a}_i, \hat{a}_j] &= \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0
\end{aligned}
$$

From these relations we construct raising and lowering operators and find a complete set of states on which these operators act. Normally we are interested in eigenstates of the Hamiltonian, because these have a definite value of the energy. A complete treatment of the quantum mechanical simple harmonic oscillator is HERE.

1.3 Normal ordering

There is one point requiring caution with Dirac quantization: *ordering ambiguity.* The problem arises when the Hamiltonian (or any other dynamical variable of interest) depends in a more complicated way on position and momentum. The simplest example is a Hamiltonian containing a term of the form

$$H_1 = \alpha \mathbf{p} \cdot \mathbf{x}$$

For the classical variables, $\mathbf{p} \cdot \mathbf{x} = \mathbf{x} \cdot \mathbf{p}$, but since operators don't commute we don't know whether to write $\hat{H}_1 = \alpha \hat{\mathbf{p}} \cdot \hat{\mathbf{x}}$ or $\hat{H}_1 = \alpha \hat{\mathbf{x}} \cdot \hat{\mathbf{p}}$, or a linear combination

$$\hat{H}_1 = \frac{\alpha}{2} \left(\hat{\mathbf{p}} \cdot \hat{\mathbf{x}} + \hat{\mathbf{x}} \cdot \hat{\mathbf{p}} \right)$$

In many circumstances an equal linear combination turns out to be preferable, and certain rules of thumb exist.

Notice the effect of this prescription when a problem involves raising and lowering operators $\hat{a}_i, \hat{a}_j^\dagger$, as we found for the simple harmonic oscillator. Substituting

$$\begin{aligned} \hat{q}_i &= \frac{1}{\sqrt{2}} \left(\hat{a}_i + \hat{a}_i^\dagger \right) \\ \hat{p}_i &= \frac{i\hbar}{\sqrt{2}} \left(\hat{a}_i - \hat{a}_i^\dagger \right) \end{aligned}$$

into $\hat{H}_1$,

$$\begin{aligned} \hat{H}_1 &= \frac{\alpha}{2} \left(\hat{\mathbf{p}} \cdot \hat{\mathbf{x}} + \hat{\mathbf{x}} \cdot \hat{\mathbf{p}} \right) \\ &= \frac{\alpha}{2} \left(\frac{i\hbar}{\sqrt{2}} \left(\hat{a}_i - \hat{a}_i^\dagger \right) \cdot \frac{1}{\sqrt{2}} \left(\hat{a}_i + \hat{a}_i^\dagger \right) + \frac{1}{\sqrt{2}} \left(\hat{a}_i + \hat{a}_i^\dagger \right) \cdot \frac{i\hbar}{\sqrt{2}} \left(\hat{a}_i - \hat{a}_i^\dagger \right) \right) \\ &= \frac{\alpha}{2} \frac{i\hbar}{2} \left(\hat{a}_i \hat{a}_i + \hat{a}_i \hat{a}_i^\dagger - \hat{a}_i^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_i^\dagger + \hat{a}_i \hat{a}_i - \hat{a}_i \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_i^\dagger \right) \\ &= \frac{1}{2} i\hbar\alpha \left(\hat{a}_i \hat{a}_i - \hat{a}_i^\dagger \hat{a}_i^\dagger \right) \end{aligned}$$

we see that the ambiguous terms $\hat{a}_i \hat{a}_i^\dagger$ and $\hat{a}_i^\dagger \hat{a}_i$ have dropped out.

For commutators, this problem means that, unlike Poisson brackets, commutators are order-specific. Thus, we can write the Leibnitz rule as

$$\left[\hat{A}, \hat{B}\hat{C} \right] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$$

but must remember that

$$\left[\hat{A}, \hat{B}\hat{C} \right] \neq \left[\hat{A}, \hat{C} \right] \hat{B} + \left[\hat{A}, \hat{B} \right] \hat{C}$$

For now it is enough to be aware of the problem.

1.4 Schrödinger picture

The rules above reproduce the Heisenberg formulation, involving commutators. We can also arrive at the Schrödinger picture by choosing a set of *functions* as our vector space of states. Let $\psi(x)$ be an element of this vector space. Then we satisfy the fundamental commutators,

$$\begin{aligned} [\hat{p}_i, \hat{x}_j] &= -i\hbar\delta_{ij} \\ [\hat{x}_i, \hat{x}_j] &= 0 \\ [\hat{p}_i, \hat{p}_j] &= 0 \end{aligned}$$

if we represent the operators as

$$\begin{aligned} \hat{x}_i &= x_i \\ \hat{p}_i &= -i\hbar\frac{\partial}{\partial x_i} \\ \hat{H} &= i\hbar\frac{\partial}{\partial t} \\ &= \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}}) \end{aligned}$$

The representation of $\hat{x}_i$ by x_i simply means we replace the operator by the coordinate. Now consider the time evolution of a state ψ. This is given by the action of the Hamiltonian operator:

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

and we immediately recognize the Schrödinger equation. Inserting the form of $\hat{H}$, in terms of $\hat{x}_i$ and $\hat{p}_i$, then substituting the expressions above,

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{x})\psi = i\hbar\frac{\partial\hat{\psi}}{\partial t} \tag{4}$$

Notice that ψ is a field. This means that even in quantum *mechanics* we are working with a type of field theory. The difference between this field theory and "quantum field theory" lies principally in the way the operators are introduced. In quantum mechanics, the dynamical variables (energy, momentum, etc.) are parameterized by a single independent variable, time, but in quantum field theory the fields are parameterized by both space and time variables. In either case, we make the dynamical quantities into operators.

Other than the greater number of independent variables, the method for quantization is the same. We demand the usual fundamental canonical commutators for the field and the field momentum *density*. We will see all of this in detail before long.

2 Quantization of fields

We have introduced several distinct types of fields, with actions that give their field equations. These include scalar fields,

$$S = \frac{1}{2}\int \left(\partial^\alpha\varphi\partial_\alpha\varphi - m^2\varphi^2\right) d^4x \tag{5}$$

and complex scalar fields,

$$S = \frac{1}{2}\int \left(\partial^\alpha\varphi^*\partial_\alpha\varphi - m^2\varphi^*\varphi\right) d^4x \tag{6}$$

These are often called *charged scalar fields* because they have a nontrivial global $U(1)$ symmetry that allows them to couple to electromagnetic fields. Scalar fields have spin 0 and mass m.

The next possible value of $W^2 \sim J^2$ is spin-$\frac{1}{2}$, which is possessed by spinors. Dirac spinors satisfy the Dirac equation, which follows from the action

$$S = \int d^4x \; \bar{\psi} \left(i\gamma^\mu \partial_\mu - m \right) \psi \tag{7}$$

Once again, the mass is m. For higher spin, we have the zero mass, spin-1 electromagnetic field, with action

$$S = \int d^4x \; \left(\frac{1}{4} F^{\alpha\beta} F_{\alpha\beta} + J^\alpha A_\alpha \right) \tag{8}$$

Electromagnetic theory has an important generalization in the Yang-Mills field, $F^A{}_{\alpha\beta}$ where the additional index corresponds to an $SU(n)$ symmetry. We could continue with the spin-$\frac{3}{2}$ Rarita-Schwinger field and the spin-2 metric field, $g_{\alpha\beta}$ of general relativity. The latter follows the Einstein-Hilbert action,

$$S = \int d^4x \; \sqrt{-\det\left(g_{\alpha\beta}\right)} g^{\alpha\beta} R^\mu{}_{\alpha\mu\beta} \tag{9}$$

where $R^\mu{}_{\nu\alpha\beta}$ is the Riemann curvature tensor computed from $g_{\alpha\beta}$ and its first and second derivatives. However, we will be plenty busy quantizing the simplest examples: scalar, charged scalar, and Dirac fields.

We need the Hamiltonian formulation of field theory to do this properly, and that will require a bit of functional differentiation. It's actually kind of fun.

2.1 Canonical quantization of a field theory

While we go into more detail later, we can see some issues that arise in the quantization of a field theory. Consider the action for the relativistic scalar field ϕ. We will use Greek indices for spacetime $\alpha, \beta, \ldots = 0, 1, 2, 3$ and Latin for space $i, j, \ldots = 1, 2, 3$, so, for example, $\partial_\alpha = (\partial_0, \partial_i)$ where

$$\partial_0 = \frac{1}{c} \frac{\partial}{\partial t}$$

The metric,

$$\eta_{\alpha\beta} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$$

is used to raise and lower indices. For example, we can write the d'Alembertian $\Box$ as

$$\begin{aligned} \Box &= \eta^{\alpha\beta} \partial_\alpha \partial_\beta \\ &= \partial^\alpha \partial_\alpha = \partial_\alpha \partial^\alpha \end{aligned}$$

where

$$\partial^\alpha = \eta^{\alpha\beta} \partial_\beta = (\partial_0, -\partial_i)$$

With this notation, the action for the relativistic wave equation is

$$\begin{aligned} S &= \frac{1}{2} \int \partial_\alpha \phi \partial^\alpha \phi \; d^4x \\ &= \frac{1}{2} \int \left(\dot{\phi}^2 - \nabla\phi \cdot \nabla\phi \right) d^4x \end{aligned}$$

The relativistic summation convention *always* involves one raised index and one lowered index. When summed, repeated indices are both in the same position the sum is *Euclidean*. Thus, $\partial_\alpha \partial_\alpha = (\partial_0)^2 + \nabla^2$ is the 4-dimensional *Euclidean* Laplacian.

Now we can illustrate the quantization. In order to set up the canonical commutator we first require its conjugate momentum. This, as usual, is the derivative of the Lagrangian with respect to the "velocity", but in this case the Lagrangian is a *functional* of $\dot{\phi}$,

$$L = \frac{1}{2}\int \left(\dot{\phi}^2 - \nabla\phi\cdot\nabla\phi\right) d^3x$$

The derivative of a functional is called, naturally, the *functional derivative.* In the present case, it takes the form,

$$\begin{aligned}
\pi\left(x^i,t\right) &= \frac{\delta}{\delta\dot{\phi}\left(x^i,t\right)} L\left[\phi,\dot{\phi}\right] \\
&= \frac{1}{2}\frac{\delta}{\delta\dot{\phi}\left(x^i,t\right)}\int\left(\dot{\phi}^2\left(y^i,t\right) - \nabla\phi\left(y^i,t\right)\cdot\nabla\phi\left(y^i,t\right)\right) d^4y \\
&= \frac{1}{2}\left(\int 2\dot{\phi}\left(y^i,t\right)\frac{\delta\dot{\phi}\left(y^i,t\right)}{\delta\dot{\phi}\left(x^i,t\right)}\ d^3y\right) \\
&= \int\dot{\phi}\left(y^i,t\right)\delta^3\left(y^i-x^i\right)\ d^3y \\
&= \dot{\phi}\left(x^i,t\right)
\end{aligned}$$

The differentiation has given us a *momentum densit*y,

$$\pi = \partial^0\phi$$

where the total momentum is

$$p = \int \pi\ d^3x$$

The canonical commutator between the momentum and the field is

$$\left[\hat{p},\hat{\phi}\left(\mathbf{x}\right)\right] = -i\hbar$$

In terms of the density, this becomes

$$\int\left[\hat{\pi}\left(\mathbf{x}'\right),\hat{\phi}\left(\mathbf{x}\right)\right]\ d^3x = -i\hbar$$

which clearly is satisfied if we set

$$\left[\hat{\pi}\left(\mathbf{x}'\right),\hat{\phi}\left(\mathbf{x}\right)\right] = -i\hbar\delta^3(\mathbf{x}-\mathbf{x}')$$