Lecture 1: Review of Quantum Mechanics

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Hermitian (self-adjoint) operators on a Hilbert space are a key concept in QM.

In classical mechanics, an observable is a real-valued quantity that may be measured from a system. Examples are position, momentum, energy, angular momentum.

In QM, a state of the system is a vector in a Hilbert space. Every classical observable *A* has a QM counterpart \widehat{A} that is a Hermitian (self-adjoint) operator. Before discussing QM we discuss operators.

Hermitian operators

If \mathfrak{H} is a Hilbert space, a bounded operator *T* is an endomorphism of \mathfrak{H} such that $|T(v)| \leq c|v|$ for some constant *c*. The minimum value of *c* is the norm |T|.

If $y \in \mathfrak{H}$ the functional $x \to \langle Tx, y \rangle$ is bounded, i.e. there is a constant *c* with $\langle Tx, y \rangle \leq c|x|$. (*c*=|*T*| will work.) By the Riesz representation theorem there exists $T^{\dagger}y$ such that

$$\langle Tx, y \rangle = \langle x, T^{\dagger}y \rangle.$$

Then T^{\dagger} is the adjoint of *T*. If $T = T^{\dagger}$ then *T* is called Hermitian (or self-adjoint).

Unbounded operators

We will also encounter unbounded operators on a Hilbert space \mathfrak{H} . An unbounded operator *T* is defined on a dense linear subspace $D \subset \mathfrak{H}$.

Let

 $D^{\dagger} = \{y \in \mathfrak{H} | x \mapsto (Tx, y) \text{ is bounded on } D\}.$

The adjoint T^{\dagger} is then defined on D^{\dagger} by

$$(Tx, y) = (x, T^{\dagger}y).$$

Since *D* is dense, $T^{\dagger}y$ is uniquely determined. *T* is symmetric if $D \subseteq D^*$ and $T^* = T$ on *D*. Thus

$$(Tx, y) = (x, Ty), \qquad x, y \in D.$$

Then *T* is Hermitian if $D^* = D$ and $T^* = T$.

Spectral theorem

Let $T: D \to \mathfrak{H}$ be an unbounded Hermitian operator. The spectrum *T* is the set of $\lambda \in \mathbb{C}$ such that $\lambda I - T$ does not have a bounded inverse. This implies that λ is real.

If *T* is a Hermitian unbounded operator, then there is a spectral theorem. First assume that the spectrum is discrete. Let λ_i be the eigenvalues of *T*. Then if *v* is in the spectrum, it is an eigenvector. Thus when the spectrum is discrete the spectrum is the set { λ_i } of eigenvalues. The spectral theorem in this case asserts that every $v \in \mathfrak{H}$ has an eigenvector expansion:

$$v = \sum_{i} v_i, \qquad Tv_i = \lambda_i v_i.$$

If the spectrum is not assumed discrete, there is still a spectral theorem but we will not formulate it.

Self-adjoint extensions

The spectral theorem applies to self-adjoint operators, not symmetric operators. So it is worth noting that every symmetric operator has a self-adjoint extension. That is, we can enlarge the domain D to obtain a Hermitian operator.

Many operators can be defined with domain the Schwartz space $S(\mathbb{R})$ consisting of functions f such that f and all its derivatives $f^{(n)}$ are of faster than polynomial decay. $S(\mathbb{R})$ has a topology as a Frechet space, and a continuous linear functional is called a tempered distribution.

Continuous spectrum: position and momentum

We consider the following unbounded operators on $\mathfrak{H} = L^2(\mathbb{R})$. Both will have domain initially $S(\mathbb{R})$.

$$\widehat{q}f(x) = xf(x), \qquad \widehat{p}f(x) = -i\hbar f'(x).$$

These are symmetric operators. For \hat{q} , this is easy. for \hat{p} , it follows by integration by parts: if f_1 and f_2 are Schwartz functions then

$$(\widehat{p}f_1, f_2) = -i\hbar \int_{-\infty}^{\infty} f_1'(x)\overline{f_2(x)} \, dx = i\hbar \int_{-\infty}^{\infty} f_1(x)\overline{f_2'(x)} \, dx = (f_1, \widehat{p}f_2).$$

The spectrum of both \hat{q} (position) and \hat{p} (momentum) are all of \mathbb{R} , and they have no eigenvectors in \mathfrak{H} . However they have eigenfunctions in the space of tempered distributions: $\delta(x-a)$ for \hat{q} , and e^{iax} for \hat{p} .

The oscillator Hamiltonian

Although the unbounded operators \hat{q} and \hat{p} do not have a discrete spectrum, by contrast (taking $\hbar = 1$) consider the Hamiltonian of the harmonic oscillator:

$$\widehat{H} = \frac{1}{2}(\widehat{p}^2 + \widehat{q}^2) = \frac{1}{2}\left(x^2 - \frac{d^2}{dx^2}\right)$$

This operator does have a discrete spectrum

$$\left\{\frac{1}{2},\frac{3}{2},\frac{5}{2},\cdots\right\}.$$

The eigenstate of the lowest eigenvalue $\frac{1}{2}$ is

$$\psi_{1/2} = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$

If $\psi_{k+1/2}$ ($k = 0, 1, 2, \cdots$) is the $k + \frac{1}{2}$ -eigenvector of norm 1, then the $\psi_{k+1/2}$ are an orthonormal basis of $L^2(\mathbb{R})$.

Proofs

To derive the properties of the oscillator Hamiltonian, introduce the creation and annihilation operators

$$a = rac{1}{\sqrt{2}}(\hat{q}+i\hat{p}), \qquad a^{\dagger} = rac{1}{\sqrt{2}}(\hat{q}-i\hat{p}).$$

Since \hat{q} and \hat{p} are Hermitian, *a* and a^{\dagger} are adjoints. They are not Hermitian, so when they arise in QM they are not observables. As we will see they give a "ladder" relating the different eigenfunctions of \hat{H} .

$$0 \xleftarrow{a} \psi_{1/2} \xleftarrow{a^{\dagger}}{a} \psi_{3/2} \xleftarrow{a^{\dagger}}{a} \psi_{5/2} \xleftarrow{a^{\dagger}}{a} \cdots$$

Proofs (continued)

Denote $N = a^{\dagger}a$. This is obviously self-adjoint and positive definite. Using $[\hat{q}, \hat{p}] = i$

$$[a, a^{\dagger}] = 1, \qquad \widehat{H} = \frac{1}{2}(aa^{\dagger} + a^{\dagger}a) = N + \frac{1}{2}.$$

Since *N* is positive-definite, the spectrum of *H* is bounded below by $\frac{1}{2}$. We can exhibit one eigenfunction

$$\psi_{1/2}(x) = \pi^{-1/4} e^{-x^2/2}, \qquad N\psi_{1/2} = 0, \qquad \widehat{H}\psi_{1/2} = \frac{1}{2}\psi_{1/2}.$$

Proofs (continued)

The eigenfunctions of N must be nonnegative integers by the following argument. We have

$$Na = a(N-1)$$

which implies that if Nv = kv then Nav = (k - 1)av. Unless *k* is a positive integer, we may repeatedly apply *a* and obtain an eigenvector with negative eigenvalue, a contradiction since *N* is positive definite.

On the other hand, using the identity

$$Na^{\dagger} = a^{\dagger}(N-1)$$

applying a^{\dagger} increases the eigenvalue of N (or of \hat{H}) by 1.

Proofs (continued)

We have

$$(a^{\dagger}\psi, a^{\dagger}\psi) = (\psi, N\psi)$$

from which we see that the eigenfunctions

$$\psi_{n+1/2}(x) = \frac{1}{\sqrt{n!}} (a^{\dagger})^n \psi_{1/2}$$

are orthonormal. In terms of the Hermite polynomials H_n we have

$$\psi_{n+1/2}(x) = \left(\sqrt{\pi}2^n n!\right)^{-1/2} H_n(x) e^{-x^2/2}$$

These are an orthonormal basis of $L^2(\mathbb{R})$. See Messiah, Quantum Mechanics Chapter XII and Appendix B.

(Note: there are different normalizations for Hermite polynomials in the literature.)

Amplitudes

A basic concept in QM is that of an amplitude. In a nutshell, an amplitude is a complex number *a* such that $|a|^2$ is the probability (density) of an event, say the probability that measuring a quantity *q* returns the value *x*. Thus a = a(x) depends on *x*.

If *X* is the measure space of all possible values of *a*, then since $|a(x)|^2$ is a probability, we must have

$$\int_X |a(x)|^2 \, dx = 1.$$

Thus $a \in L^2(X)$. We already see that QM will involve Hilbert space.

Bra-Ket notation

The bra-ket notation was invented by Dirac. In mathematics it is customary for an inner product (,) to be linear in the first component and anti linear in the second. In physics the expression $\langle x|y \rangle$ is linear in the second component and antilinear in the second. So

$$\langle x|y\rangle = (y,x).$$

If $x \in \mathfrak{H}$ we denote $|x\rangle = x$; in this notation $|x\rangle$ is called a ket.

Let \mathfrak{H}^* be the Hilbert space dual of bounded linear functionals on \mathfrak{H} . As a real vector space it is isomorphic to \mathfrak{H} . Indeed the Riesz representation theorem asserts that every bounded linear functional on \mathfrak{H} is of the form $x \mapsto (x, y) = \langle y | x \rangle$ for some $y \in \mathfrak{H}$. Denote this functional $\langle y | \in \mathfrak{H}^*$. It is called a bra.

QM systems

A quantum mechanical system presupposes a Hilbert space \mathfrak{H} . A vector v of length 1 in \mathfrak{H} determines a state of the system. Note what happens to amplitudes when we multiply the vector representing the vector v by a complex number λ of absolute value 1. The amplitude a is replaced by λa but its probabilistic interpretation that $|a|^2$ is a probability (or probability density) is unchanged. Since all physical meaning of the state v is derived from the amplitudes, the physical meaning of the state is unchanged.

Thus a state of the system is a ray in \mathfrak{H} , that is, a one-dimensional subspace. By the above all vectors of length 1 in the ray have the same physical meaning, this is reasonable.

Classical limit

Quantum mechanics depends on a quantity \hbar , Planck's constant. Classical Mechanics, which in its simplest form is Newton's law F = ma (force equals mass times acceleration) is the limiting theory $\hbar \rightarrow 0$. Since \hbar is small compared to the observer, the universe appears to the observer to obey the laws of classical mechanics.

There is another parameter c that appears in both quantum and classical mechanics. This is the speed of light. The limit $c \to \infty$ is nonrelativistic (classical or quantum) mechanics. Our first examples will be nonrelativistic but ultimately one must find relativistic formulations.

Observables

Given a classical system, there should be a corresponding QM system. In many cases this can be obtained by applying a simple recipe. Let \mathfrak{H} be the underlying Hilbert space of the QM system.

In classical mechanics, an observable is a real-valued quantity A that can be measured from the state of a system. But in QM an observable is a Hermitian operator \widehat{A} on \mathfrak{H} .

Now if we can find a state $\phi \in \mathfrak{H}$ that is an Eigenvector of \widehat{A} , say $\widehat{A}\phi = \lambda\phi$ then λ is real since \widehat{A} is Hermitian (self-adjoint). In this case the observable *A* has a definite value, λ . That means that if the observable *A* is measured the value will be λ , with probability 1.

Eigenfunction expansions

Let us consider the case where \widehat{A} has discrete spectrum. This means that there is a sequence $\lambda_1 < \lambda_2 < \cdots$ of eigenvalues such that

$$\mathfrak{H} = \bigoplus V_{\lambda_i}$$

where V_i is the λ_i -eigenspace. Given a state ϕ we expand $\phi = \sum_i a_i \phi_i$ where $\phi_i \in V_i$. Then a_i is the amplitude of obtaining the value λ_i on measuring A, so $|a_i|^2$ is the probability of this measurement. Note that

$$\sum |a_i|^2 = |\varphi|^2 = 1,$$

as required by this probabilistic interpretation.

Commuting operators

Suppose that *A* and *B* are observables whose corresponding operator \widehat{A} and \widehat{B} commute. Then each \widehat{A} eigenspace is invariant under \widehat{B} so the two operators can be simultaneously diagonalized. This means that \mathfrak{H} has a basis of elements that are simultaneously eigenvectors for both operators, that is, for which both observables have definite values. The converse is also obviously true: if such a basis exists then \widehat{A} and \widehat{B} commute.

In terms of measurements, this means that \widehat{A} and \widehat{B} commute if and only if the observables A and B can be measured simultaneously. An example of operators that do not commute are the angular momenta of a particle in two different directions.

The Hamiltonian

In classical mechanics, Emmy Noether proved that corresponding to every one-parameter subgroup of symmetries of a physical system there is a corresponding conserved quantity, an observable. The observable corresponding to symmetry under space translations, is momentum; corresponding to space rotations is angular momentum; and corresponding to time translations is energy.

The QM observable corresponding to energy is the Hamiltonian operator \hat{H} . Let $\Psi(t)$ be the state of the system at time *t*. The time evolution of the (nonrelativistic) system is given by Schrödinger's equation

$$i\hbar \frac{\partial}{dt} \Psi(t) = \hat{H} \Psi(t).$$

Eigenstates of the Hamiltonian

From Schrödinger's equation,

$$i\hbar \frac{\partial}{dt} \Psi(t) = \hat{H} \Psi(t) ,$$

if Ψ_0 is an eigenstate of the Hamiltonian, say $\hat{H}\Psi_0 = E\Psi_0$, we have a stationary solution of the Hamiltonian with $\Psi(0) = \Psi_0$:

$$\Psi(t) = e^{i\hbar Et}\Psi_0.$$

This is a solution with a definite energy *E*.

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Assume that the Hamiltonian has a discrete spectrum. To be physically realistic, should have a smallest eigenvalue λ_0 . The corresponding eigenstate (typically unique up to phase) is called the vacuum typically denoted $|0\rangle$ or $|\lambda_0\rangle$.

Canonical quantization

A method of converting a classical system to a QM one is as follows. Consider particles moving in \mathbb{R}^d . Suppose that $x_i = (x_i^1, \dots, x_i^d)$ $(i = 1, \dots, N)$ are the positions of the particles of mass m_i and p_i are the corresponding momenta. These are all observables. Consider the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}^{Nd})$, where x_i^j are the coordinate functions on \mathbb{R}^{Nd}). The operators \hat{q}_i^j and \hat{p}_i^j are unbounded operators, defined on the Schwartz space $\mathfrak{S}(\mathbb{R}^{Nd})$ of smooth functions f that are, with all their derivatives, of faster-than-polynomial decay.

The *i*-th position operator \hat{q}_i^j multiplies $f \in S(\mathbb{R}^{Nd})$ by the (i,j)-th coordinate function. And the *i*-th momentum operator

$$\widehat{p}_i^j = -i\hbar \frac{\partial}{\partial x_i^j}.$$

Heisenberg Lie algebra

The operators \hat{q}_i and \hat{p}_i defined by

$$[\widehat{q}_i f(x_1, \cdots, x_d) = x_i f(x), \qquad \widehat{p}_i^j f(x) = -i\hbar \frac{\partial f}{\partial x_i^j}$$

satisfy the Heisenberg commutation relations

$$[\widehat{q}_i, \widehat{q}_j] = [\widehat{p}_i, \widehat{p}_j] = 0, \qquad [\widehat{q}_i, \widehat{p}_j] = \delta_{ij}.$$

These relations define the (2d + 1)-dimensional Heisenberg Lie algebra.

Example: The particle in one dimension

Let us consider the system consisting of a single particle moving in a potential V(x) in one dimension. In the classical system, if the particle has position x and momentum p, its kinetic and potential energies are

$$T = \frac{p^2}{2m}, \qquad V = V(x)$$

and as the system evolves in time energy T + V is conserved.

To obtain the corresponding quantum mechanical Hamiltonian we substitute for x and p the position and momentum operators

$$\hat{q}\psi(x) = x\psi(x), \qquad \hat{p} = -i\hbar\frac{\partial}{\partial x}.$$

Example: The harmonic oscillator

The classical harmonic oscillator corresponds to a quadratic potential, $V(x) = \frac{k}{2}x^2$. The classical energy is

$$T+V = \frac{p^2}{2m} + \frac{k}{2}x^2.$$

Thus we obtain the Hamiltonian

$$-\hbar^2\frac{\partial^2}{\partial x^2}+\frac{k}{2}x^2\;.$$

This is the operator we gave as an example of an unbounded Hermitian operator with a discrete spectrum.

From quantum to classical

We have given a recipe for turning a classical system into a quantum one. But why does this work? Why does sending $\hbar \rightarrow 0$ recover the classical system?

In quantum mechanics, position and velocity of a particle are not localized. But if \hbar is small the position can be described by a wave packet such as a Gaussian, localized in a small region of space. As the system evolves by Schrödinger's equation, the wave packet may move but stay compact, approximating the motion of the classical particle.

But how can we see this in practice?

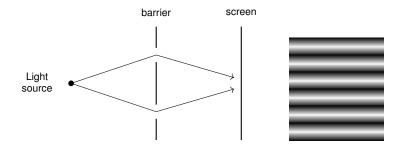
The path integral

The path integral formulation of quantum mechanics originated in Feynman's dissertation, though it may have been understood earlier by Dirac. It has advantages:

- It easily gives relativistic formulations
- It works well in quantum field theory

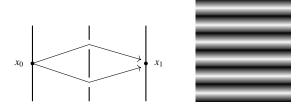
Roughly a particle moves from an initial state to a final state. To calculate the amplitude of this process, one sums the amplitudes for every possible path.

The slit experiment



In the two-slit experiment particles (photons or massive particles such as electrons or atoms) are fired towards a barrier containing two slits. A diffraction pattern appears.

The slit experiment (continued)



This is understood as a wave associated with the particle stream interfering with itself. The phenomenon persists even if the particles are sent only one at a time. This is paradoxical, but if we accept it we are led to the conclusion that both paths are followed. And this conclusion remains if the screen is removed entirely: every possible path is followed.

Action

The path integral formulation is closely related to the principle of least action in classical mechanics. Consider a classical particle of mass *m* moving in \mathbb{R}^N subject to a potential *V*. Assume the particle moves from q_0 at time t_0 to q_1 at time t_1 . Thus it follows a path q(t). Its kinetic and potential energies are

$$T = \frac{1}{2}m\dot{q}^2, \qquad V = V(q).$$

The Lagrangian is $\mathfrak{L}(q, \dot{q}) = T - V$. The action is

$$S = \int_{t_0}^{t_1} \mathfrak{L}(q, \dot{q}) \, dt.$$

q and \dot{q} are independent variables in the definition of \mathfrak{L} but given a path q(t) both have definite values for $t_0 \leq t \leq t_1$.

About *q*

The meaning of \dot{q} in these formulas depends on context.

In the definition of the Lagrangian,

$$\mathfrak{L}(q,\dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$$

 \dot{q} is an independent variable. But when q(t) is a parametrized path, as in the definition of action:

$$S = \int_{t_0}^{t_1} \mathfrak{L}(q, \dot{q}) \, dt,$$

the parameter \dot{q} has a definite value for all t, namely

$$\dot{q}(t) = \frac{dq}{dt}(t).$$

The principle of least action

We continue to consider a particle moving in a potential well, but the principle of least action has greater generality.

Principle of Least Action

Among all the paths between q_0 and q_1 , the path of motion is a local minimum of the action *S*.

Assume that the action is minimal. For simplicity take N = 1. We perturb the path q(t) by an infinitessimal deformation $\delta q(t)$. Note that $\delta(t_0) = \delta(t_1) = 0$.

$$0 = \delta S = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} \delta(t) + \frac{\partial L}{\partial \dot{q}} \delta'(t) \right) dt = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{q}} \right) \delta(t) dt$$

where we integrated by parts.

Euler Lagrange equations

Thus we obtain the Euler-Lagrange equation:

$$\frac{\partial L}{\partial q} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{q}} = 0.$$

Let us check that these give the right equations of motion for a particle in a potential well. In this case

$$\frac{\partial L}{\partial q} = -V'(q) = \text{force on the particle},$$
$$\frac{\partial L}{\partial \dot{q}} = \frac{\partial}{\partial \dot{q}}T = \frac{\partial}{\partial \dot{q}}\frac{1}{2}m\dot{q}^2 = m\dot{q}, \qquad \frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{q}} = m\ddot{q}$$

so the Euler Lagrange equation boils down to:

" Force equals mass times acceleration."

From classical to quantum

We have considered the classical system of a particle moving in a potential V on \mathbb{R}^N . A state of the classical system assigns values in \mathbb{R}^N to q and \dot{q} , positition and velocity. The subsequent evolution of the system as a function of t is then determined by the Euler-Lagrange equations.

The analog in nonrelativistic quantum mechanics depends on a Hilbert space \mathcal{H} which we can take to be $L^2(\mathbb{R}^N)$. A state of the system is a one-dimensional subspace, represented by a vector ψ . We normalize ψ so its L^2 norm $\langle \psi | \psi \rangle = 1$. Multiplying ψ by a phase factor $e^{i\theta}$ does not change its physical meaning.

Review: Amplitudes

To reiterate a unit vector in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^N)$ represents a state of the system consisting of a single particle in \mathbb{R}^N . The inner product is written

$$\langle \psi_1 | \psi_2 \rangle = \int_{\mathbb{R}^N} \overline{\psi_1(x)} \psi_2(x) \, dx.$$

The precise location of the particle is not determined by ψ . Instead, the probability density of the particle being at the point *x* is $|\psi(x)|^2$. The value $\psi(x)$ is called an amplitude.

More generally an amplitude is a complex number whose norm square has interpretation as a probability or probability density.

Position versus momentum

The relation between the quantum and classical systems is controlled by a positive number \hbar . The classical system emerges when $\hbar \longrightarrow 0$.

The momentum similarly has a wave function φ which is the Fourier transform of ψ :

$$\Phi(p) = \frac{1}{(2\pi\hbar)^{N/2}} \int_{\mathbb{R}^N} \psi(q) e^{-ip \cdot q/\hbar} dq.$$

The Fourier transform is an isometry $L^2(\mathbb{R}^N) \longrightarrow L^2(\mathbb{R}^N)$ so we may regard either ψ or ϕ as a vector in an abstract Hilbert space \mathcal{H} . The position and momentum realizations of \mathcal{H} may be thought of different views of the same system.

Hermitian operators and the spectral theorem

A bounded operator $T: \mathcal{H} \to \mathcal{H}$ is Hermitian or self-adjoint if

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\langle T\psi_1|\psi_2\rangle = \langle \psi_1|T\psi_2\rangle.
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In this case we use the notation $\langle \psi_1 | T | \psi_2 \rangle$.

Theorem

T is compact and Hermitian, then \mathcal{H} decomposes into the eigenspaces of *T*, which are all finite-dimensional (except perhaps the 0-eigenspace) and orthogonal.

We also encounter unbounded operators, defined on a dense subspace. There is a spectral theorem for unbounded Hermitian operators.

Review: Observables

An observable is a quantity *A* such as position, momentum, energy, or angular momentum that can be measured from a physical system.

In a quantum system the observable *A* corresponds to a Hermitian operator \hat{A} . If ψ is an eigenfunction then its eigenvalue λ is the measured value of *A*. If ψ is not an eigenfunction then measuring *A* does not have a deterministic outcome. Two observables can be measured simultaneously if and only if their operators commute.

The operator \hat{H} corresponding to energy is called the Hamiltonian.

Review:: The particle in one dimension

Let us consider the system consisting of a single particle moving in a potential V(x) in one dimension. Position becomes the unbounded operator \hat{q} which is multiplication by *x*:

$$\hat{q}\psi(x) = x\psi(x).$$

The momentum operator is

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

and we have the Heisenberg commutation relation $[\hat{x}, \hat{p}] = i\hbar$. The operator corresponding to the classical energy $E = T + V = \frac{p^2}{2m} + V(x)$ is the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

Review: The Hamiltonian as an evolution operator

In nonrelativistic quantum mechanics the Hamiltonian is an evolution operator.

A system prepared in state ψ_0 at time $t = t_0$ evolves according to Schrödinger's equation. Let $\Psi(x, t)$ be the state at time t so $\psi(x) = \Psi(x, t_0)$.

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \hat{H} \Psi(x,t).$$
 (1)

Schrödinger's equation describes the evolution of ψ . Thus the state $\psi_1(q) = \Psi(q, t_1)$ at a later time t_1 is

$$\psi_1 = U(t_1, t_0)\psi_0, \qquad U(t_1, t_0) = e^{i\hbar(t_1 - t_2)\hat{H}}.$$

The propagator amplitude as a Green's function

Suppose the particle is prepared to be at location q_0 at time t_0 and is found to be at q_0 at time t_1 . The amplitude for this process is an amplitude $\langle q_1 | U(t_1, t_0) | q_0 \rangle$. This propagator can be understood as a kernel

$$K(q_1,t_1,q_0,t_0) = \langle q_1 | U(t_1,t_0) | q_0 \rangle$$

for propogating solutions of the (nonrelativistic) Schrödinger equation. It is itself a solution (in either x_0 or x_1 and has a mild singularity when x_0 and x_1 coincide.

Intuitively $\langle q_1 | U(t_1, t_0) | q_0 \rangle$ is the amplitude of the process, that the particle moves from x_0 to x_1 .

The path integral

So what is this amplitude? According to Feynman, it is a path integral. For every possible path x(t) from $x_0 = (q_0, t_0)$ to $x_1 = (q_1, t_1)$ there is an action

$$S(x(t)) = \int_{t_0}^{t_1} \mathcal{L}(q, \dot{q}) dt$$

where \mathcal{L} is the Lagrangian. According to the path integral formulation of quantum mechanics there is a measure [dx] on the space of all possible paths x(t) from x_0 to x_1 such that:

$$\langle q_1|U(t_1,t_0)|q_0\rangle = \int \exp\left(\frac{i}{\hbar}S(x(t))\right)[dx]$$

The wandering particle

The path integral

$$\langle q_1|U(t_1,t_0)|q_0\rangle = \int \exp\left(\frac{i}{\hbar}S(x(t))\right) [dx]$$

is unintuitive from the viewpoint of classical mechanics since it many of the paths will be quite nonphysical ones violating the conservation laws of energy and momentum.



Stationary phase

Now let us recall the principle of stationary phase. This says that that given an oscillatory integral the main contribution to the integral is where the oscillations are least. For example consider

$$\int_{a}^{b} e^{i\lambda \Phi(x)} f(x) dx.$$

Suppose that there is a unique $c \in (a, b)$ where $\phi'(x) = 0$, and $\phi''(c) > 0$. Then if λ is large, the integral is approximately

$$e^{i\lambda\Phi(c)}f(c)\sqrt{\frac{2\pi}{\lambda\Phi''(c)}}e^{i\pi/4}.$$

Classical limit

Another manifestation of stationary phase is that if \hbar is small, the main contribution to the path integral

$$\langle q_1|U(t_1,t_0)|q_0\rangle = \int \exp\left(\frac{i}{\hbar}S(x(t))\right) [dx]$$

is from the classical path of least action, that is, from the path x(t) that minimizes the action.

References for the path integral.

- Polchinski, String Theory Vol.1, Appendix A: a short course in path integrals
- DiFrancesco, Senechal and Mathieu, Conformal Field Theory, Chapter 2
- Zee, Quantum Field Theory in a Nutshell, Chapter I.2.