

THE SCHRÖDINGER EQUATION

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1. THE SCHRÖDINGER EQUATION

In mathematical physics, the Schrödinger equation (and the closely related Heisenberg equation) are the most fundamental equations in non-relativistic quantum mechanics, playing the same role as Hamilton's laws of motion (and the closely related Poisson equation) in non-relativistic classical mechanics. (In relativistic quantum mechanics, it is the equations of quantum field theory which replace the role of Heisenberg's equation, while Schrödinger's equation does not directly have a natural analogue.) In pure mathematics, the Schrödinger equation and its variants is one of the basic equations studied in the field of partial differential equations, and has applications to geometry, to spectral and scattering theory, and to integrable systems. There are actually two (closely related) variants of Schrödinger's equation, the *time dependent* Schrödinger equation and the *time independent* Schrödinger equation; we will begin with the discussion of the time-dependent equation.

Let us begin with the physical motivation, reviewing both the classical and quantum mechanics of a simple physical system. While the Schrödinger equation can be used to describe the quantum dynamics of many-particle systems under the influence of a variety of forces, let us for simplicity just consider a single particle with some mass $m > 0$ in n -dimensional space \mathbf{R}^n moving subject to the influence of a potential, which for us will be a function $V : \mathbf{R}^n \rightarrow \mathbf{R}$. To avoid technicalities we shall assume implicitly that all functions in this discussion are smooth (i.e. infinitely differentiable).

In classical mechanics, this particle would have a specific position $q(t) \in \mathbf{R}^n$ and a specific momentum¹ $p(t) \in \mathbf{R}^n$ for each time t . (Eventually we shall observe the familiar law $p(t) = mv(t)$, where $v(t) := q'(t)$ is the velocity of the particle.) Thus the state of this system at any given time t is described by the element $(q(t), p(t))$ of *phase space* $\mathbf{R}^n \times \mathbf{R}^n$. The *energy* of this state is described by the *Hamiltonian function* $H : \mathbf{R}^n \times \mathbf{R}^n \rightarrow \mathbf{R}$ on phase space, defined in this case by

$$H(q, p) := \frac{|p|^2}{2m} + V(q).$$

¹To be more precise, the momentum $p(t)$ should live in the cotangent space $T_{q(t)}^* \mathbf{R}^n$ of \mathbf{R}^n at $q(t)$, but we shall ignore this subtlety for sake of simplicity in this discussion.

(Physically, the quantity $\frac{|p|^2}{2m} = \frac{1}{2}m|v|^2$ represents kinetic energy, while $V(q)$ represents potential energy.) The system then evolves by *Hamilton's equations of motion*

$$q'(t) := \frac{\partial H}{\partial p}; \quad p'(t) := -\frac{\partial H}{\partial q},$$

where we keep in mind that p and q are vectors and so these derivatives are thus gradients. Hamilton's equations of motion are valid for any classical system, but in our specific case of a particle in a potential well, they become

$$q'(t) := \frac{1}{m}p(t); \quad p'(t) = -\nabla V(q).$$

The first equation is asserting that $p = mv$; the second equation is basically Newton's second law (the left-hand side is equal to $ma(t) = mq''(t)$, and the right-hand side has the physical interpretation of the force exerted by the potential). One consequence of Hamilton's equations of motion is that one has *conservation of energy*

$$\frac{d}{dt}H(q(t), p(t)) = 0;$$

more generally, given any *classical observable* $A : \mathbf{R}^n \times \mathbf{R}^n \rightarrow \mathbf{R}$, we have *Poisson's equation of motion*

$$\frac{d}{dt}A(q(t), p(t)) = \{H, A\}(q(t), p(t))$$

where $\{H, A\} : \mathbf{R}^n \times \mathbf{R}^n \rightarrow \mathbf{R}$ is the *Poisson bracket* of H and A , defined as

$$\{H, A\} := \frac{\partial H}{\partial p} \cdot \frac{\partial A}{\partial q} - \frac{\partial A}{\partial p} \cdot \frac{\partial H}{\partial q}.$$

One can easily show that Hamilton and Poisson's equations of motion are in fact equivalent to each other. From conservation of energy, we see that there is a quantity E (independent of time) such that

$$H(q(t), p(t)) = E$$

for all $t \in \mathbf{R}$; we will refer to this as the *time-independent Hamilton equation*, for reasons which will be clearer later.

Now we analyze the quantum mechanical analogue of the above classical system. We need a small parameter $\hbar > 0$, known as *Planck's constant*. The state of the particle at a time t is no longer described by a single point $(q(t), p(t))$ in phase space, but is instead described by a *wave function*, which in this case is a complex-valued function $\psi(t) : \mathbf{R}^n \rightarrow \mathbf{C}$ obeying the normalization $\langle \psi(t), \psi(t) \rangle = 1$, where $\langle \cdot, \cdot \rangle$ denotes the inner product

$$\langle \phi, \psi \rangle := \int_{\mathbf{R}^n} \phi(q) \overline{\psi(q)} dq.$$

Unlike classical mechanics, a wave function $\psi(t)$ does not necessarily have a specific position $q(t)$, however it does have an *average position* $\langle q(t) \rangle$, defined as

$$\langle q(t) \rangle := \langle Q\psi(t), \psi(t) \rangle = \int_{\mathbf{R}^n} q|\psi(t, q)|^2 dq,$$

where the *position operator* Q is the operation of multiplication by q , thus $Q\psi(t, q) := q\psi(t, q)$. Similarly, while ψ does not have a specific momentum $p(t)$, it does have

an *average momentum* $\langle p(t) \rangle$, defined as

$$\langle p(t) \rangle := \langle P\psi(t), \psi(t) \rangle = \frac{\hbar}{i} \int_{\mathbf{R}^n} (\nabla_q \psi(t, q)) \overline{\psi(t, q)} dq,$$

where the *momentum operator* P is defined by *Planck's law*

$$P\psi(t, q) := \frac{\hbar}{i} \nabla_q \psi(t, q).$$

Note that while at first glance $\langle p(t) \rangle$ appears to be a complex-valued vector, it is in fact a real-valued vector because all the components of P are self-adjoint. More generally, given any *quantum observable* - by which we mean a self-adjoint operator A acting on the space $L^2(\mathbf{R}^n)$ of complex-valued square integrable functions - we can define the *average value* $\langle A(t) \rangle$ of A at time t by the formula

$$\langle A(t) \rangle := \langle A\psi(t), \psi(t) \rangle.$$

The analogue of Hamilton's equations of motion is now the *time-dependent Schrödinger equation*

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

where H is now a quantum observable rather than a classical one, and more precisely

$$H = \frac{|P|^2}{2m} + V(Q).$$

In other words, we have

$$i\hbar \frac{\partial \psi}{\partial t}(t, q) = H\psi(t, q) = -\frac{\hbar^2}{2m} \Delta_q \psi(t, q) + V(q)\psi(t, q)$$

where $\Delta_q \psi = \sum_{j=1}^n \frac{\partial^2 \psi}{\partial q_j^2}$ is the *Laplacian* of ψ . In pure mathematics it is not uncommon to normalize $\hbar = m = 1$ and write x instead of q , thus writing Schrödinger's equation in the form

$$i \frac{\partial \psi}{\partial t}(t, x) = -\Delta_x \psi(t, x) + V(x)\psi(t, x).$$

The analogue of Poisson's equation of motion is the *Heisenberg equation*

$$\frac{d}{dt} \langle A(t) \rangle = \left\langle \frac{i}{\hbar} [H(t), A(t)] \right\rangle$$

for any observable A , where $[A, B] = AB - BA$ is the *commutator* or *Lie bracket* of A and B . (The quantity $\frac{i}{\hbar} [A, B]$ is occasionally referred to as the *quantum Poisson bracket* of A and B .) Thus for instance we have the conservation of energy law

$$\frac{d}{dt} \langle H(t) \rangle = 0.$$

In classical mechanics, this would imply that there exists a real number E such that the Hamiltonian H always takes the value of E . This is sometimes, but not always, the case in quantum mechanics. It is possible that the quantum state ψ oscillates in time according to the formula $\psi(t, q) = e^{\frac{E}{i\hbar}t} \psi(0, q)$ for some real number E in which case it is true that

$$H\psi(t) = E\psi(t) \text{ for all times } t.$$

The equation $H\psi = E\psi$ is then known as the *time-independent Schrödinger equation*, and E is referred to as the *energy level* or *eigenvalue* of the state ψ . However, in general ψ does not have such a simple oscillation behavior in time, but is instead

a *superposition* or *linear combination* of such oscillating states, for instance one possibility is that ψ has a representation of the form

$$\psi(t, q) = \sum_{k=1}^K e^{\frac{E_k}{i\hbar}t} \psi_k(q)$$

for a finite number of energy levels E_1, \dots, E_K , and a finite number of functions ψ_1, \dots, ψ_K each obeying the time-independent Schrödinger equation $H\psi_k = E_k\psi_k$ at energy level E_k . In fact a general solution ψ to the time-dependent Schrödinger equation always has a representation of the above form, except that the finite summation may have to be replaced by an infinite summation or a continuous integral (or a combination of both). Thus knowing all the solutions to the time-independent Schrödinger equation gives (at least in principle) all the solutions to the time-dependent Schrödinger equation. (One can also view the two equations as Fourier transforms of each other; the quantity $\frac{E}{\hbar}$ is essentially the frequency variable dual to the time variable t .)

At first glance it is not immediately apparent that Schrödinger's equations and Hamilton's equations are at all related, although there is certainly some similarity between Heisenberg's equation and Poisson's equation. Nevertheless, strong analogies exist between the two equations. For instance, one can deduce from the Heisenberg equation that

$$\frac{d}{dt}\langle q(t) \rangle = \frac{1}{m}\langle p(t) \rangle; \quad \frac{d}{dt}\langle p(t) \rangle = -\langle \nabla_q V(q)(t) \rangle,$$

which is certainly very similar to Hamilton's equations of motion. Also, given any classical solution $t \mapsto (q(t), p(t))$ to Hamilton's equation of motion, one can construct a corresponding family of *approximate* solutions $\psi(t)$ to Schrödinger's equation, for instance by the formula²

$$\psi(t, q) := e^{\frac{i}{\hbar}L(t)} e^{\frac{i}{\hbar}p(t)\cdot(q-q(t))} \varphi(q - q(t))$$

where $L(t) := \int_0^t \frac{p(s)^2}{2m} - V(q(s)) ds$ is the *classical action* and φ is any slowly varying function (thus the derivatives of φ are small) which is normalized in the sense that $\int_{\mathbf{R}^n} |\varphi(q)|^2 dq = 1$. Indeed, one can verify that $\psi(t, q)$ solves the approximate Schrödinger's equation

$$i\hbar \frac{\partial \psi}{\partial q}(t, q) = H\psi(t, q) + \frac{\hbar^2}{2m} e^{\frac{i}{\hbar}L(t)} e^{\frac{i}{\hbar}p(t)\cdot(q-q(t))} \Delta \varphi(q - q(t)).$$

The error term on the right-hand side will be small if $\hbar^2 \Delta \varphi$ is small. In physics, this fact is an example of the *correspondence principle*, which asserts that classical mechanics can be used to approximate quantum mechanics accurately if Planck's constant is small and one is working at macroscopic scales (which is what allows us to use slowly varying functions φ). In mathematics (and more precisely in the fields of *microlocal analysis* and *semi-classical analysis*), there are a number of

²Intuitively, this function $\psi(t, q)$ is localized in position near $q(t)$ and localized in momentum near $p(t)$, and is thus localized near $(q(t), p(t))$ in phase space. Such a localized function, exhibiting such "particle-like" behavior as having a reasonably well defined position and velocity is sometimes known as a "wave packet". In general, most solutions of the Schrödinger equation do not behave like wave packets, but can be decomposed as a *superposition* or *linear combination* of wave packets; such decompositions are a useful tool in analyzing general solutions of such equations.

formalizations of this principle that allow us to use knowledge about the behavior of Hamilton's equations of motion in order to analyze the Schrödinger equation. For example if the classical equations of motion have periodic solutions, then often the Schrödinger equation also has nearly-periodic solutions, whereas if the classical equations have very chaotic solutions, then the Schrödinger equation typically does also (this phenomenon is known as *quantum chaos* or *quantum ergodicity*).

The time-independent Schrödinger equation $H\psi = E\psi$ is of course an eigenvalue equation for the operator H . If H was a self-adjoint transformation on a *finite-dimensional* space then as is well known, there would only be a finite number of eigenvalues E for which the equation $H\psi = E\psi$ had a non-trivial solution; however since H acts on an infinite-dimensional space, the situation can be more complicated. Indeed, H can have eigenfunctions ψ which lie in the domain $L^2(\mathbf{R}^n)$ of H (consisting of square-integrable complex-valued functions), but it is also possible to have solutions $H\psi = E\psi$ which do not decay at infinity, but instead are bounded or grow at infinity; in fact, the behavior at infinity depends crucially on the value of E , and in particular whether it lies in one or more components of the *spectrum* of H , defined as the set of energies E for which the operator $H - E$ fails to be invertible with a bounded inverse. This leads to the *spectral theory* of Schrödinger operators and their variants, which is a vast and active area of current research.

Closely related to spectral theory is *scattering theory*, which is of importance in both physics and mathematics. If the potential function V decays sufficiently quickly at infinity, and $k \in \mathbf{R}^n$ is a non-zero frequency vector, then setting the energy level as $E := \frac{\hbar^2 |k|^2}{2m}$, the time-dependent Schrödinger equation $H\psi = E\psi$ admits solutions $\psi(q)$ which behave asymptotically as $|q| \rightarrow \infty$ as

$$\psi(q) \approx e^{ik \cdot q} + f\left(\frac{q}{|q|}, k\right) \frac{e^{i|k||q|}}{r^{(n-1)/2}}$$

for some canonical function $f : S^{n-1} \times \mathbf{R}^n \rightarrow \mathbf{C}$, known as the *scattering amplitude function*. This scattering amplitude depends (in a non-linear fashion) on the potential V , and the map from V to f is known as the *scattering transform*, and can be viewed as a non-linear variant of the Fourier transform. A major area of study in scattering theory is understanding the relationship between properties of the potential V and properties of the scattering amplitude f , and in particular whether one can reconstruct the potential V from the scattering amplitudes. This theory is important not just for the study of the Schrödinger equation, but is (rather surprisingly) also useful for studying a number of *integrable systems*, for instance one can explicitly write the solution to the *Korteweg-de Vries* equation

$$\frac{\partial V}{\partial t} + \frac{\partial^3 V}{\partial t^3} = 6V \frac{\partial V}{\partial x}$$

by means of the one-dimensional scattering and inverse scattering transforms.

There are many generalizations and variants of the Schrödinger equation; one can generalize to many-particle systems, or add other forces such as magnetic fields or even non-linear terms. One can also couple this equation to other physical equations such as Maxwell's equations of electromagnetism, or replace the domain \mathbf{R}^n by another space such as a torus, a discrete lattice, a manifold, or alternatively one

could place some impenetrable obstacles in the domain (thus effectively removing those regions of space from the domain). The study of all of these variants is a vast and diverse field in both pure mathematics and in mathematical physics.

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