# *Geometry, Topology, and Physics* Chapter 1: Quantum Physics

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# 1 Introduction

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# 2 Analytical Mechanics

## 2.1 Newtonian Mechanics

Let $\mathbf{x}(t)$ denote the position of a mass $m$ at time $t$. Suppose the particle is moving under an external force $\mathbf{F}(\mathbf{x})$. Then $\mathbf{x}(t)$ satisfies the second-order differential equation

$$m\frac{d^2\mathbf{x}(t)}{dt^2} = \mathbf{F}(\mathbf{x}(t)) \tag{1}$$

called **Newton's equation** or simply the **equation of motion**.

A **conserved force** is one that can be expressed as the gradient of a scalar function: $\mathbf{F}(\mathbf{x}) = -\nabla V(\mathbf{x})$ (the negative sign is present simply in order to use the physically-realized force $\mathbf{F}$ and scalar potential $V$ – mathematically it could be absorbed into $V$, and we'd recover the definition of a conservative vector field).

An example of a non-conserved force is friction: $F = -\eta \frac{dx}{dt}$.For a conserved force, the following scalar quantity is also conserved:

$$E = \frac{m}{2}\Big(\frac{d\mathbf{x}}{\mathbf{t}}\Big)^2 + V(\mathbf{x}) \tag{2}$$

In order to see this fact, we simply take the derivative of (2) with respect to time and use the equation of motion (1):

$$\frac{dE}{dt} = \sum_{k=1,2,3}\left[m\frac{dx_k}{dt}\frac{d^2x_k}{dt^2} + \frac{\partial V}{\partial x_k}\frac{dx_k}{dt}\right] = \sum_k\left(m\frac{d^2x_k}{dt^2} + \frac{\partial V}{\partial x_k}\right)\frac{dx_k}{dt} = 0 \tag{3}$$

where the last equality comes from (1). Of course, we can now *define* the quantity $E$ as the (mechanical) energy.

## 2.2 Lagrangian Formalism

As students of physics, we already know of the many difficulties working in the Newtonian formalism: vectors are difficult to work with (especially in a non-orthogonal coordinate system), second-order ODEs are not ideal if we can solve the problem with a first-order ODE, constraints are difficult to systematically take into account, etc. Perhaps the only convincing we need that we must search for a formalism beyond the Newtonian scheme is that quantum physics can't be directly derived from Newtonian mechanics. Thus, here we introduce the Lagrangian and Hamiltonian formalisms, starting with the former.

Consider a system whose state[1] is described by $N$ paramters $\{q_i\}_{i=1}^N$ in some space (really, manifold) $M$. $M$ is referred to as the **configuration space** of the **generalized coordinates** $\{q_i\}$.

Suppose a particle has a trajectory described by $q(t)$, $t \in [t_i, t_f]$ with $q(t_i) = q_i$ and $q(t_f) = t_f$. Then we can consider the functional

$$S[q(t), \dot{q}(t)] = \int_{t_i}^{t_f} L(q, \dot{q})dt \tag{4}$$

which we will define as the **action**. Nakahara makes the odd choice to define $S$ before we've defined the **Lagrangian** $L$ which shows up in the integrand of (4), but following his style, I will simply choose to state that the Lagrangian must be chosen such that **Hamilton's principle** (otherwise known as the **principle of least action**) is satisfied. This principle states that the physically realized trajectory[2] corresponds to an extremum of the action.

Let's see if we can get any mathematics to come from Hamilton's principle. Let $q(t)$ be a path that realizes the extremum of $S$ (this is, therefore, the physically-realized path). Consider now a variation $\delta q(t)$ of this trajectory such that $\delta q(t_i) = \delta q(t_f) = 0$ (i.e., $q_i$ and $q_f$ do not change). The reason for imposing this condition will become clear later. The action therefore changes under this variation by:

$$\begin{aligned}\delta S &= \int_{t_i}^{t_f} L(q+\delta q, \dot{q}+\delta\dot{q})dt - \int_{t_i}^{t_f} L(q,\dot{q}) \\ &= \int_{t_i}^{tf} \delta L \\ &= \int_{t_i}^{t_f} \Big(\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta\dot{q}\Big)dt \end{aligned} \tag{5}$$

Anticipating the result we wish to obtain, we will now use integration by parts on the second term in (5):

$$\int_{t_i}^{t_f} \frac{\partial L}{\partial \dot{q}}\delta\dot{q}dt = \delta q\frac{\partial L}{\partial \dot{q}}\Bigg|_{t_i}^{t_f} - \int_{t_i}^{t_f}\delta q\frac{d}{dt}\frac{\partial L}{\partial \dot{q}}dt = -\int_{t_i}^{t_f}\delta q\frac{d}{dt}\frac{\partial L}{\partial \dot{q}}dt \tag{6}$$

[1]The term *state* here is not well-defined. More often than not, generalized coordinates describe position in some way (whether that's linear displacement $x$, angular displacement $\theta$, or otherwise). The precise definition here is not as important as recognizing that generalized coordinates allow us to very easily and systematically eliminate the use of Cartesian coordinates (which can be inconvenient in certain contexts).

[2]It is worthwile mentioning that the action $S$ can in fact be defined for *any* trajectory, and this fact becomes relevant later.

We therefore see the reasoning behind that nebulous demand that $\delta q(t_i) = \delta q(t_f) = 0$: it is what gives the second equality in (6) so that we can plug this into (5) and recover:

$$\delta S = \int_{t_i}^{t_f} \Big(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\Big)\delta q dt \tag{7}$$

If you've never done this calculation, you may be wondering why equation (7) is so special. Here's the kicker: $q(t)$ realizes an extremum of $S$, so (7) must vanish. We therefore have derived the all-important **Euler-Lagrange equation**:

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0 \tag{8}$$

which can be generalized to $N$ degrees of freedom indexed by $k$ in the obvious way:

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} = 0 \tag{9}$$

A physicist may be inclined to write that $\frac{\delta S}{\delta q}$ is equivalent to the Euler-Lagrange equations. Indeed this is correct to some degree, but in order to make this notion rigorous, we employ the **functional derivative**. It is defined via

$$\frac{\delta f(t_2)}{\delta f(t_1)} = \delta(t_1 - t_2) \tag{10}$$

For our purposes, we have

$$\frac{\delta S[q,\dot{q}]}{\delta q(s)} \stackrel{\text{def}}{=} \lim_{\varepsilon \to 0} \frac{S[q(t) + \varepsilon\delta(t-s), \dot{q}(t) + \varepsilon \frac{d}{dt}\delta(t-s)] - S[q(t),\dot{q}(t)]}{\varepsilon} \tag{11}$$

where

$$\begin{aligned} S[q(t) + \varepsilon\delta(t-s), \dot{q}(t) + \varepsilon\frac{d}{dt}\delta(t-s)] &= \int dt L\Big(q(t) + \varepsilon\delta(t-s), \dot{q} + \varepsilon\frac{d}{dt}\delta(t-s)\Big) \\ &= \int dt L(q,\dot{q}) + \varepsilon \int dt\Big(\frac{\partial L}{\partial q}\delta(t-s) + \frac{\partial L}{\partial \dot{q}}\frac{d}{dt}\delta(t-s)\Big) + \mathcal{O}(\varepsilon^2) \\ &= S[q,\dot{q}] + \varepsilon\Big(\frac{\partial L}{\partial q}(s) - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}(s)\Big) + \mathcal{O}(\varepsilon^2) \end{aligned} \tag{12}$$

Thus we indeed see that the Euler-Lagrange equation may be written as

$$\frac{\delta S}{\delta q(s)} = \frac{\partial L}{\partial q}(s) - \frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}}\Big)(s) = 0 \tag{13}$$

Define the **conjugate momentum** as $\frac{\partial L}{\partial \dot{q}}$. A coordinate $q_k$ of which the Lagrangian is independent is called **cyclic**. The conjugate momentum to a cyclic coordinate is conserved. That is, if $q_k$ is cyclic, then

$$\frac{dp_k}{dt} = \frac{\partial L}{\partial q_k} = 0 \tag{14}$$

One last quick remark before we move onto Hamiltonians: If $Q(q)$ is an arbitrary function of $q$, then the Lagrangians $L$ and $L + dQ/dt$ yield the same Euler-Lagrange equation. I don't show this here, but Nakahara makes this very explicitly clear.

## 2.3 Hamiltonian Formalism

The Hamiltonian formalism discussed in this section offers several advantages over the Lagrangian formalism, most of which will be apparent later. Suffice to say that anyone with an elementary understanding of quantum mechanics understands the importance of the Hamiltonian.

Suppose a Lagrangian $L$ is given. Then the **Hamiltonian** (as a function of momentum $p$ and coordinate $q$) is defined by the Legendre transform:

$$H(q,p) \stackrel{\text{def}}{=} \sum_k p_k \dot{q}_k - L(q,\dot{q}) \tag{15}$$

Formally, note that we must require that the Jacobian satisfies

$$\det\left(\frac{\partial p_i}{\partial \dot{q}_j}\right) \neq 0 \tag{16}$$

Just as before with Hamilton's principle, we will consider an infinitesimal change (this time both in $q_k$ and $p_k$) in order to obtain some useful differential equations. In this case (excluding terms second-order in infinitesimal changes):

$$H(q+\delta q, p+\delta p) - H(q,p) = \sum_k \left(\dot{q}_k \dot{p}_k + \dot{q}_k \delta p_k + \delta \dot{q}_k p_k\right) + L(q,\dot{q}) - L(q+\delta q, \dot{q}+\delta\dot{q})$$

$$= \sum_k \left(\dot{q}_k \delta p_k + \delta \dot{q}_k p_k - \frac{\partial L}{\partial q_k}\delta q_k - \frac{\partial L}{\partial \dot{q}_k}\delta \dot{q}_k\right)$$

We could then go through the rigorous functional derivative calculations of (11)-(12) in order to show that

$$\frac{\partial H}{\partial p_k} = \dot{q}_k \tag{17}$$

$$\frac{\partial H}{\partial q_k} = -\frac{\partial L}{\partial q_k} = -\dot{p}_k \tag{18}$$

which are **Hamilton's equations of motion**.

Note that we define the space with coordinates $(q_k, p_k)$ as the **phase space**. Let $A(q,p)$ and $B(q,p)$ be two functions defined on the phase space of a Hamiltonian $H$. Then the Poisson bracket[3] is defined by

$$[A,B] \stackrel{\text{def}}{=} \sum_k \left(\frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k}\frac{\partial B}{\partial q_k}\right) \tag{19}$$

The Poisson bracket is a **Lie bracket**, meaning it satisfies linearity, skew-symmetry, and the **Jacobi identity**:

$$[[A,B],C] + [[B,C],A] + [[C,A],B] = 0 \tag{20}$$

as a general note: don't memorize this! Each term here is just one of the three cyclic permutations of $\{A, B, C\}$.

Clearly, the fundamental Poisson brackets are

$$[p_i, p_j] = [q_i, q_j] = 0 \tag{21}$$

$$[q_i, p_j] = \delta_{ij} \tag{22}$$

since in phase space, $q$ and $p$ are independent coordinates.

Let $A(q,p)$ be a physical quantity. Then its time derivative is given by

$$\frac{dA}{dt} = \sum_k \left(\frac{dA}{dq_k}\frac{dq_k}{dt} + \frac{dA}{dp_k}\frac{dp_k}{dt}\right)$$

$$= \sum_k \left(\frac{dA}{dq_k}\frac{\partial H}{\partial p_k} - \frac{dA}{dp_k}\frac{\partial H}{\partial q_k}\right)$$

$$= [A,H] \tag{23}$$

That is to say, **if** $[A,H]=0$, **then** $A$ **is conserved**.

[3] I generally prefer to use {} to denote the Poisson bracket since it gets promoted to the commutator [] in quantum mechanics, and I don't like to confuse the two (then again, {} could also be easily confused with the anticommutator which becomes much more important in quantum field theory).

**Theorem 1** (Noether's Theorem)**.** *Let $H(q_k, p_k)$ be a Hamiltonian that is invariant under the infinitesimal coordinate transformation $q_k \to q'_k = q_k + \varepsilon f_k(q)$. Then*

$$Q = \sum_k p_k f_k(q) \tag{24}$$

*is conserved.*

*Proof.* The Jacobian $\Lambda_{ij}$ (up to $\mathcal{O}(\varepsilon)$) associated with the $q_k \to q'_k$ is

$$\Lambda_{ij} = \frac{\partial q'_i}{\partial q_j} \simeq \delta_{ij} + \varepsilon \frac{\partial f_i(q)}{\partial q_j} \tag{25}$$

The momentum transforms as

$$p_i \to \sum_j p_j \Lambda^{-1}_{ji} \simeq p_i - \varepsilon \sum_j p_j \frac{\partial f_j}{\partial q_i} \tag{26}$$

Therefore:

$$\begin{aligned} 0 &= \delta H \\ &= \frac{\partial H}{\partial q_k} \varepsilon f_k(q) - \frac{\partial H}{\partial p_j} \varepsilon p_i \frac{\partial f_i}{\partial q_j} \\ &= \varepsilon \Big[ \frac{\partial H}{\partial q_k} f_k(q) - \frac{\partial H}{\partial p_j} p_i \frac{\partial f_i}{\partial q_j} \Big] \\ &= \varepsilon [H, Q] = \varepsilon \frac{dQ}{dt} \end{aligned} \tag{27}$$

which shows that $Q$ is conserved. ■

Maybe what we've just done doesn't seem significant, but it is arguably the greatest discovery in mathematical physics. Putting it simply: **conserved quantities leave the Hamiltonian invariant**. What's more is that the conserved quantity $Q$ is the **generator of the transformation** that leaves the Hamiltonian invariant. To see what we mean:

$$\begin{aligned} [q_i, Q] &= \sum_k \Big[ \frac{\partial q_i}{\partial q_k} \frac{\partial Q}{\partial p_k} - \frac{\partial q_i}{\partial p_k} \frac{\partial Q}{\partial q_k} \Big] \\ &= \sum_k \delta_{ik} f_k(q) = f_i(q) \end{aligned} \tag{28}$$

In other words, $\delta q_i = \varepsilon f_i(q) = \varepsilon [q_i, Q]$.

Perhaps this is a little too abstract, and you're having trouble visualizing what $Q$ would be in a physical example. Consider a particle $m$ moving in a two-dimensional plane with an axial symmetric potential $V(r)$. The Lagrangian (which, again, is simply defined so far as being the function which allows the action $S$ to satisfy the Euler-Lagrange equations in (9)) is

$$L(r, \theta) = \frac{1}{2} m(\dot{r}^2 + r^2 \dot{\theta}^2) - V(r) \tag{29}$$

and the conjugate momenta are

$$\begin{aligned} p_r &= m\dot{r} \\ p_\theta &= mr^2 \dot{\theta} \end{aligned} \tag{30}$$

so the Hamiltonian is

$$H = p_r \dot{r} + p_\theta \dot{\theta} - L = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + V(r) \tag{31}$$

Because $H$ is independent of $\theta$, it is invariant under the (infinitesimal) transformation

$$\theta \to \theta + \varepsilon \cdot 1 \tag{32}$$

which leaves $p_\theta$ invariant. Notice that $f(\theta) = 1$ in this case, so by Noether's Theorem, the quantity

$$Q = p_\theta \cdot 1 = mr^2 \dot{\theta} \tag{33}$$

is conserved. Indeed, this quantity is the angular momentum.

# 3 Canonical Quantization

## 3.1 Hilbert Space, Bras, and Kets

A **Hilbert space** $\mathscr{H}$ is a vector space defined over $\mathbb{C}$ that contains **ket vectors** (e.g., $|\psi\rangle$).

Define a **bra** $\langle\psi| : \mathscr{H} \to \mathbb{C}$ as a linear functional that sends kets to a complex number. Bras belong to the dual Hilbert space $\mathscr{H}^* \stackrel{\text{def}}{=} \{\chi : \mathscr{H} \to \mathbb{C} : \chi \text{ is linear}\}$. The action of a bra $\langle\phi|$on a ket $|\psi\rangle$ is denoted $\langle\phi|\psi\rangle$

Let $\{|e_1\rangle, |e_2\rangle, \dots\}$ be a basis of $\mathscr{H}$ (that is at most countably infinite by assumption). Thus any vector $|\psi\rangle \in \mathscr{H}$ can be expanded as $|\psi\rangle = \sum_k \psi_k |e_k\rangle$, where $\psi_k \in \mathbb{C}$ is the $k$-th component of $|\psi\rangle$. Now introduce the dual basis $\{\langle e_1|, \langle e_2|, \dots\} \subseteq \mathscr{H}^*$, where "**dual**" implies that

$$\langle e_i|e_j\rangle = \delta_{ij} \tag{34}$$

Let $\langle\alpha| \in \mathscr{H}^*$, and note that it can be written as $\langle\alpha| = \sum_k \alpha_k \langle e_k|$. Then

$$\langle\alpha|\psi\rangle = \sum_{ij} \alpha_i \psi_j \langle e_i|e_j\rangle = \sum_i \alpha_i \psi_i \tag{35}$$

i.e., we simply sum the product of each component of $\langle\alpha|$ and $|\psi\rangle$. Thus, if we define any dual vector $\langle\psi|$ to a ket $|\psi\rangle$ to take the complex conjugate of each component (i.e., if $|\psi\rangle = \sum_k \psi_k |e_k\rangle$, then $\langle\psi| = \sum_k \psi_k^* \langle e_k|$), then we see that a natural definition for a complex **inner product** on our Hilbert space emerges:

$$(|\phi\rangle, |\psi\rangle) \stackrel{\text{def}}{=} \langle\phi|\psi\rangle = \sum_k \phi_k^* \psi_k \tag{36}$$

Now that we have an inner product, we can also define the **norm** of a vector $|psi\rangle$:

$$\| |\psi\rangle \| \stackrel{\text{def}}{=} \sqrt{\langle\psi|\psi\rangle} \tag{37}$$

Finally, an inner product allows us to define an orthonormal basis (ONB) $\{|e_k\rangle\}$ such that $\langle e_i|e_j\rangle = \delta_{ij}$. We then see that

$$|\psi\rangle = \sum_k \psi_k |e_k\rangle = \sum_k \langle e_k|\psi\rangle |e_k\rangle = \sum_k |e_k\rangle \langle e_k|\psi\rangle \tag{38}$$

which implies that

$$\sum_k |e_k\rangle \langle e_k| = \mathbb{1} \tag{39}$$

If you are unfamiliar with (39), get used to it – introducing a **complete set of states** that sums to $\mathbb{1}$ is perhaps the single most-used trick[4] of physicists in quantum mechanics.

[4]The only trick?

## 3.2 Axioms of Canonical Quantization

Despite being a highly accurate model for reality, quantum mechanics is not yet proven in the rigorous mathematical sense. As such, we devise a set of five[5] axioms that quantum systems must follow:

1. There exists a Hilbert space $\mathscr{H}$ for a quantum system, and the state of the system is described by a vector $|\psi\rangle \in \mathscr{H}$. Moreover, $|\psi\rangle$ and $c\,|\psi\rangle$ ($c \in \mathbb{C}\backslash\{0\}$) describe the same state (we most often use this point for phase factors, i.e., $|c| = 1$).

2. A physical quantity $A$ in classical mechanics is replaced by a Hermitian operator $A : \mathscr{H} \to \mathscr{H}$[6]. The operator $A$ is called an **observable**, and the result obtained when making a measurement of $A$ is one of its eigenvalues (hermiticity guarantees that this is always a real number).

3. The Poisson bracket in CM is replaced by $-i/\hbar$ times the **commutator**:

$$[A, B] \stackrel{\text{def}}{=} AB - BA \tag{40}$$

   We will henceforth use $\hbar = 1$ units.

   The fundamental commutation relations are therefore

$$[q_i, q_j] = 0 \tag{41}$$
$$[p_i, p_j] = 0 \tag{42}$$
$$[q_i, p_j] = i\delta_{ij} \tag{43}$$

   and equation (23) becomes

$$\frac{dA}{dt} = \frac{1}{i}[A, H] \tag{44}$$

4. Let $|\psi\rangle \in \mathscr{H}$ be an arbitrary state. Suppose one prepares many systems, each of which is in this state. The observation of $A$ in these systems at time $t$ yields random results in general, and the expectation value of the results is

$$\langle A\rangle_t = \frac{\langle\psi|A(t)|\psi\rangle}{\langle\psi|\psi\rangle} \tag{45}$$

5. For any physical state $|\psi\rangle \in \mathscr{H}$, there exists an observable[7] for which $|\psi\rangle$ is one of the eigenstates.

Let's look at Axiom 4. Suppose that $|\psi\rangle \in \mathscr{H}$ is normalized as $\langle\psi|\psi\rangle = 1$, and suppose that $\{|n\rangle\}$ is an ONB[8] for an observable $A(t)$ with associated *discrete* eigenvalues $\{a_n\}$. Then the expectation value $A$ in $|\psi\rangle$ is

$$\langle\psi|A(t)|\psi\rangle = \sum_{m,n} \psi_m^* \psi_n \langle m|A(t)|n\rangle = \sum_n a_n |\psi_n|^2 \tag{46}$$

where we see that we have defined

$$|\psi_n|^2 = |\langle n|\psi\rangle|^2 \tag{47}$$

as the **probability** that $|\psi\rangle$ exists in state $|n\rangle$ (since this would produce the value of $a_n$ that appears in (46)). Thus, the quantity $\langle n|\psi\rangle$ is known as the **probability amplitude**

What if the spectrum of $A$ is not discrete but rather continuous? Let $a$ be the index of this continuous set of eigenvalues/eigenvectors, and write

$$|\psi\rangle = \int da\psi(a)\,|a\rangle = \int da\,|a\rangle\,\langle a|\psi\rangle \tag{48}$$

[5]Typically there are 4 listed axioms, but I'm a big fan of Nakahara's additional axiom.
[6]I am choosing to omit hats on all of my operators. It should always be clear from context what I mean.
[7]While Nakahara uses the term "operator" in this context, it's worth noting that he is referring to observables.
[8]Since $A$ is hermitian, we can always choose a basis such that $\{|n\rangle\}$ is orthonormal (Spectral Theorem).

Thus our completeness relation analogous to (39) is

$$\int da\,|a\rangle\,\langle a| = \mathbb{1} \tag{49}$$

A consequence of (49) is that $\int da'\,|a'\rangle\,\langle a'|a\rangle = |a\rangle$, so $\langle a'|a\rangle = \delta(a'-a)$, the Dirac $\delta$ function. Now write the analogue to (46):

$$\langle\psi|A|\psi\rangle = \int a|\psi(a)|^2 da \tag{50}$$

which implies that the probability that a measured value of $A$ is in the interval $[a, a+da]$ is $|\psi(a)|^2 da$. Therefore, in the continuous case, the **probability density** is

$$\rho(a) = |\,\langle a|\psi\rangle\,|^2 \tag{51}$$

Notice that the role of the probability in the discrete case is replaced by the probability density in the continuous case!

As for why we need Axiom 5, we already saw that in the discrete case, the probability of $|\psi\rangle$ to be in the state of some observable's eigenstate $|n\rangle$ is $|\,\langle n|\psi\rangle\,|$. Axiom 5 assures us that we can replace $|n\rangle$ with any arbitrary $|\phi\rangle \in \mathscr{H}$.

### 3.3 Heisenberg and Schrödinger

It is straightforward to check that the solution to (44) is

$$A(t) = e^{iHt}A(0)e^{-iHt} \tag{52}$$

where it is worth noting that the operator $U(t) = e^{-iHt}$ is unitary. In this **Heisenberg picture**, we see that the operator takes on the time-dependence instead of the state. We can instead take the expectation value of (52) with respect to some state $|\psi\rangle$ and define

$$|\psi(t)\rangle \stackrel{\text{def}}{=} e^{-iHt}\,|\psi\rangle \tag{53}$$

Then

$$\langle A(t)\rangle = \langle\psi(t)|A(0)|\psi(t)\rangle \tag{54}$$

which is referred to as the **Schrödinger picture**, where the states take on time-dependence instead of the operators.

Now it may have been a seemingly-arbitrary definition, but differentiating (53) with respect to $t$ gives us the most well-known equation in all of quantum mechanics: the **Schrödinger equation**:

$$i\frac{d}{dt}\,|\psi(t)\rangle = H\,|\psi(t)\rangle \tag{55}$$

### 3.4 The Wavefunction

Consider a particle moving on the real line $\mathbb{R}$, and let $x$ be the position operator with eigenvalue $x$ and eigenvector $|x\rangle$: $x\,|x\rangle = x\,|x\rangle$. Assume standard normalization: $\langle x|y\rangle = \delta(x-y)$. Similarly let $q$ and $|q\rangle$ be the eigenvalue/vector of the momentm operator $p$. We weren't very explicit about it, but we can see from (48) that $\psi(x) = \langle x|\psi\rangle$ for some $|\psi\rangle \in \mathscr{H}$ is the component of $|\psi\rangle$ in the $|x\rangle$ basis; i.e.,

$$|\psi\rangle = \int dx\,|x\rangle\,\langle x|\,|\psi\rangle = \int dx\,|x\rangle\,\psi(x) \tag{56}$$

where the coefficient $\psi(x) \in \mathbb{C}$ is the **wavefunction**. From our discussion of the axioms, we see that it is the probability amplitude of finding a particle in the state $|\psi\rangle$ at position $x$. Thus:

$$\int dx|\psi(x)|^2 = |\psi|\psi\rangle = 1 \tag{57}$$

Notice then that the inner product between arbitrary vectors $|\psi\rangle, |\phi\rangle \in \mathscr{H}$ is

$$\langle\psi|\phi\rangle = \int dx \,\langle\psi|x\rangle \langle x|\phi\rangle = \int dx \psi^*(x)\phi(x) \tag{58}$$

where we've once again simply applied the completeness relation in (49) (see footnote 4 on page 6). We can also see rather easy that $\langle x|x|\psi\rangle = x\langle x|\psi\rangle = x\psi(x)$, which will be handy to know for future calculations.

**Lemma 1.** *The unitary operator*

$$U(a) = e^{-iap}$$

*satisfies*

$$U(a)|x\rangle = |x+a\rangle \tag{59}$$

*Proof.* Given in Nakahara. It's worthwile to go through the calculation, but doing so is not necessary here. The key fact used is that $[x, p^n] = inp^{n-1}$ which easily follows from induction. ■

The main point of Lemma 1 is that *momentum is the generator of translations.*

We can now consider an infinitesimal translation $\varepsilon$:

$$U(\varepsilon)|x\rangle = |x+\varepsilon\rangle \simeq (1 - i\varepsilon p)|x\rangle \tag{60}$$

Thus

$$p|x\rangle = \frac{|x+\varepsilon\rangle - |x\rangle}{-i\varepsilon} \xrightarrow{\varepsilon\to 0} i\frac{d}{dx}|x\rangle \tag{61}$$

and taking the hermitian conjugate gives

$$\langle x|p = \frac{\langle x+\varepsilon| - \langle x|}{i\varepsilon} \xrightarrow{\varepsilon\to 0} -i\frac{d}{dx}\langle x| \tag{62}$$

It immediately follows from (62) that

$$\langle x|p|\psi\rangle = -i\frac{d}{dx}\langle x|\psi\rangle = -i\frac{d}{dx}\psi(x) \tag{63}$$

which is often written as

$$p \xrightarrow{x \text{ basis}} -i\frac{d}{dx} \tag{64}$$

**Proposition 1.** *The following hold:*

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}e^{ipx} \tag{65}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}}e^{-ipx} \tag{66}$$

Nakahara proves (65), so we will prove (66). Before we do so, however, we need to do Exercise 1.2:

**Exercise** (1.2)**.** *Firstly, $p|p\rangle = p|p\rangle$ is a defining equation we can take as fact. Second, consider:*

$$\langle x|x|p\rangle = \frac{x}{\sqrt{2\pi}}e^{ipx} \tag{67}$$

*and*

$$\langle x|\Big(-i\frac{d}{dp}\Big)|p\rangle = -i\frac{d}{dp}\langle x|p\rangle = \frac{x}{\sqrt{2\pi}}e^{ipx} \tag{68}$$

*where we can pull out the derivative in the first equality of (68) since $\frac{d}{dp}\langle x| = 0$ (since $p$ and $x$ are independent variables in phase space). The equality of (67) and (68) proves that*

$$x|p\rangle = -i\frac{d}{dp}|p\rangle \tag{69}$$

*Taking the hermitian conjugate of (69) and multiplying by $|\psi\rangle$ gives $\langle p|x|\psi\rangle = -\frac{d}{dp}\psi(p)$, and doing the same to $p|p\rangle = p|p\rangle$ gives $\langle p|p|\psi\rangle = p\psi(p)$.*

Now that we've proven some useful identities in momentum space, we can prove equation (66).

*Proof.* We could simply take the complex conjugate of (65), but perhaps it's more instructive to go through a proof.

We consider the quantity

$$\langle p|x|x\rangle = x\,\langle p|x\rangle = i\frac{d}{dp}\,\langle p|x\rangle$$

which is a simple ODE with solution

$$\langle p|x\rangle = Ce^{-ipx}$$

As always, we fix the constant $C$ via normalization:

$$\begin{aligned}\delta(p-q) = \langle p|q\rangle &= \int dx\,\langle p|x\rangle\,\langle x|q\rangle \\ &= \int dx|C|^2 e^{-ix(p-q)} \\ &= |C|^2 2\pi\delta(p-q)\end{aligned} \tag{70}$$

where we can now assume $C \in \mathbb{R}$, so $C = 1/\sqrt{2\pi}$. ■

Proposition 1 is powerful because it tells us that $\psi(p) = \langle p|\psi\rangle$ is simply the Fourier Transform of $\psi(x)$:

$$\psi(p) = \langle p|\psi\rangle = \int dx\,\langle p|x\rangle\,\langle x|\psi\rangle = \int dx\frac{1}{\sqrt{2\pi}}e^{-ipx}\psi(x) \tag{71}$$

By projecting the Schrödinger equation (55) into the $x$ basis and solving the PDE via separation of variables (i.e., assuming that $\psi(x,t) = T(t)X(x)$), we can obtain the **time-independent Schrödinger equation**. In 3d:

$$-\frac{1}{2m}\nabla^2 X(\mathbf{x}) + V(\mathbf{x})X(\mathbf{x}) = EX(\mathbf{x}) \tag{72}$$

where $E$ is the energy eigenvalue of the Hamiltonian given by $H = -\frac{1}{2m}\nabla^2 + V(\mathbf{x})$. This gives the spatial dependence of $\psi(x,t)$, and the time dependence is given by

$$T(t) = e^{-iEt} \tag{73}$$

### 3.5 The Harmonic Oscillator

Perhaps the most instructive and useful model for nonrelativistic quantum mechanics is the harmonic oscillator. This is due to the harmonic oscillator's quadratic potential energy term, meaning that if a theory has a local minimum, we can use the harmonic oscillator to approximate a solution. Furthermore, the harmonic oscillator is exactly solvable.

The Hamiltonian for the harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{74}$$

After a change of variables, $\xi = x\sqrt{m\omega}$ and $\varepsilon = E/\omega$, the time-independent Schrödinger equation is

$$\psi'' + (\varepsilon - \xi^2)\psi = 0 \tag{75}$$

This ODE is more difficult than it looks. Any good quantum mechanics textbook will flesh out the full details, but here I will simply outline its solution[9]. We start with the following ansatz:

$$\psi(\xi) = R(\xi)u(\xi) \tag{76}$$

[9] Nakahara omits all of these details, but I think that given the importance of the solution, especially for the energy spectrum, it's worth seeing how it comes about.

where $u(\xi)$ is an asymptotic solution, and $R(\xi)$ is a polynomial. We begin with solving for $u(\xi)$. The asymptotic form of (75) is

$$u'' - \xi^2 u = 0$$

which is still somewhat formidable. Consider a varied version of (77):

$$u'' - \gamma\xi u - \xi^2 u = 0 \tag{77}$$

which has the benefit of still yielding a valid $u$ since our solution need only be asymptotically exact, and the added $\gamma\xi u$ term is nonleading for large $\xi$. Equation (78) can be easily solved with the following ansatz: $u(\xi) = \exp(\sum_{n=0}^{\infty} \alpha_n \xi^n)$:

$$\frac{d^2u}{d\xi^2} = u(\xi)\bigg(\sum_n n(n-1)\xi^{n-2} + \Big(\sum_n n\alpha_n \xi^{n-1}\Big)^2\bigg)$$

Why is (79) helpful? By comparing with (78), we see that we are permitted powers of $\xi$ no greater than 2! Therefore, only the $n = 0$, $n = 1$, and $n = 2$ terms survive in our ansatz. Furthermore, the coefficient of the $\xi^2$ term must be one. Thus:

$$1 = (2\alpha_2)^2 \Rightarrow \alpha_2 = \pm\frac{1}{2}$$

We will choose $\alpha_2 = -1/2$ and therefore obtain $u(\xi) = \exp(\alpha_0 + \alpha_1\xi - \xi^2/2)$. The $\alpha_0$ term is a constant that will be fixed by normalzation, and the $\alpha_1$ term can be ignored since it is subleading and is incompatible with the reflection symmetry of the harmonic potential. Therefore:

$$u(\xi) = e^{-\xi^2/2} \tag{78}$$

Thus, the wavefunction of the harmonic oscillator is asymptotically Gaussian.

In order to determine $R(\xi)$, we assume a power series ansatz and plug in $\psi = Ru$ into (75). If we write $R(\xi) = \sum_n a_n \xi^n$, then we obtain the recursion relation:

$$a_{n+2} = \frac{1 + 2n - 2\varepsilon}{(n+1)(n+2)} a_n \tag{79}$$

where we see that $a_{n+2}/a_n \sim 2/n$. Therefore, for $R$ to converge, we need this power series to terminate; i.e., we need a value of $n$ such that $1 + 2n - 2\varepsilon = 0$, or:

$$\varepsilon = n + \frac{1}{2} \tag{80}$$

which therefore means that our eigenenergies are

$$E_n = \Big(n + \frac{1}{2}\Big)\omega \tag{81}$$

where $n = 0, 1, 2, \ldots$. Given this condition on the power series coefficients, $R(\xi)$ is given by the Hermite polynomials $H_n(\xi)$. Thus, the solution to the harmonic oscillator is

$$\psi(\xi) = \sqrt{\frac{m\omega}{2^n n! \sqrt{\pi}}} H_n(\xi) e^{-\xi^2/2} \tag{82}$$

We can alternatively analyze the harmonic oscillator via the **creation operator** $a^\dagger$ and **annihilation operator** $a$:

$$a = \sqrt{\frac{m\omega}{2}} x + i\sqrt{\frac{1}{2m\omega}} p \tag{83}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2}} x - i\sqrt{\frac{1}{2m\omega}} p \tag{84}$$

as well as the **number operator**

$$N = a^\dagger a \tag{85}$$

It is straightforward to show that $[a, a^\dagger] = 1$, $[N, a] = -a$, $[N, a^\dagger] = a^\dagger$, and $H = (N + \frac{1}{2})\omega$. If $|n\rangle$ is a normalized eigenvector of $N$:

$$N|n\rangle = n|n\rangle \tag{86}$$

then it is also straightforward to determine the action of the annihilation and creation operators on $|n\rangle$ using commutation relations:

$$\begin{aligned} N(a|n\rangle) &= (aN - a)|n\rangle = (n-1)(a|n\rangle) \\ N(a^\dagger|n\rangle) &= (a^\dagger N + a^\dagger)|n\rangle = (n+1)(a^\dagger|n\rangle) \end{aligned}$$

which shows that $a|n\rangle = \beta_n|n-1\rangle$ and $a^\dagger|n\rangle = \gamma_n|n+1\rangle$, where $\beta_n$ and $\gamma_n$ are constants that can be obtained via:

$$\begin{aligned} \|a|n\rangle\|^2 &= \langle n|a^\dagger a|n\rangle = n = \beta_n^2 \\ \|a^\dagger|n\rangle\|^2 &= \langle n|aa^\dagger|n\rangle = \langle n|(1 + a^\dagger a)|n\rangle = n + 1 = \gamma_n^2 \end{aligned}$$

Thus:

$$a|n\rangle = \sqrt{n}|n-1\rangle \tag{87}$$
$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{88}$$

Furthermore, the harmonic oscillator has a ground state given by $n = 0$ and $a|0\rangle = 0$ since, according to (87), $n = \|a|n\rangle\|^2 \geq 0$, so by contradiction, we cannot further lower the state $|0\rangle$ in order to obtain $n < 0$.

**Exercise** (1.4)**.** *Straightforward induction shows that*

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle \tag{89}$$

*is valid way to write the state $|n\rangle$. Before we show the main result, we use induction to prove the intermediate result: $N(a^\dagger)^n = (a^\dagger)^n N + n(a^\dagger)^n$. The base case $n = 0$ is trivially true, and if we assume the induction hypothesis is true, then we see that*

$$\begin{aligned} N(a^\dagger)^{n+1} = N(a^\dagger)^n a^\dagger &= (a^\dagger)^n N a^\dagger + n(a^\dagger)^{n+1} \\ &= (a^\dagger)^{n+1} N + (n+1)(a^\dagger)^{n+1} \end{aligned}$$

*which completes the proof of our intermediate result by the Principle of Mathematical Induction.*

*Using this result, we can now use induction to show that $N|n\rangle = n|n\rangle$. Once again, the base $n = 0$ case is trivial, so assuming the induction hypothesis allows us to write:*

$$\begin{aligned} N|n+1\rangle &= N\left(\frac{1}{\sqrt{(n+1)!}}(a^\dagger)^{n+1}|0\rangle\right) \\ &= \frac{1}{\sqrt{(n+1)!}}\Big((a^\dagger)^{n+1}N + (n+1)(a^\dagger)^{n+1}\Big)|0\rangle \\ &= \frac{n+1}{\sqrt{(n+1)!}}(a^\dagger)^{n+1}|0\rangle \\ &= (n+1)|n+1\rangle \end{aligned} \tag{90}$$

*which completes the proof.*

*For normalization, we note that*

$$a^n (a^\dagger)^n = n! + A_n \tag{91}$$

*where $A_n$ is a nontrivial linear combination of $a$'s and $a^\dagger$'s of the form $(a^\dagger)^p a^q$; i.e.,* ***with the annihilation operator*** *$a$* ***following the creation operator*** *$a^\dagger$*[10]*. This means that when we do the operation $\langle 0 | a^n (a^\dagger)^n | 0 \rangle$, we see that it is equal to $n! + \langle 0 | A_n | 0 \rangle = n!$ (since $a\,|0\rangle = 0$). Thus*

$$\langle n | n \rangle = \frac{1}{n!} \langle 0 | a^n (a^\dagger)^n | 0 \rangle = 1 \tag{92}$$

*completing the proof.*

We therefore see that the spectrum of $N$ is given by $\{0, 1, 2, \dots\}$, so the spectrum of $H$ is $\{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots\}$.

# 4 Path Integral Quantization of a Bose Particle

[10] I don't prove this here since it's something of a headache to do so. I would appreciate if someone had a relatively short proof of this fact.