Mathematical Formulation of Quantum Mechanics and Electrodynamics

Christian Schmeiser[1]

1 The formulation of quantum mechanics

All physical theories are based on fundamental laws formulated in a mathematical framework and on correspondence rules mapping elements of the mathematical theory to physical objects. Compared to classical mechanics, the mathematical framework for quantum mechanics is difficult and the correspondence rules are less intuitive. We start be providing the mathematical basis for the *Schrödinger representation* of quantum mechanics.

Mathematical prerequisites

A vector space $\mathcal{H}$ over the field $\mathbb{C}$ of complex numbers, equipped with a scalar product $\langle\cdot,\cdot\rangle$, which is complete with respect to the norm $\|\psi\| := \sqrt{\langle\psi,\psi\rangle}$ induced by the scalar product, is called a *Hilbert space*.

A Hilbert space $\mathcal{H}$ is called *separable*, if it contains a denumerable complete orthonormal system, i.e. a sequence $\{u_i\}_{i\in\mathbb{N}} \subset \mathcal{H}$ such that

$$(i) \quad \langle u_i, u_j\rangle = \delta_{ij} \qquad \forall\, i,j \in \mathbb{N}\,,$$
$$(ii) \quad \psi = \sum_{i=1}^{\infty} \langle\psi, u_i\rangle u_i \qquad \forall\, \psi \in \mathcal{H}\,.$$

A linear map $A:\ D(A) \subset \mathcal{H} \to \mathcal{H}$ is called a *linear operator in* $\mathcal{H}$. It is *bounded* if there exists a constant $M \geq 0$, such that

$$\|A\psi\| \leq M\|\psi\| \qquad \forall\, \psi \in \mathcal{H}\,.$$

Bounded linear operators can always be extended to $\mathcal{H}$, and therefore for bounded linear operators we shall always consider the situation $D(A) = \mathcal{H}$.

A bounded linear operator is *nonnegative*, iff

$$\langle A\psi, \psi\rangle \geq 0 \qquad \forall\, \psi \in \mathcal{H}\,.$$

[1]Institut für Analysis und Scientific Computing, TU Wien, Wiedner Hauptstraße 8–10, 1040 Wien, Austria. Christian.Schmeiser@tuwien.ac.at

Let A be a nonnegative operator and $\{u_i\}_{i\in\mathbb{N}}$ a complete orthonormal set. Then the *trace* of A is defined by (the finite or infinite value)

$$\mathrm{tr}(A) = \sum_{i=1}^{\infty} \langle Au_i, u_i\rangle\,.$$

A simple computation shows that the value of the trace is independent from the choice of the complete orthonormal system. With a little care this definition can be extended to bounded but not necessarily nonnegative operators. Operators with a finite trace are called *trace (class) operators*.

For a linear operator A, the *adjoint operator* A^* is defined by

$$\langle A^*u, v\rangle = \langle u, Av\rangle \qquad \forall\, u \in D(A^*),\ v \in D(A)\,,$$

where the domain of A^* is defined by

$$D(A^*) = \{u \in \mathcal{H} :\ \exists\, w \in \mathcal{H} :\ \langle u, Av\rangle = \langle w, v\rangle\ \forall\, v \in D(A)\}\,.$$

By the Riesz theorem, $D(A^*) = \mathcal{H}$ holds for all bounded operators A. A bounded operator U satisfying $UU^* = U^*U = I$ is called *unitary*. Under a unitary transformation, the scalar product is invariant:

$$\langle Uu, Uv\rangle = \langle u, v\rangle \qquad \forall\, u, v \in \mathcal{H}\,.$$

A linear operator A is called *self adjoint*, iff $A^* = A$ and $D(A^*) = D(A)$ holds. *Symmetry*, i.e.,

$$\langle Au, v\rangle = \langle u, Av\rangle \qquad \forall\, u, v \in D(A)\,,$$

is neccessary for self adjointness. Obviously, for bounded operators it is also sufficient.

The *resolvant set* of a linear operator A is the set of all $\lambda \in \mathbb{C}$ such that the *resolvant*

$$R(\lambda, A) := (\lambda I - A)^{-1}$$

is a bounded operator. The complement (in $\mathbb{C}$) of the resolvant set is called the *spectrum* of A and is denoted by $\sigma(A)$. Self adjoint operators A satisfy $\sigma(A) \subset \mathbb{R}$.

The *point spectrum* $\sigma_p(A) \subset \sigma(A)$ is the set of all *eigenvalues*, i.e.,

$$\lambda \in \sigma_p(A) \quad\Longleftrightarrow\quad \exists\, u \in D(A),\ u \neq 0 :\ Au = \lambda u\,.$$

It has to be noted that in general the inclusion $\sigma_p(A) \subset \sigma(A)$ is strict and that, in particular, a *continuous spectrum* may occur along with a discrete point spectrum.

For a self adjoint operator A in a finite dimensional Hilbert space (say, $\dim\mathcal{H} = n$), there exists an orthonormal basis $\{u_1, \ldots, u_n\}$ of $\mathcal{H}$ consisting of eigenvectors of A, i.e., $Au_k = \lambda_k u_k$, $k = 1, \ldots, n$. Denoting the projection onto the k-th eigenspace of A by $P_k u = \langle u, u_k\rangle u_k$, we have the formula

$$A = \sum_{k=1}^{n} \lambda_k P_k \,, \tag{1.1}$$

which can be written in the form

$$A = \int_{-\infty}^{\infty} \lambda \, dE(\lambda) \,, \tag{1.2}$$

with the *spectral family* of projections

$$E(\lambda) = \sum_{\lambda_k \leq \lambda} P_k \,.$$

The spectral family satisfies the properties

$$\begin{aligned} &(i) \quad E(\lambda)E(\mu) = E(\lambda) \quad \text{for } \lambda \leq \mu \,, \\ &(ii) \quad E(-\infty) = 0 \,, \quad E(\infty) = I \,, \\ &(iii) \quad E(\lambda + 0) = E(\lambda) \,. \end{aligned} \tag{1.3}$$

This setting can be transferred to the infinite dimensional case. The *spectral theorem* asserts that for self adjoint operators in arbitrary Hilbert spaces a spectral family of projections with the properties (1.3) exists, such that (1.2) holds. The differential $dE(\lambda)$ vanishes away from $\sigma(A)$ and, thus, the integral in (1.2) only contains contributions from the spectral values of A.

The spectral theorem provides a framework for applying functions to self adjoint operators:

$$f(A) := \int_{-\infty}^{\infty} f(\lambda) dE(\lambda) \,.$$

The postulates

One of the experimental observations leading to the development of quantum mechanics was the fact that certain physical quantities, which should take

values from a continuum according to classical physics, take only discrete (or *quantized*) values in certain experiments. This is the case, for example, for the energy emitted by an electron in an atom. Free electrons, on the other hand, have a continuous range of energies. This should be a motivation for the first two postulates:

Postulate 1: To every quantum mechanical system there corresponds a separable Hilbert space $\mathcal{H}$.

Postulate 2: Every physical quantity (*observable*) is represented by a self adjoint operator A in $\mathcal{H}$. The physical quantity can only take values in the spectrum of A.

Another experimental observation shows that the outcome of experiments of quantum mechanical systems cannot be predicted deterministically, but only in a probabilistic sense. The same could be said within the framework of classical mechanics as a result of measurement errors and/or the complexity of a system. In quantum mechanics, however, the probabilistic nature is seen as a basic principle and, therefore, has to be part of every quantum mechanical theory.

The *state* of a system is therefore always understood as the description of an *ensemble* of systems with identical experimental conditions. To motivate the representation of states, let us consider a situation with a finite dimensional $\mathcal{H}$ and a self adjoint operator A with spectral decomposition (1.1). We shall compute the expected value of the observable corresponding to A. By postulate 2, the observable can only take one of the values $\lambda_1, \ldots, \lambda_n$. If the system is in a fixed state, these values are taken with probabilities $p_1, \ldots, p_n \geq 0$ ($p_1 + \cdots + p_n = 1$). The expected value of A is, thus,

$$\langle A \rangle = \sum_{k=1}^{n} p_k \lambda_k = \sum_{k=1}^{n} p_k \langle A u_k, u_k \rangle = \operatorname{tr}(\varrho A)\,,$$

$$\text{with } \varrho_{ij} = \sum_{k=1}^{n} p_k u_{k,i} \overline{u_{k,j}}\,.$$

The operator ϱ is nonnegative and satisfies $\operatorname{tr}(\varrho) = 1$.

Postulate 3: The state of a quantum mechanical system is represented by a nonnegative trace operator ϱ with $\operatorname{tr}(\varrho) = 1$, the *state operator* (or *density matrix*). The expectation value of an observable A is given by

$$\langle A \rangle = \operatorname{tr}(\varrho A)\,.$$

The definition of the probabilistic setting is completed by using the spectral family $E(\lambda)$ corresponding to the observable A. We define the distribution function for A by

$$\text{prob}(A \subset (-\infty, \lambda]) \quad = \quad \text{tr}(\varrho E(\lambda)) \, .$$

The spectral theorem shows that this is consistent with the formula for the expectation value in postulate 3.

The properties of the state operator immediately imply $\sigma(\varrho) \subset [0, 1]$. The projection onto a normalized vector $\psi \in \mathcal{H}$, $\|\psi\| = 1$, defines a *pure state*

$$\varrho u = \langle u, \psi \rangle \psi \, .$$

For a pure state, the formula for the distribution function and for the expectation value is simple:

$$\text{prob}(A \subset (-\infty, \lambda]) = \langle E(\lambda)\psi, \psi \rangle \, , \quad \langle A \rangle = \langle A\psi, \psi \rangle \, .$$

Non-pure states are called *mixed states*. The spectral theorem applied to state operators has the interpretation that mixed states can be written as convex combinations of pure states (at least in the case of a discrete $\sigma(\varrho) = \sigma_p(\varrho)$).

Note that for arbitrary real ω, ψ and $e^{i\omega}\psi$ define the same state. For a pure state, the vector ψ is only unique up to a *phase factor* $e^{i\omega}\psi$.

Space-time symmetries

We aim at a nonrelativistic theory, invariant with respect to the *Galilei group*. A general Galilei transformation τ we write as

$$\begin{pmatrix} x' \\ t' \end{pmatrix} = \tau \begin{pmatrix} x \\ t \end{pmatrix} = \begin{pmatrix} R_1(\vartheta_1)R_2(\vartheta_2)R_3(\vartheta_3)x + a + vt \\ t + s \end{pmatrix} . \tag{1.4}$$

Here $R_j(\vartheta_j)$ is an orthogonal matrix describing a rotation by the angle ϑ_j around the x_j-axis. So the Galilei transformation consists of a rotation, a translation by the vector a, a velocity shift by the velocity v, and a time shift by s. It can be further decomposed into 10 basic transformations, each depending on a scalar parameter. All these basic transformations $T(\lambda)$ with scalar parameter λ satisfy the group properties $T(0) = I$, $T(\lambda_1 + \lambda_2) = T(\lambda_1)T(\lambda_2)$, and they are continuous with respect to the parameter.

Requiring Galilei invariance of our theory, we represent Galilei transformations by unitary operators U_τ and the basic transformations by groups of unitary operators in $\mathcal{H}$ (see below). The combination of two Galilei transformations τ_1 and τ_2 can be represented by either $U_{\tau_1\tau_2}$ or by $U_{\tau_1}U_{\tau_2}$. For a normalized ψ, the vectors $U_{\tau_1\tau_2}\psi$ and $U_{\tau_1}U_{\tau_2}\psi$ have to represent the same pure state. This leads to the requirement

$$U_{\tau_1\tau_2} = e^{i\omega(\tau_1,\tau_2)}U_{\tau_1}U_{\tau_2} , \tag{1.5}$$

with a phase factor $e^{i\omega(\tau_1,\tau_2)}$.

Mathematical sidestep: continuous groups of unitary operators

A family $\{U(s) : \ s \in \mathbb{R}\}$ *of bounded operators in* $\mathcal{H}$ *is called a* continuous group, *iff*

$$\begin{aligned} &U(0) = I , \quad U(s_1 + s_2) = U(s_1)U(s_2) , \\ &\lim_{s\to 0} U(s)u = u \quad \forall\, u \in \mathcal{H} . \end{aligned}$$

The generator K *of a continuous group is defined by*

$$iKu := \lim_{s\to 0} \frac{U(s)u - u}{s} ,$$

for all $u \in D(K)$, i.e., such that the limit on the right hand side exists. We write $U(s) = e^{iKs}$. It can be shown that $u(s) = e^{iKs}u_0$ solves the initial value problem

$$\frac{du}{ds} = iKu\,, \quad u(0) = u_0\,.$$

Let $\{U(s) : \ s \in \mathbb{R}\}$ be a continuous group of unitary operators and consider the identity

$$0 = \frac{U(s)^*U(s) - I}{s} = U(s)^*\frac{U(s) - I}{s} + \frac{U(s)^* - I}{s}\,.$$

For $u, v \in D(K)$, we apply the right hand side to u and take the scalar product with v:

$$0 = \left\langle \frac{U(s)u - u}{s}, U(s)v \right\rangle + \left\langle u, \frac{U(s)v - v}{s} \right\rangle\,.$$

The limit $s \to 0$ gives

$$\langle iKu, v\rangle + \langle u, iKv\rangle = 0\,,$$

showing that the generators of continuous groups of unitary operators are symmetric.

In the following table we introduce the names of the generators of the groups of unitary operators corresponding to the basic Galilei transformations:

transformation	group
$x \to R_j(\vartheta_j)x$	$\exp(i\vartheta_j J_j)$
$x_j \to x_j + a_j$	$\exp(-ia_j P_j)$
$x_j \to x_j + v_j t$	$\exp(iv_j G_j)$
$t \to t + s$	$\exp(isH)$

The signs in the exponents are just conventions. The 10 generators in the right column are also denoted by $K_1, \ldots, K_{10}$. In the following, the requirement (1.5) will be used to derive relations between the K_n. However, the computations are purely formal. They would only be rigorously justified, if the generators were bounded operators.

Commutation relations will be derived by considering transformations of the form

$$e^{i\varepsilon K_m} e^{i\varepsilon K_n} e^{-i\varepsilon K_m} e^{-i\varepsilon K_n} = I + \varepsilon^2 [K_n, K_m] + O(\varepsilon^3)\,,$$

where $[\cdot,\cdot]$ denotes the *commutator* $[K_n, K_m] = K_n K_m - K_m K_n$. By (1.5), this transformation can also be written as

$$\exp(i\varepsilon^2 \omega_{mn}) U_\tau = I + i\varepsilon^2 \sum_{r=1}^{10} c_{nmr} K_r + i\varepsilon^2 \omega_{nm} I + O(\varepsilon^3)\,,$$

resulting in

$$[K_m, K_n] = i \sum_{r=1}^{10} c_{mnr} K_r + i\omega_{mn} I\,.$$

We shall evaluate the coefficients on the right hand side in two steps. First the c_{mnr} will be found by computing the space-time transformation τ.

Obviously, translations commute with each other, with velocity shifts, and with time shifts:

$$[P_j, P_k] = i\omega I\,, \quad [P_j, G_k] = i\omega I\,, \quad [P_j, H] = i\omega I\,,$$

where ω is still unknown and takes possibly different values in each of the above equations. It is also easy to see that velocity shifts commute with each other and that rotations commute with time shifts:

$$[G_j, G_k] = i\omega I\,, \quad [J_j, H] = i\omega I\,.$$

Furthermore, rotations commute with translations and velocity shifts along their axes:

$$[J_j, P_j] = i\omega I\,, \quad [J_j, G_j] = i\omega I\,.$$

All other pairs of basic transformations do not commute. The space-time transformation corresponding to

$$e^{i\varepsilon H} e^{i\varepsilon G_j} e^{-i\varepsilon H} e^{-i\varepsilon G_j}$$

is carried out step by step:

$$\begin{aligned} (x,t) &\to (x - \varepsilon t e_j, t) \to (x - \varepsilon t e_j, t - \varepsilon) \\ &\to (x - \varepsilon t e_j + \varepsilon(t-\varepsilon), t - \varepsilon) \to (x - \varepsilon^2 e_j, t)\,, \end{aligned}$$

where $\{e_1, e_2, e_3\}$ denotes the canonical basis of $\mathbb{R}^3$. The resulting transformation is a translation, resulting in

$$[G_j, H] = iP_j + i\omega I\,.$$

Finally, we have to work on the rotations. The rotation matrices are given by

$$R_1(\vartheta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\vartheta & \sin\vartheta \\ 0 & -\sin\vartheta & \cos\vartheta \end{pmatrix}, \quad R_2(\vartheta) = \begin{pmatrix} \cos\vartheta & 0 & -\sin\vartheta \\ 0 & 1 & 0 \\ \sin\vartheta & 0 & \cos\vartheta \end{pmatrix},$$

$$R_3(\vartheta) = \begin{pmatrix} \cos\vartheta & \sin\vartheta & 0 \\ -\sin\vartheta & \cos\vartheta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Taylor expansion gives $R_j(\varepsilon) = I + i\varepsilon M_j + O(\varepsilon^2)$ with

$$M_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad M_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Computation of the commutators gives

$$[M_j, M_k] = i\varepsilon_{jkl} M_l\,,$$

where the summation convention and the epsilon-tensor is used: $\varepsilon_{jkl} = 1$ if (j,k,l) is an even permutation of $(1,2,3)$, $\varepsilon_{jkl} = -1$ if (j,k,l) is an odd permutation of $(1,2,3)$, and $\varepsilon_{jkl} = 0$ otherwise. As a consequence we have

$$[J_j, J_k] = i\varepsilon_{jkl} J_l + i\omega I\,.$$

The space transformation corresponding to

$$e^{i\varepsilon G_k} e^{i\varepsilon J_j} e^{-i\varepsilon G_k} e^{-i\varepsilon J_j}$$

is carried out step by step:

$$\begin{aligned} x &\to R_j(-\varepsilon)x - \varepsilon t e_k \to x - \varepsilon t R_j(\varepsilon) e_k + \varepsilon t e_k \\ &= x + \varepsilon t (I - R_j(\varepsilon)) e_k = x - i\varepsilon^2 t M_j e_k + O(\varepsilon^3) = x + \varepsilon^2 t \varepsilon_{jkl} e_l\,. \end{aligned}$$

The resulting transformation is a velocity shift, resulting in

$$[J_j, G_k] = i\varepsilon_{jkl} G_l + i\omega I \,.$$

Very similarly, we derive

$$[J_j, P_k] = i\varepsilon_{jkl} P_l + i\omega I \,.$$

For the evaluation of the various ωs, two properties of the commutator are used: The antisymmetry,

$$[K_m, K_n] + [K_n, K_m] = 0 \,,$$

and the *Jacobi identity*,

$$[[K_m, K_n], K_l] + [[K_n, K_l], K_m] + [[K_l, K_m], K_n] = 0 \,.$$

For example, the Jacobi identity for the triple (G_j, H, P_k) leads to

$$[P_j, P_k] = 0 \,.$$

Here we used the fact that the identity commutes with every other operator. Similarly, with the triples (J_j, P_k, H), (J_j, G_k, G_j), and (J_j, J_k, H), we obtain

$$[P_j, H] = [G_j, G_k] = [J_j, H] = 0 \,.$$

By the antisymmetry of the commutator, the matrix with the entries ω_{jk} from

$$[J_j, J_k] = i\varepsilon_{jkl} J_l + i\omega_{jk} I$$

must be antisymmetric and can therefore be written as $\omega_{jk} = \varepsilon_{jkl} b_l$ with an appropriate vector (b_1, b_2, b_3). Redefining the rotation generators by $J_j + b_j I \to J_j$ leads to

$$[J_j, J_k] = i\varepsilon_{jkl} J_l \,.$$

The redefinition of the generators changes the rotation operators only by phase factors and, thus, does not have any physical significance.

As the next step, we apply the Jacobi identity to the triple (J_1, J_2, G_3), resulting in

$$[J_3, G_3] = [J_1, G_1] + [J_2, G_2] \,.$$

Rotation of the indices in this computation gives

$$[J_1, G_1] = [J_2, G_2] + [J_3, G_3]\,, \quad [J_2, G_2] = [J_3, G_3] + [J_1, G_1]\,.$$

These 3 equations imply

$$[J_j, G_j] = 0\,.$$

This and the Jacobi identity for the triple (J_j, J_k, G_j) proves the antisymmetry of $[J_j, G_k]$. With an argument as above, we can write

$$[J_j, G_k] = i\varepsilon_{jkl} G_l + i\varepsilon_{jkl} b_l\,,$$

and, with the redefinition $G_j + b_j \to G_j$, produce the final commutation relation

$$[J_j, G_k] = i\varepsilon_{jkl} G_l\,.$$

Similarly, we obtain

$$[J_j, P_k] = i\varepsilon_{jkl} P_l\,,$$

after a redefinition of the P_j.

The Jacobi identity for (J_j, G_k, H) now leads to

$$[G_j, H] = iP_j\,.$$

Finally, with the triples (J_j, G_k, P_j) with $j \neq k$ and (J_j, G_k, P_l) with (j, k, l) pairwise different, we get

$$[G_j, P_k] = i\delta_{jk} MI\,,$$

with an arbitrary constant M, which cannot be determined within our algebraic framework. It turns out that this fact has physical significance, which will be discussed further below.

Dynamics of a single free particle

If the quantum mechanical system consists of a single particle, we introduce the vector valued *position operator* $\mathbf{Q} = (Q_1, Q_2, Q_3)$, with $\sigma(Q_j) = \mathbb{R}$, $j = 1, 2, 3$, and the Q_j have common eigenvectors: For every $x \in \mathbb{R}^3$ there is a $u(x) \in \mathcal{H}$ such that $Q_j u(x) = x_j u(x)$, $j = 1, 2, 3$. The *velocity operator* $\mathbf{V} = (V_1, V_2, V_3)$ is then defined by the requirement

$$\frac{d}{dt}\langle \mathbf{Q} \rangle = \langle \mathbf{V} \rangle \,.$$

In particular, for a time dependent pure state, given by $\psi(t) \in \mathcal{H}$ this gives

$$\langle \mathbf{V}\psi, \psi \rangle = \frac{d}{dt}\langle \mathbf{Q}\psi, \psi \rangle = \left\langle \mathbf{Q}\frac{d\psi}{dt}, \psi \right\rangle + \left\langle \mathbf{Q}\psi, \frac{d\psi}{dt} \right\rangle$$

Since H is the generator of the time shift transformation, we have $\exp(isH)\psi(t) = \psi(t+s)$. Comparing the generators of both sides (derivatives with respect to s at $s = 0$) gives

$$\frac{d\psi}{dt} = iH\psi \,,$$

and, thus,

$$\mathbf{V} = i[\mathbf{Q}, H] \,. \tag{1.6}$$

We shall need commutation relations between $\mathbf{Q}$ and $\mathbf{P} = (P_1, P_2, P_3)$. We start by postulating the action of the space shift operator on the eigenvectors of $\mathbf{Q}$:

$$e^{-ia\cdot\mathbf{P}} u(x) = u(x + a)$$

with the consequence

$$e^{ia\cdot\mathbf{P}} Q e^{-ia\cdot\mathbf{P}} u(x) = (x + a)u(x) \,,$$

giving

$$e^{ia\cdot\mathbf{P}} \mathbf{Q} e^{-ia\cdot\mathbf{P}} = \mathbf{Q} + aI \,.$$

Taylor expansion for small a leads to the commutation relations

$$[Q_j, P_k] = i\delta_{jk} I \,.$$

As a next step we postulate the following relations between operators:

$$\mathbf{J} = \mathbf{Q} \times \mathbf{P}\,, \qquad H = -\frac{\mathbf{P} \cdot \mathbf{P}}{2M}\,,$$

with $\mathbf{J} = (J_1, J_2, J_3)$. These satisfy all the commutation relations stated so far. Substitution of the second relation into (1.6) gives

$$\begin{aligned} &\mathbf{P} = M\mathbf{V}\,, \quad \text{and, thus,} \\ &-H = \frac{1}{2} M\mathbf{V} \cdot \mathbf{V}\,, \\ &\mathbf{J} = \mathbf{Q} \times M\mathbf{V}\,. \end{aligned}$$

If M where the mass of the particle, these where reasonable definitions of momentum, kinetic energy, and angular momentum. However, comparison of dimensions shows that M has to be measured in $\frac{sec}{cm^2}$. It is plausible that M can be written as

$$M = \frac{m}{\hbar}\,,$$

where m is the mass of the particle and $\hbar$ is a fundamental constant with the dimension of an action (Wirkung). It is called the *Planck constant* (Planckssches Wirkungsquantum), and its value has been determined experimentally: $\hbar \approx 1.054573 \times 10^{-34}$ joule-seconds.

At this point we conveniently redefine the operators $\mathbf{P} \to \mathbf{P}/\hbar$, $H \to -H/\hbar$, $\mathbf{J} \to \mathbf{J}/\hbar$, such that the new operators correspond to momentum, kinetic energy, and angular momentum.

Referring to classical mechanics, the *Hamiltonian* H for a particle moving in a position dependent external field given by the vector potential $A(x)$ and a scalar potential $W(x)$ is defined as

$$H = \frac{1}{2} m(\mathbf{V} - A(Q)) \cdot (\mathbf{V} - A(Q)) + W(Q)\,.$$

The equations of motion and conservation laws

With the Hamiltonian given above, the state vector $\psi(t)$ of a time dependent pure state satisfies the abstract ordinary differential equation

$$i\hbar \frac{d\psi}{dt} = H\psi \,.$$

For the corresponding density matrix defined by $\varrho u = \langle u, \psi \rangle \psi$ a straightforward computation shows

$$i\hbar \frac{d\varrho}{dt} = [H, \varrho] \,,$$

which will also be assumed to hold for general (mixed) states.

For an observable A the evolution of the expected value is governed by

$$i\hbar \frac{d}{dt} \langle A \rangle = \langle [A, H] \rangle \,,$$

with the consequence that the expected values of all observables, which commute with the Hamiltonian, are conserved in time. Examples for the free particle are the identity, $\mathbf{P}$, $\mathbf{J}$, and H, corresponding to conservation of mass, momentum, angular momentum, and energy.

2 Coordinate representation and the Schrödinger equation

For a one particle system we choose the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$, i.e. state vectors are complex valued square integrable *wave functions* $\psi(x)$ satisfying

$$1 = \|\psi\|^2 = \int_{\mathbb{R}^3} |\psi(x)|^2 \, dx \,.$$

The action of the position and translation operators are defined as

$$(\mathbf{Q}\psi)(x) = x\psi(x) \quad \text{and} \quad (e^{ia\cdot\mathbf{P}/\hbar}\psi)(x) = \psi(x+a) \,.$$

Consequently, the momentum and angular momentum operators are given by

$$(\mathbf{P}\psi)(x) = -i\hbar\nabla\psi(x) \,, \quad (\mathbf{J}\psi)(x) = -i\hbar x \times \nabla\psi(x) \,,$$

and the Hamiltonian of a particle in an external field by

$$(H\psi)(x) = \frac{m}{2}\left(\frac{i\hbar}{m}\nabla + A(x)\right)\cdot\left(\frac{i\hbar}{m}\nabla\psi(x) + A(x)\psi(x)\right) + W(x)\psi(x)\,.$$

For vanishing vector potential A, the equation of motion for a time dependent wave vector becomes the *Schrödinger equation*

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + W\psi\,. \tag{2.1}$$

The density matrix $\varrho(x,y,t)$ of a pure state is

$$\varrho(x,y,t) = \psi(x,t)\overline{\psi(y,t)}\,.$$

For a mixed state its trace also has to be unity:

$$\mathrm{tr}(\varrho) = \int_{\mathbb{R}^3}\varrho(x,x,t)dx = 1\,.$$

The density matrix of a time dependent state has to satisfy the *von Neumann equation*

$$i\hbar\frac{\partial\varrho}{\partial t} = -\frac{\hbar^2}{2m}(\Delta_x\varrho - \Delta_y\varrho) + (W(x) - W(y))\varrho\,.$$

Returning to pure states, the probability to find the particle at time t in the domain $\Omega\subset\mathbb{R}^3$ is given by

$$\int_\Omega |\psi(x,t)|^2\,dx\,.$$

Computing the rate of change of this quantity, and using the arbitrariness of Ω we derive the conservation equation

$$\frac{\partial}{\partial t}|\psi|^2 + \nabla\cdot j = 0\,, \tag{2.2}$$

with the *probability flux*

$$j = \frac{\hbar}{m}\mathrm{Im}(\overline{\psi}\nabla\psi)\,.$$

Let us know check some of the properties stated in the abstract setting of the previous sections. For example, a Galilei transformation $x' = x - vt$, $t' = t$, should leave the Schrödinger equation invariant, if the wave function is multplied by a phase factor: $\psi(x,t) = e^{i\omega(x,t)}\psi'(x',t')$. Substitution in the Schrödinger equation (2.1) shows that the appropriate choice for the phase is $\omega(x,t) = \frac{m}{\hbar} v \cdot (x - vt)$.

Now we turn to the conservation laws. Integration of (2.2) shows that the property $\int_{\mathbb{R}^3} |\psi|^2 dx = 1$ is conserved. The expectation value for the momentum is

$$\langle \mathbf{P} \rangle = \langle -i\hbar\nabla\psi, \psi \rangle = \hbar \operatorname{Im} \int_{\mathbb{R}^3} \overline{\psi} \nabla\psi \, dx \,.$$

A straightforward computation shows that $\frac{d}{dt}\langle \mathbf{P} \rangle = 0$ holds if the potential vanishes, as expected. On the other hand, the energy

$$\langle H \rangle = \int_{\mathbb{R}^3} \left(\frac{\hbar^2}{2m} |\nabla\psi|^2 + W|\psi|^2 \right) dx$$

is conserved, when ψ solves (2.1): $\frac{d}{dt}\langle H \rangle = 0$.

A fundamental consequence of the quantum theory is the *Heisenberg uncertainty principle*, i.e., the fact that certain pairs of observables cannot be measured simultaneously with arbitrary accuracy. One of these pairs is position and momentum.

The *variance* ΔA of the observable A is determined by

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \| (A - \langle A \rangle)\psi \|^2$$

The uncertainty principle for position and momentum then takes the form of the inequality

$$\Delta Q_j \Delta P_j \geq \frac{\hbar}{2} \,,$$

for every pure state. The proof relies on the commutation relation

$$\frac{i}{\hbar}[P_j, Q_k] = \delta_{jk} I \,,$$

and on the identities

$$[A - \langle A \rangle, B - \langle B \rangle] = [A, B] \,, \qquad i\langle [A, B] \rangle = 2 \operatorname{Im} \langle A\psi, B\psi \rangle \,,$$

where the latter holds for symmetric operators A and B:

$$
\begin{aligned}
1 = \langle I \rangle &= \frac{i}{\hbar}\langle [P_j, Q_j] \rangle = \frac{i}{\hbar}\langle [P_j - \langle P_j \rangle, Q_j - \langle Q_j \rangle] \rangle \\
&= \frac{2}{\hbar}\,\mathrm{Im}\langle (P_j - \langle P_j \rangle)\psi, (Q_j - \langle Q_j \rangle)\psi \rangle \leq \frac{2}{\hbar}\,\|(P_j - \langle P_j \rangle)\psi\|\,\|(Q_j - \langle Q_j \rangle)\psi\| \\
&= \frac{2}{\hbar}\Delta P_j \Delta Q_j\,.
\end{aligned}
$$

Simple solutions of the Schrödinger equations can be obtained from eigenfunctions of the Hamiltonian: Let $(E, u(x))$ denote an eigenvalue-eigenfuction-pair, i.e., $Hu = Eu$. Then

$$\psi(x,t) = e^{-iEt/\hbar}u(x) \tag{2.3}$$

is a solution of the Schrödinger equation. Since the time dependence only occurs in a phase factor, all observables of this solution are constant in time. Therefore a solution of this form is called a *steady state solution with energy* E.

Eigenfunctions are only solutions of $Hu = Eu$ with $u \in L^2(\mathbb{R}^3)$. However, it can be shown that the continuous spectrum can also be recovered by solving this equation, looking for solutions u, not necessarily in $L^2(\mathbb{R}^3)$, but satisfying certain growth conditions at infinity. These so called *spectral functions* also correspond to pysically meaningful states of the form (2.3).

For example, the functions $u_k(x) = e^{ik\cdot x}$, $k \in \mathbb{R}^3$, are spectral functions of the Hamiltonian of a free particle ($W = 0$) corresponding to the spectral values

$$E_k = \frac{\hbar^2|k|^2}{2m}\,.$$

Tunnelling

The tunnelling effect is one of the striking differences between classical and quantum mechanics. A particle may cross a potential barrier higher than the energy of the particle.

Let us consider a rectangular potential barrier:

$$W(x) = \begin{cases} V_0 & \text{for } 0 < x < a\,, \\ 0 & \text{elsewhere.} \end{cases}$$

The one-dimensional steady state Schrödinger equation with energy E is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + W\psi = E\psi\,, \tag{2.4}$$

where we assume $0 < E < V_0$. A classical particle with energy E, travelling towards $x = 0$ from the left, would be reflected by the barrier. Setting $E = \frac{\hbar^2 k^2}{2m}$, $k > 0$, and $V_0 - E = \frac{\hbar^2\beta^2}{2m}$, solutions of (2.4) have the form

$$\psi(x) = \begin{cases} A_1 e^{ikx} + B_1 e^{-ikx}\,, & x \le 0\,, \\ Ce^{\beta x} + De^{-\beta x}\,, & 0 \le x \le a\,, \\ A_2 e^{ikx} + B_2 e^{-ikx}\,, & x \ge a\,. \end{cases}$$

The number of free constants is reduced to 2 by requiring ψ to be continuously differentiable.

The probability flux, computed in the three regions, is given by

$$j = \frac{\hbar}{m}\,\mathrm{Im}\left(\overline{\psi}\frac{d\psi}{dx}\right) = \frac{\hbar k}{m}(|A_1|^2 - |B_1|^2) = \frac{2\hbar\beta}{m}\,\mathrm{Im}(C\overline{D}) = \frac{\hbar k}{m}(|A_2|^2 - |B_2|^2)\,.$$

Away from the barrier (i.e., for $x < 0$ and $x > a$), the contribution $A_j e^{ikx}$ produces a rightgoing flux, and $B_j e^{-ikx}$ a leftgoing flux. The two remaining constants are determined by requiring a certain behaviour at infinity. We fix the incoming fluxes by choosing $A_1 = 1$, $B_2 = 0$. This should reflect a situation, where electrons move towards the barrier from the left. Then the part $B_1 e^{-ikx}$ can be interpreted as a reflection, and the part $A_2 e^{ikx}$ as a transmission. From the representations for the flux we obtain the equation

$$R + T = 1$$

with the reflection coefficient $R = |B_1|^2$ and the transmission coefficient $T = |A_2|^2$. These can be interpreted as probabilities for the electron to be reflected and transmitted, respectively. The term *tunnelling* is used for the fact that the transmission coefficient is positive in general, i.e., the electron crosses the barrier with positive probability although its kinetic energy would lead to reflection in a classical description. Solving for the coefficients in the representation of the wave function gives

$$B_1 = \frac{|z|^2(e^{a\beta} - e^{-a\beta})}{z^2 e^{-a\beta} - \overline{z}^2 e^{a\beta}}\,,$$

showing that the reflection coefficient tends to zero with the width a of the barrier.

Wigner transformation — The classical limit

In this section a connection between quantum and classical mechanics is established. We start with a nondimensionalization of the von Neumann equation

$$i\hbar\frac{\partial\varrho}{\partial t} = -\frac{\hbar^2}{2m}(\Delta_x\varrho - \Delta_y\varrho) + (W(x) - W(y))\varrho\,.$$

Let W_0 denote a typical potential difference such that the dimensionless $W_s = W/W_0$ takes moderate values. Then we introduce reference values L_0 and t_0 for length and time, respectively, and the corresponding scaling $x_s = x/L_0$, $t_s = t/t_0$. Here L_0 is chosen as a length scale which is typical for an experiment. We assume that L_0 is large enough such that the action $L_0\sqrt{mW_0}$ is large compared to $\hbar$, i.e.,

$$\varepsilon = \frac{\hbar}{L_0\sqrt{mW_0}} \ll 1\,.$$

Then t_0 is determined such that $\varepsilon = \hbar/(t_0W_0)$. Carrying out the scaling in the von Neumann equation and dropping the subscripts s for simplicity, we obtain

$$i\varepsilon\frac{\partial\varrho}{\partial t} = -\frac{\varepsilon^2}{2}(\Delta_x\varrho - \Delta_y\varrho) + (W(x) - W(y))\varrho\,.$$

We are interested in approximating this equation for small values of ε. This is made possible by the so called *Wigner transformation* (Eugene Wigner, 1932). It consists of two steps: First, a coordinate transformation in the 6-dimensional (x, y)-space is introduced:

$$x = \xi + \frac{\varepsilon\eta}{2}\,, \quad y = \xi - \frac{\varepsilon\eta}{2}\,.$$

In terms of (ξ, η), the von Neumann equation becomes

$$i\frac{\partial\varrho}{\partial t} = -\nabla_\eta\cdot\nabla_\xi\varrho + \frac{W(\xi + \varepsilon\eta/2) - W(\xi - \varepsilon\eta/2)}{\varepsilon}\varrho\,.$$

The second step is a Fourier transformation: The *Wigner function* is introduced by

$$w(\xi, k, t) = (2\pi)^{-3}\int_{\mathbf{R}^3}\varrho(\xi + \varepsilon\eta/2, \xi - \varepsilon\eta/2, t)e^{-ik\cdot\eta}d\eta\,.$$

The inversion formula then gives

$$\varrho(\xi+\varepsilon\eta/2,\xi-\varepsilon\eta/2,t)=\int_{\mathbb{R}^3} w(\xi,k,t)e^{ik\cdot\eta}dk =: \widehat{w}(\xi,\eta,t)\,.$$

Observing $\nabla_\eta\widehat{w}=\widehat{ikw}$, the Wigner function satisfies the *Wigner equation*

$$\frac{\partial w}{\partial t}+k\cdot\nabla_\xi w-(2\pi)^{-3}\int_{\mathbb{R}^3}\frac{W(\xi+\varepsilon\eta/2)-W(\xi-\varepsilon\eta/2)}{i\varepsilon}\widehat{w}e^{-ik\cdot\eta}\,d\eta=0\,.$$

In this equation, we may let the small parameter ε tend to zero. Observing $\eta\widehat{w}=i\widehat{\nabla_k w}$, the *classical limit* $\varepsilon\to 0$ gives formally

$$\frac{\partial w_0}{\partial t}+k\cdot\nabla_\xi w_0-\nabla_\xi W\cdot\nabla_k w_0=0\,, \tag{2.5}$$

for $w_0=\lim_{\varepsilon\to 0} w$.

The physical significance of the Wigner function is easily seen for a pure state $\varrho(x,y,t)=\psi(x,t)\overline{\psi(y,t)}$. Then the probability density for the position of the particle is given by

$$|\psi(x,t)|^2=\varrho(x,x,t)=\widehat{w}(x,0,t)=\int_{\mathbb{R}^3} w(x,k,t)dk\,,$$

and the probability flux (or momentum density) by

$$\varepsilon\mathrm{Im}(\overline{\psi(x,t)}\nabla\psi(x,t))=-i\nabla_\eta\widehat{w}(x,0,t)=\int_{\mathbb{R}^3} kw(x,k,t)dk\,.$$

These two relations show that the new independent variable k can be interpreted as a momentum, and the Wigner function has some properties of a probability distribution in phase space (i.e., position-momentum space). Its zeroth order moment with respect to k is the probability density in position space and its first order moment the momentum density. However, there is one problem with this view. It can be shown that the Wigner function may take negative values in general.

In the classical limit, on the other hand, there is no problem like this. Solutions of (2.5) remain positive if they are positive at some point in time. The *Liouville equation* (2.5) is the correct equation for a probabilistic description of classical mechanics. Let $(x(t),k(t))$ denote a classical particle trajectory, i.e., a solution of

$$\dot{x}=k\,,\quad \dot{k}=-\nabla_x W(x)\,.$$

Then, for solutions $w_0(x,k,t)$ of (2.5), $\frac{d}{dt}w_0(x(t),k(t),t)=0$ holds.