An introduction to the Schrödinger equation

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + V\left[(\vec{r},t)\right]\Psi(\vec{r},t)$$

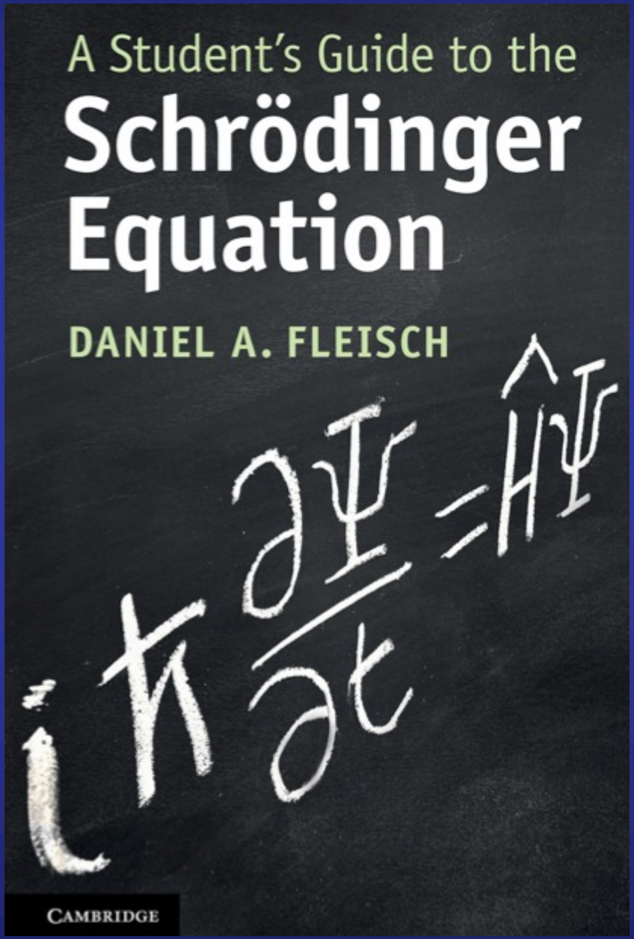
Javier Junquera

UC
UNIVERSIDAD
DE CANTABRIA

CITIMAC

Preschool ASESMA, February 27th 2025

The most important reference followed in this lecture



A Student's Guide to the

Schrödinger Equation

DANIEL A. FLEISCH

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

CAMBRIDGE

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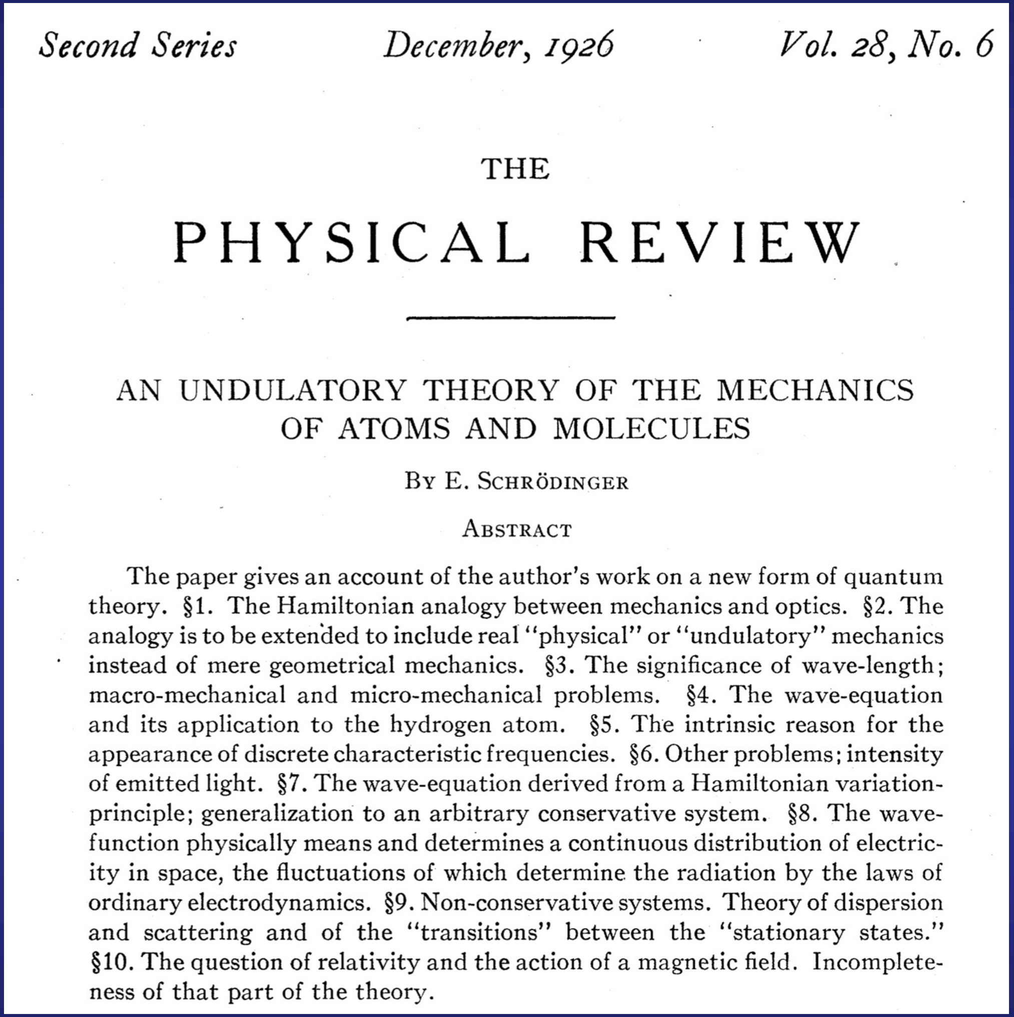
A little bit of history



Second Series *December, 1926* *Vol. 28, No. 6*

THE

PHYSICAL REVIEW

AN UNDULATORY THEORY OF THE MECHANICS OF ATOMS AND MOLECULES

By E. Schrödinger

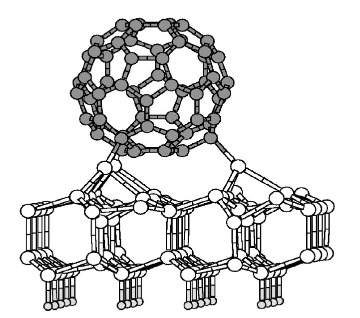
Abstract

The paper gives an account of the author's work on a new form of quantum theory. §1. The Hamiltonian analogy between mechanics and optics. §2. The analogy is to be extended to include real "physical" or "undulatory" mechanics instead of mere geometrical mechanics. §3. The significance of wave-length; macro-mechanical and micro-mechanical problems. §4. The wave-equation and its application to the hydrogen atom. §5. The intrinsic reason for the appearance of discrete characteristic frequencies. §6. Other problems; intensity of emitted light. §7. The wave-equation derived from a Hamiltonian variation-principle; generalization to an arbitrary conservative system. §8. The wave-function physically means and determines a continuous distribution of electricity in space, the fluctuations of which determine the radiation by the laws of ordinary electrodynamics. §9. Non-conservative systems. Theory of dispersion and scattering and of the "transitions" between the "stationary states." §10. The question of relativity and the action of a magnetic field. Incompleteness of that part of the theory.

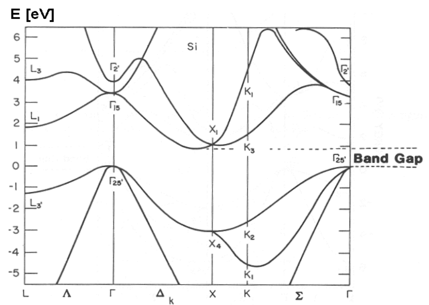
Paper published in 1926

Erwin Schrödinger
(1887-1961)

Goal: Describe properties of matter from theoretical methods firmly rooted in fundamental equations



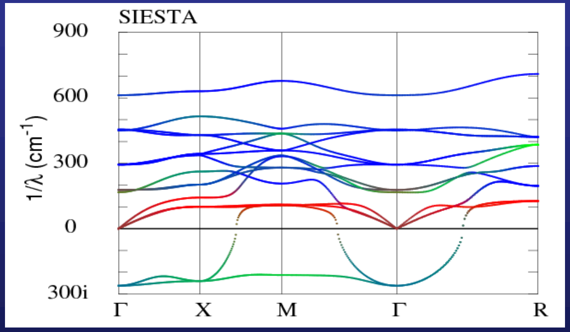
structural



electronic

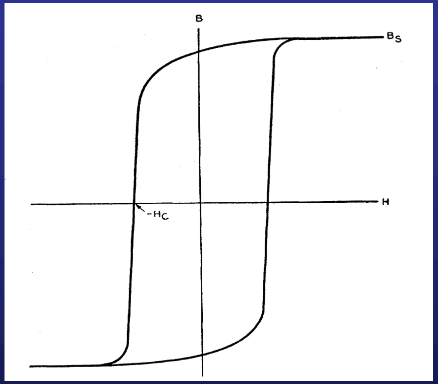
PROPERTIES

vibrational



optical

magnetic



Goal: Describe properties of matter from theoretical methods firmly rooted in fundamental equations

Quantum Mechanics: Schrödinger equation (assuming no relativistic)

$$i\hbar \frac{\partial \Psi\left(\{\vec{x}_i\}, \{\vec{R}_\alpha\}; t\right)}{\partial t} = \hat{H}\Psi\left(\{\vec{x}_i\}, \{\vec{R}_\alpha\}; t\right)$$

Coordinates of electron i $\vec{x}_i$ comprise

$$\begin{cases} \text{Space coordinates} & \vec{r}_i \\ \text{Spin coordinates} & \sigma_i \end{cases}$$

Electromagnetism: Coulomb's law

For a pair of charged particles

$$\hat{H} = \hat{T} + \hat{V}_{Coulomb}$$

$$\hat{V}_{Coulomb} = \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}$$

This hamiltonian can not be solved exactly: practical and fundamental problems

Fundamental problem:

Schrödinger’s equation is exactly solvable for

- Harmonic oscillator (analytically)
- Two particles (analytically)
- Very few particles (numerically)

The complexity wall is the treatment of the electron-electron interaction

Practical problem:

The number of electrons and nuclei in a pebble is of the order of 10^{23}

The computational cost grows exponentially with the number of electrons

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Outline:

What the Schrödinger equation means

Characteristics of the Schrödinger equation

Time independent Schrödinger equation in 1D

Schrödinger equation in 3D

What does the electronic wavefunction represents.
Principles of Copenhagen interpretation

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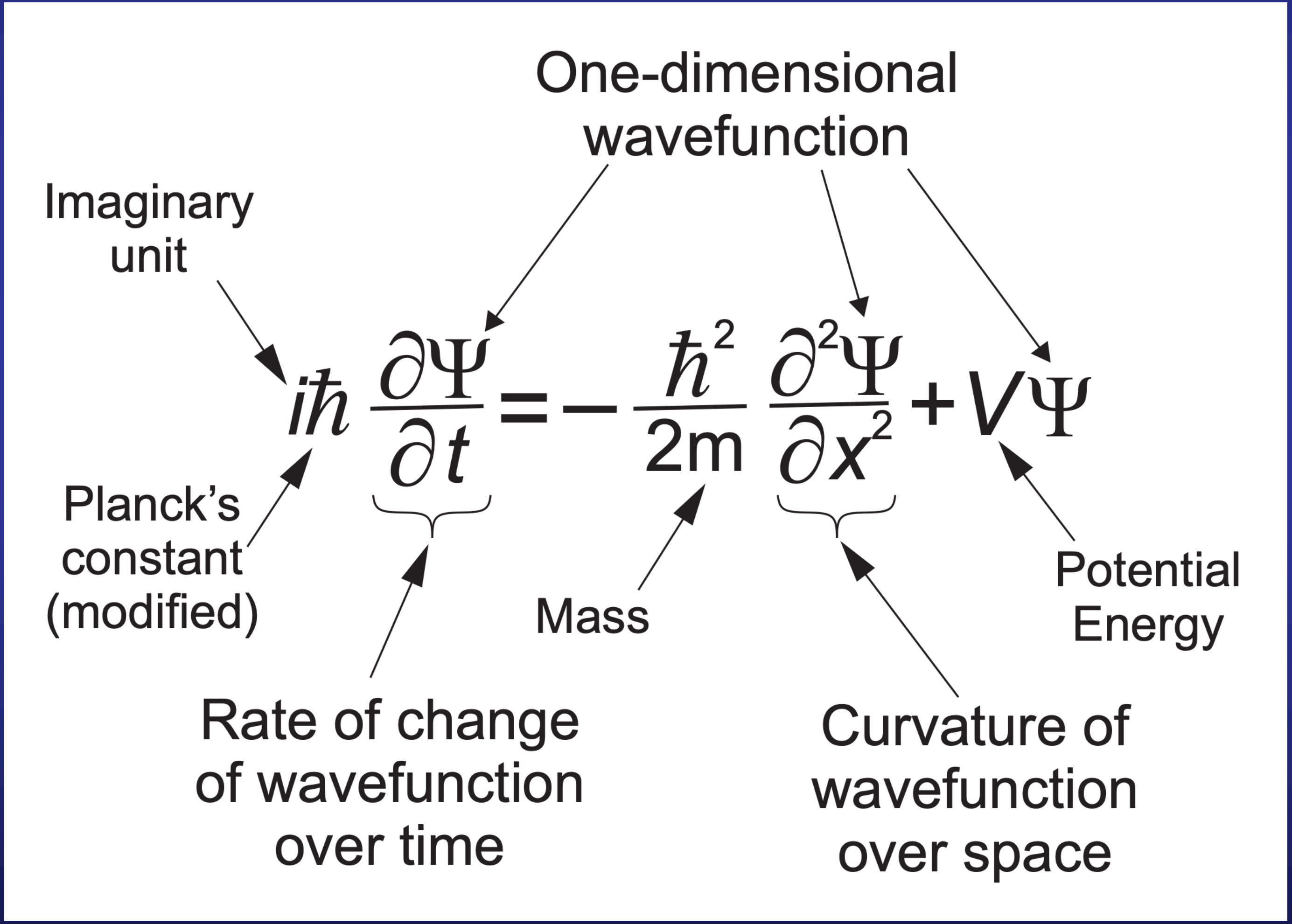
What the Schrödinger equation means

Time dependent Schrödinger equation in one-dimension



One-dimensional wavefunction

Imaginary unit

$$i\hbar \underbrace{\frac{\partial \Psi}{\partial t}} = -\frac{\hbar^2}{2m} \underbrace{\frac{\partial^2 \Psi}{\partial x^2}} + V\Psi$$

Planck's constant (modified)

Mass

Potential Energy

Rate of change of wavefunction over time

Curvature of wavefunction over space

$\frac{\partial \Psi}{\partial t}$ Partial derivative of the wave function with respect to time

The quantum wavefunction $\Psi(x,t)$ is a function of both the spatial position x and time t

$\frac{\partial \Psi}{\partial t}$ Represents the change of the wave function over time only (it is a partial derivative)

In a graph of the wavefunction at a given location as a function of time, this term is the slope of the graph

Units (in one dimension and in the international system)

$$\frac{1}{s\sqrt{m}}$$

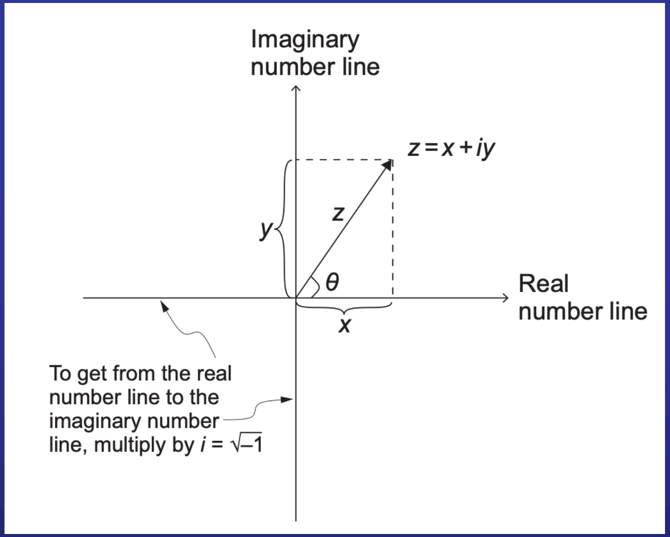
s = seconds
m = meters

i numerical value of the imaginary unit (adimensional)

$$i = \sqrt{-1}$$

Multiplication by i has the effect of causing a 90° rotation in the complex plane

It moves numbers from the positive real axis to the positive imaginary axis, ot from the positive imaginary axis to the negative real axis



To get from the real number line to the imaginary number line, multiply by $i = \sqrt{-1}$

Its presence means that the quantum wavefunction solutions might be complex (this has a significant impact on the results of combining two wave functions)

$\hbar$ the modified Planck constant

$$\hbar = \frac{h}{2\pi} = 1.05457 \times 10^{-34} \ \frac{\mathrm{Js}}{\mathrm{rad}}$$

s = seconds
J = Joules

It is the constant of proporciontality between the energy and the angular frequency

$$E = \hbar\omega$$

It is the constant of proporciontality between the momentum and the wave number

$$p = \hbar k$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

Linear dependency here because it appears linearly in the energy expression

Quadratic dependency here because it appears linearly in the momentum expresión and the kinetic energy is quadratic to the momentum

m mass of the particle or system associated with the quantum wavefunction

It is a measure of inertia
(resistance to acceleration)

Units in kg in the international system

$\frac{\partial^2 \Psi}{\partial x^2}$ curvature of the wavefunction over space

$$\frac{\partial \Psi}{\partial x}$$

Change of wavefunction over space
(the slope of the wave function plotted against x)

$$\frac{\partial^2 \Psi}{\partial x^2}$$

Change in the slope of the wavefunction over space
(curvature of the wavefunction)

Units on the international system

$$\frac{1}{m^{5/2}}$$

m = meters

V potential energy of the system

$V(x,t)$ **may vary over space and time**

In quantum mechanics, the particle's total energy may be less than the potential energy in some regions

$E < V$ **Classically "unallowed regions"**
Evanescent solutions

$E > V$ **Classically "allowed regions"**
Oscillating solutions

Units on the international system: Joules

$$\mathrm{J} = \frac{\mathrm{kg\ m^2}}{\mathrm{s^2}}$$

m **= meters**
s **= seconds**
kg **= kilograms**

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Characteristics of the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

Differential: involves the change of the wavefunction over space and time

Partial: because the wavefunction depends on both space and time

Second-order: because the highest-order in the equation is a second derivative

Parabolic: because the combination of a first-order differential term in time and a second-order differential term in space is analogous to the combination of a first-order algebraic term and a second-order algebraic term in a parabola

Relationship with difussion equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

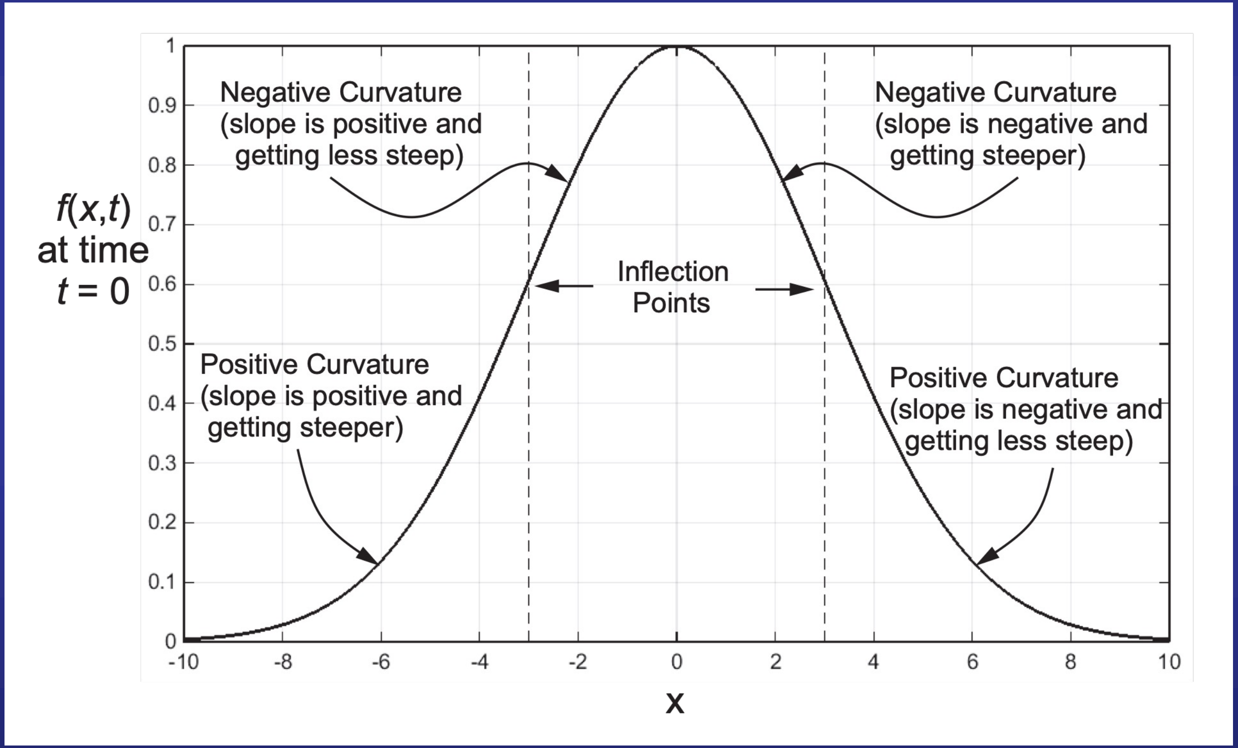
$$\frac{\partial\left[f(x,t)\right]}{\partial t} = D\frac{\partial^2\left[f(x,t)\right]}{\partial x^2}$$

$$\frac{\partial\left[\Psi(x,t)\right]}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\left[\Psi(x,t)\right]}{\partial x^2}$$

Relationship with difussion equation

$$\frac{\partial\left[f(x,t)\right]}{\partial t} = D\frac{\partial^2\left[f(x,t)\right]}{\partial x^2}$$

Consider a function at $t = 0$ that might represent, for instance, the initial temperature distribution of a fluid with a warm spot at the origin



The curvature is the change in the slope (second derivative of the function)

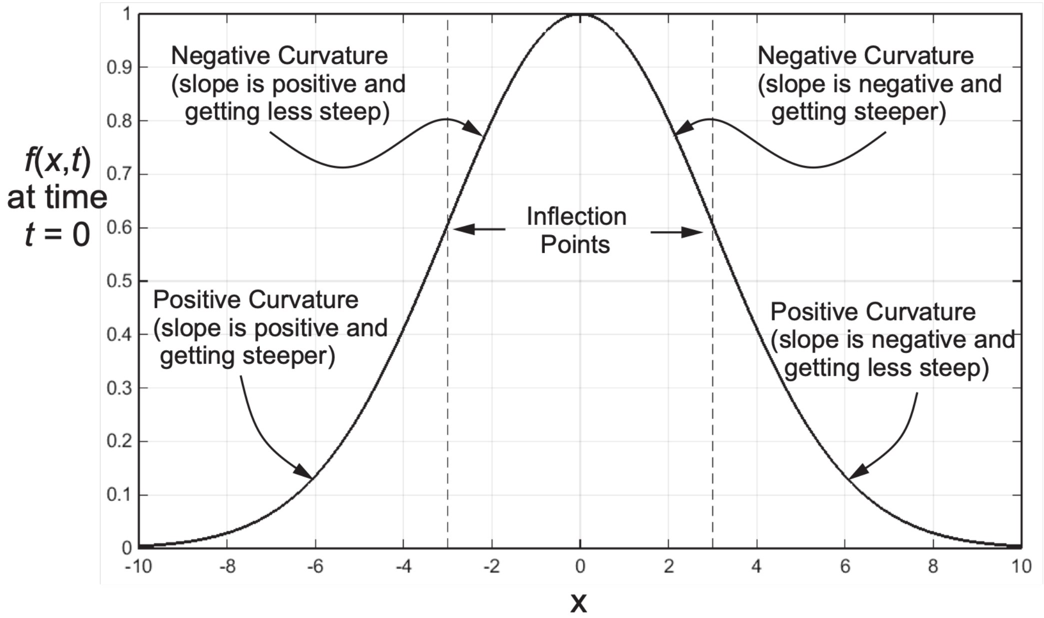
How this temperature will evolve over time?

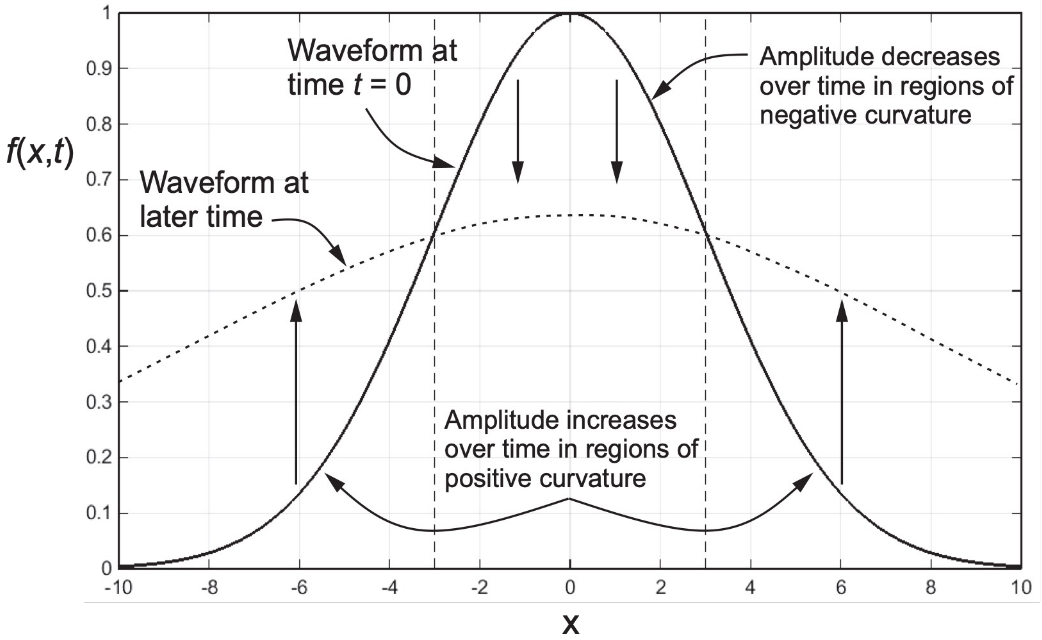
From the diffusion equation, we should consider the curvature of the function in various regions

Relationship with difussion equation

$$\frac{\partial\left[f(x,t)\right]}{\partial t} = D\frac{\partial^2\left[f(x,t)\right]}{\partial x^2}$$

Since the difussion equation tells that the time rate of change of the function is proportional to the curvature of the function, the function will evolve as…





The temperature increases in regions of positive curvature

The temperature decreases in regions of negative curvature

(the energy from the initially warm regions diffuses into the cooler neighboring regions)

Would all the quantum particles and systems diffuse or spread out in space as time passes?

Sometimes, but no always

The difference between the Schrödinger equation and the difussion equation is a factor of “i” in the former

The wavefunctions might be complex

They may exhibit oscillatory behaviour rather than diffusing under some circumstances

Interpretation of the wavefunction as a probability amplitude

Due to Max Born (1926)

The module squared of a particle's position wavefunction

$$|\Psi|^2 = \Psi^* \times \Psi$$

gives the particle's position probability density function

In the one-dimensional case this is the probability per unit length

The integral of the probability density function over any spatial interval gives the probability of finding the particle within that interval

When the wavefunction oscillates or diffuses,
it is the probability's distribution that is changing

The wavefunctions that satisfy the Schrödinger eq. represent "all you can ever know" about the state of a particle of system

The time derivative is first order $\frac{\partial\Psi}{\partial t}$

The first-order tells you how fast the wavefunction itself is changing over time

If we integrate once, only one constant of integration is required

The knowledge of the wavefunction at some instant in time completely specifies the state if the particle or system at all future times

This is at odds with the classical wave equation,
where both the time and spatial derivatives are second order

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Time-independent Schrödinger equation

Assumption: separation of variables

The solution $\Psi(x,t)$ can be written as the product of two separate functions:

- One depending only on the spatial coordinates (x)
- Another depending only on t

$$\Psi(x,t) = \psi(x)T(t)$$

There is no a-priori reason why this approach should work.
But it often does.

In any situation in which the potential energy varies only over space (and not over time), you can use separtation of variables to solve the Schrödinger equation

Time-independent Schrödinger equation

$$\Psi(x,t) = \psi(x)T(t)$$

Inserting this into the Schrödinger equation

$$i\hbar\frac{\partial\left[\psi(x)T(t)\right]}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\left[\psi(x)T(t)\right]}{\partial x^2} + V(x)\left[\psi(x)T(t)\right]$$

Since $\psi(x)$ does not depend on time,
and $T(t)$ does not depend on position,
they can be taken out from the partial derivatives

$$i\hbar\psi(x)\frac{d\left[T(t)\right]}{dt} = -\frac{\hbar^2 T(t)}{2m}\frac{d^2\left[\psi(x)\right]}{dx^2} + V(x)\left[\psi(x)T(t)\right]$$

Now the partial derivatives have become total derivatives

Time-independent Schrödinger equation

$$i\hbar\psi(x)\frac{d\left[T(t)\right]}{dt} = -\frac{\hbar^2 T(t)}{2m}\frac{d^2\left[\psi(x)\right]}{dx^2} + V(x)\left[\psi(x)T(t)\right]$$

Dividing both sides of the equation by $\Psi(x,t) = \psi(x)T(t)$

$$\frac{1}{\cancel{\psi(x)}T(t)}i\hbar\cancel{\psi(x)}\frac{d[T(t)]}{dt} = -\frac{1}{\psi(x)\cancel{T(t)}}\frac{\hbar^2\cancel{T(t)}}{2m}\frac{d^2[\psi(x)]}{dx^2} + \frac{1}{\cancel{\psi(x)T(t)}}V[\cancel{\psi(x)T(t)}]$$

$$i\hbar\frac{1}{T(t)}\frac{d[T(t)]}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2[\psi(x)]}{dx^2} + V.$$

This side of the equation
only depends on time

If the potential does not depend on time,
this side of the equation
only depends on space

For that to be true, each side must be constant

Time-independent Schrödinger equation: time part

$$\frac{1}{\cancel{\psi(x)}T(t)}i\hbar\cancel{\psi(x)}\frac{d[T(t)]}{dt}=-\frac{1}{\psi(x)\cancel{T(t)}}\frac{\hbar^2\cancel{T(t)}}{2m}\frac{d^2[\psi(x)]}{dx^2}+\frac{1}{\cancel{\psi(x)T(t)}}V[\cancel{\psi(x)T(t)}]$$

$$i\hbar\frac{1}{T(t)}\frac{d[T(t)]}{dt}=-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2[\psi(x)]}{dx^2}+V.$$

Taking a look to the left hand side

$$i\hbar\frac{1}{T(t)}\frac{d\left[T(t)\right]}{dt}=(\text{constant}) \qquad \frac{1}{T(t)}\frac{d\left[T(t)\right]}{dt}=\frac{(\text{constant})}{i\hbar}$$

Integrating both sides over time

$$\int_0^t\frac{1}{T(t)}\frac{d\left[T(t)\right]}{dt}dt=\int_0^t\frac{(\text{constant})}{i\hbar}dt \qquad \ln\left[T(t)\right]=\frac{(\text{constant})}{i\hbar}t=\frac{-i(\text{constant})}{\hbar}t$$

Calling the constant of integration E

$$T(t)=e^{-\frac{i(\text{constant})}{\hbar}t} \qquad T(t)=e^{-\frac{iE}{\hbar}t}$$

Time-independent Schrödinger equation: spatial part

Taking a look to the right hand side

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\left[\psi(x)\right]}{dx^2}+V=E$$

The same as in the time equation

Multiplying both sides by $\psi(x)$ we arrive to the
time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\left[\psi(x)\right]}{dx^2}+V\left[\psi(x)\right]=E\left[\psi(x)\right]$$

Its solutions $\psi(x)$ describe only the spatial behaviour of the quantum wavefun.

They depend on the behaviour of the potential in the region of interest

Time-independent Schrödinger equation: spatial part

$$-\frac{\hbar^2}{2m}\frac{d^2\left[\psi(x)\right]}{dx^2}+V\left[\psi(x)\right]=E\left[\psi(x)\right]$$

It is an eigenvalue equation
Consider the operator

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V$$

Then, the TISE can be written as

$$\hat{H}\left[\psi(x)\right]=E\left[\psi(x)\right]$$

Eigenvalue

Eigenfunction

Time-independent Schrödinger equation: stationary states

The wave function $\Psi(x,t)$ depends both on time and space
It changes over time

So, what is the meaning of stationary?

Stationary means that the wave function $\Psi(x,t)$ may be separated into spatial and temporal functions,

$$\Psi(x,t) = \psi(x)T(t)$$

And quantities such as the probability density and expectation values do not vary over time

Time-independent Schrödinger equation: stationary states

Stationary means that the wave function $\Psi\ (x,t)$
may be separated into spatial and temporal functions,

$$\Psi(x,t) = \psi(x)T(t)$$

And quantities such as the probability density and expectation
values do not vary over time

Compute the inner product of such a separable wavefunction with itself

$$\begin{aligned}
\langle\Psi(x,t)|\Psi(x,t)\rangle \propto \Psi^*\Psi &= [\psi(x)T(t)]^*[\psi(x)T(t)] \\
&= [\psi(x)e^{-i\frac{E}{\hbar}t}]^*[\psi(x)e^{-i\frac{E}{\hbar}t}] \\
&= [\psi(x)]^*e^{i\frac{E}{\hbar}t}[\psi(x)]e^{-i\frac{E}{\hbar}t} = [\psi(x)]^*[\psi(x)],
\end{aligned}$$

The time dependence has disappeared
Any quantity involving $\Psi^*\Psi$ will not change over time (it will be “stationary”)
if the wave function is separable

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Time independent Schrödinger equation in 1D

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Three-dimensional Schrödinger equation

Now the wavefunction must be written as $\Psi(\vec{r}, t)$

To specify positions in 3D requires a position vector with three components
In Cartesian coordinates

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$

The second spatial derivatives will be replaced by the Laplacian operator

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Three-dimensional Schrödinger equation

Applying these changes

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V\left[(x,t)\right]\Psi(x,t)$$

$$\Downarrow$$

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + V\left[(\vec{r},t)\right]\Psi(\vec{r},t)$$

Time independent Schrödinger equation in three-dimensions

Using a similar approach (separation of variables)
to that used in the one-dimensional case

$$\Psi(\vec{r},t) = \psi(\vec{r})T(t)$$

Spatial part

$$-\frac{\hbar^2}{2m}\nabla^2\left[\psi(\vec{r})\right] + V\left[\psi(\vec{r})\right] = E\left[\psi(\vec{r})\right]$$

Temporal part

$$T(t) = e^{-i\frac{E}{\hbar}t}$$

The 3D Hamiltonian now takes the shape

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$$

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What does the electronic wave function represents?

Schrödinger interpretation (wrong):
the wavefunction of a charged particle might be
related to the spatial distribution of electric charge

Max Born

1954

Grandfather of
Olivia Newton John

Born's rule (1926):
the wavefunction represents a "probability amplitude" whose magnitude squared determines the probability that a certain result will be obtained when an observation is made

What does the electronic wave function represents?

The wavefunction is not a measurable disturbance in a physical medium

The wavefunction can be used to determine the possible results of measurements of quantum observables and to calculate the probabilities of those results

Principles of the Copenhagen interpretation (I)

Information content
The quantum state includes all possible information about a quantum system – there are no "hidden variables" with additional information.

Time evolution
Overtime, quantum states evolve smoothly in accordance with the Schrödinger equation unless a measurement is made.

Wavefunction collapse
Whenever an measurement of a quantum state is made, the state "collapses" to an eigenstate of the operator associated with the observable being measured.

Measurement results
The value measured for an observable is the eigenvalue of the eigenstate to which the original quantum state has collapsed.

Principles of the Copenhagen interpretation (II)

Uncertainty principle

Certain "incompatible" observables (such as position and momentum) may not be simultaneously known with arbitrarily great precisión

Born rule

The probability that a quantum state will collapse to a given eigenstate upon measurement is determined by the square of the amount of that eigenstate present in the original state (the wavefunction)

Correspondence principle

In the limit of very large quantum numbers, the results of measurements of quantum observables must match the results of classical physics.

Complementarity

Every quantum system includes complementary wave-like and particle-like aspects; whether the system behaves like a wave or like a particle when measured is determined by the nature of the measurement.

Physical meaning of the wave function

The wave function (ψ) in quantum mechanics is a fundamental mathematical entity that contains all the information about a quantum system.

While its square ($|\psi|^2$) represents the probability density,
the wave function itself has deeper physical implications

Encodes All Observable Properties:

The wave function contains information about a system’s position, momentum, energy, and other observable properties.

By applying the corresponding quantum mechanical operators
(e.g., position $\hat{x}$, momentum $\hat{p}$ Hamiltonian $\hat{H}$),
we can extract expectation values and probabilities for these quantities

Physical meaning of the wave function

The wave function (ψ) in quantum mechanics is a fundamental mathematical entity that contains all the information about a quantum system.

While its square ($|\psi|^2$) represents the probability density,
the wave function itself has deeper physical implications

Superposition Principle:

The Schrödinger equation is linear and homogeneous.
Therefore, the solutions can be superposed linearly

The wave function allows for quantum superposition,
meaning a system can exist in multiple states simultaneously until measured.
This leads to interference effects seen in phenomena like the double-slit experiment.

Physical meaning of the wave function

The wave function (ψ) in quantum mechanics is a fundamental mathematical entity that contains all the information about a quantum system.

While its square ($|\psi|^2$) represents the probability density, the wave function itself has deeper physical implications

Phase and Interference Effects:

The phase of the wave function plays a crucial role in quantum interference. Even if two wave functions have the same probability distribution, their relative phases can change how they combine (constructive or destructive interference).

Physical meaning of the wave function

The wave function (ψ) in quantum mechanics is a fundamental mathematical entity that contains all the information about a quantum system.

While its square ($|\psi|^2$) represents the probability density,
the wave function itself has deeper physical implications

Quantum Evolution and Determinism:
The wave function evolves deterministically according to the Schrödinger equation, meaning that while measurement introduces probabilities, the evolution of ψ itself is completely determined by the system’s Hamiltonian.

Physical meaning of the wave function

The wave function (ψ) in quantum mechanics is a fundamental mathematical entity that contains all the information about a quantum system.

While its square ($|\psi|^2$) represents the probability density, the wave function itself has deeper physical implications

Collapse and Measurement:

Upon measurement, the wave function “collapses” to a specific eigenstate of the measured observable, leading to the probabilistic nature of quantum mechanics.

Physical meaning of the wave function

While the wave function itself is not directly observable, it serves as the core mathematical and conceptual tool for understanding quantum phenomena.

the Copenhagen interpretation treats it as a tool for predicting measurement outcomes.