E QUANTA

E.1 *Schrödinger-equation as a Helmholtz-differential equation*

The iconic Schrödinger-equation

$$\mathrm{i}\hbar\partial_t\psi = \mathrm{H}\psi \tag{E.231}$$

determines the time-evolution of the wave function ψ with the Hamilton-operator H of the system. If you'd categorise the Schrödinger equation, it is elliptical rather than hyperbolical, so we need to provide boundary conditions to make the solution for ψ unique. Please remember the example about particles in an infinitively deep square potential well where $\psi = 0$ at the edges: This is effectively a Dirichlet boundary condition, likewise, the wave functions for the Coulomb-potential in the hydrogen-problem vanish for $r \to \infty$, in fulfilment of Dirichlet boundaries.

Separating out the time-dependent part by a separation of variables $\psi(x,t) = \exp(\mathrm{i}\mathrm{E}t/\hbar)\phi(x)$ recovers the time-independent Schrödinger equation,

$$\mathrm{H}\phi(x) = \mathrm{E}\phi(x) \tag{E.232}$$

where the phase of the wave function undergoes oscillations with $\exp(\mathrm{i}\mathrm{E}t/\hbar)$. Working in a position representation the Schrödinger equation becomes

$$\left(-\frac{\hbar^2\Delta}{2m} + \Phi(x)\right)\phi = \mathrm{E}\phi \quad \to \quad \left(\Delta + \frac{2m}{\hbar^2}\left[\mathrm{E} - \Phi\right]\right)\phi = 0 \tag{E.233}$$

which is the archetypical form of a Helmholtz-differential equation $\left(\Delta + k^2\right)\phi = 0$ for constant Φ. Weirdly enough, one would arrive at exactly this differential equation starting from a properly hyperbolic wave equation, even though the Schrödinger equation is elliptical, but with the added benefit that because the range of values has been extended to complex numbers, k^2 can be negative and one can switch between oscillatory behaviour for positive energies to exponentially decaying solutions for negative energies.

Non-relativistic quantum mechanics is based on Galilei-invariant classical mechanics, where time is a universal parameter to describe evolution, and as such it is not an observable. Thinking of expectation values $\langle t\rangle$ is pretty much devoid of meaning, and that's the reason why the energy-time uncertainty is just a different expression of the momentum-position uncertainty. From $\mathrm{E} = p^2/(2m)$ we can conclude that $\Delta\mathrm{E} = \mathrm{d}\mathrm{E}/\mathrm{d}p\ \Delta p = p/m\ \Delta p$ and $x = p/m\ t$ implies $\Delta x = \mathrm{d}x/\mathrm{d}t\ \Delta t = p/m\ \Delta t$ such that

$$\Delta\mathrm{E}\Delta t = \Delta p\Delta x \geq \frac{\hbar}{2} \tag{E.234}$$

without the need of defining an uncertainty Δt from (non-existent!) expectation values $\langle t^2\rangle$ and $\langle t\rangle$.

E.2 *Born's postulate and the conservation of probability*

Born's postulate gives a probabilistic interpretation to the wave function: $\rho(x) = \psi^*(x)\psi(x)$ is the probability to find the particle at position x in a localisation. With this interpretation, the total probability should be conserved in time evolution

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \mathrm{d}^3x\ \psi^*\psi = 0 \tag{E.235}$$

if the particles are stable and do not decay. From the time derivative $\partial_t\rho$ of of the probability density one can in fact derive a continuity relation:

$$\partial_t\rho = \partial_t(\psi^*\psi) = (\partial_t\psi^*)\psi + \psi^*\partial_t\psi = -\frac{\mathrm{i}}{\hbar}(\mathrm{H}\psi^*)\psi + \frac{\mathrm{i}}{\hbar}\psi^*(\mathrm{H}\psi) \tag{E.236}$$

by substituting the Schrödinger-equation and its conjugate (keeping in mind that H is hermitean, $\mathrm{H}^+ = \mathrm{H}$). For a standard form of the Hamilton-operator in position representation

$$\mathrm{H} = \frac{p^2}{2m} + \Phi = -\frac{\hbar^2\Delta}{2m} + \Phi \tag{E.237}$$

one can immediately see that the Φ-term is not relevant, such that with $\Delta = \partial_i\partial^i$ one gets

$$\partial_t\rho = \frac{\hbar}{2m\mathrm{i}}\left[(\Delta\psi^*)\psi - \psi^*\Delta\psi\right] = \frac{\hbar}{2m\mathrm{i}}\partial_i\left[(\partial^i\psi^*)\psi - \psi^*\partial^i\psi\right] = \partial_i j^i \tag{E.238}$$

with the probability current density j^i

$$j^i = \frac{\hbar}{2m\mathrm{i}}\left[(\partial^i\psi^*)\psi - \psi^*\partial^i\psi\right] \tag{E.239}$$

Please be careful here: Schrödinger-quantum mechanics is built on Galilean relativity and it's *not possible* to combine the time derivative of ρ with the divergence of j^i in to an expression like $\partial_\mu j^\mu = 0$.

One could violate the probability conserving continuity equation by adding an anti-hermitean term to the Hamilton-operator, for instance $\mathrm{H} \to \mathrm{H} - \mathrm{i}\Gamma$, with $(\mathrm{i}\Gamma)^+ = -\mathrm{i}\Gamma \neq \mathrm{i}\Gamma$ with a real-valued Γ. Then, focusing on this term alone, we would get

$$\partial_t\rho = (\partial_t\psi^*)\psi + \psi^*\partial_t\psi = -\left(\frac{\Gamma}{\hbar}\psi^*\right)\psi - \psi^*\left(\frac{\Gamma}{\hbar}\psi\right) = -2\frac{\Gamma}{\hbar}\psi^*\psi = -2\frac{\Gamma}{\hbar}\rho \tag{E.240}$$

which, depending on the sign of Γ, leads to exponential increase or decrease: The Γ-term would be suitable to describe creation or decay of particles.

E.3 *Ehrenfest's theorem*

The transition from quantum mechanics to classical mechanics is conceptually very complicated but needs in some way take care of the fact that in the limit $\hbar \to 0$ classical mechanics should be recovered. The transition is gradual as $\hbar$ provides a scale for the action S, as will be explained in Sect. E.5. But there is a more direct relation between quantum mechanics and classical mechanics in the form of Ehrenfest's theorem: For any hermitean operator A, $\mathrm{A}^+ = \mathrm{A}$, one can derive the time evolution of its expectation value $\langle\mathrm{A}\rangle$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathrm{A}\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\int \mathrm{d}^3x\ \psi^*\mathrm{A}\psi = \int \mathrm{d}^3x\ \partial_t\psi^*\mathrm{A}\psi + \psi^*\mathrm{A}\partial_t\psi \tag{E.241}$$

if A is stationary. The time derivatives $\partial_t \psi$ and $\partial_t \psi^*$ can be replaced by the Schrödinger-equation and its complex conjugate, keeping in mind that the Hamilton-operator H is itself hermitean, $H^+ = H$,

$$\frac{d}{dt}\langle A\rangle = \int d^3x\, \frac{H\psi^*}{-i\hbar} A\psi + \psi^* A \frac{H\psi}{i\hbar} = \frac{i}{\hbar}\int d^3x\, \psi^* [H, A]\, \psi = \frac{i}{\hbar}\langle [H, A]\rangle \tag{E.242}$$

which is very reminiscent of the Poisson-equation of motion. Let's go through a couple of particular cases: The simplest choice would be the identity operator A = id, which commutes with everything, [H, id] = 0, so the statement we'd derive would be

$$\frac{d}{dt}\langle \mathrm{id}\rangle = \frac{d}{dt}\int d^3x\, \psi^*\psi = \frac{d}{dt}\int d^3x\, \rho = 0 \tag{E.243}$$

such that the normalisation of the wave function is conserved in time evolution and the probability density $\rho = \psi^*\psi$ integrates up to one at every instant in time. Similarly easy is the choice A = H, and as H commutes with itself, [H, H] = 0 and the expectation value of energy is conserved,

$$\frac{d}{dt}\langle H\rangle = 0 \tag{E.244}$$

which is the quantum mechanical version of the Poisson-bracket $d\mathcal{H}/dt = \{\mathcal{H}, \mathcal{H}\}$ applied to the Hamilton-function $\mathcal{H}$. A slightly more interesting case is $A = x$ with the position operator x: Then,

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle [H, x]\rangle \tag{E.245}$$

and evaluating the commutator proceeds like this. The potential Φ in H commutes with x because it is just a function of position, so $[p^2, x]$ is left over: Working in the position-representation

$$[p^2, x]\psi = p^2 x\psi - x p^2\psi = (i\hbar)^2\left[\partial_x^2(x\psi) - x\partial_x^2\psi\right] = (i\hbar)^2\left[\partial_x(\psi + x\partial_x\psi) - x\partial_x^2\psi\right] \tag{E.246}$$

which simplifies to

$$[p^2, x]\psi = (i\hbar)^2\left[\partial_x\psi + \partial_x\psi + x\partial_x^2\psi - x\partial_x^2\psi\right] = 2(i\hbar)^2\partial_x\psi = 2i\hbar p\psi \tag{E.247}$$

such that

$$\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m} \tag{E.248}$$

taking care of the $-1/(2m)$-prefactor in the Hamilton-operator. The result implies that the expectation value of position changes in time with the expecation value of momentum,

$$\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m} \quad \rightarrow \quad m\langle x\rangle = \int dt\, \langle p\rangle \tag{E.249}$$

as one would expect in classical mechanics. Similarly, the evolution of $\langle p\rangle$ can be evaluated: This time, p commutes with the kinetic energy, $[p, p^2] = 0$ but does not

commute with the potential energy, $[p, \Phi] \neq 0$ because Φ is a function of x. Using again the position representation of p shows

$$[p,\Phi]\psi = p\Phi\psi - \Phi p\psi = \mathrm{i}\hbar\left[\partial_x(\Phi\psi) - \Phi\partial_x\psi\right] = \mathrm{i}\hbar\left[\partial_x\Phi\ \psi + \Phi\partial_x\psi - \Phi\partial_x\psi\right] = \mathrm{i}\hbar\partial_x\Phi\ \psi \tag{E.250}$$

such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = -\langle\partial_x\Phi\rangle \quad \rightarrow \quad \langle p\rangle = -\int \mathrm{d}t\,\langle\partial_x\Phi\rangle \tag{E.251}$$

as a Newton-equation of motion for the expectation values. Perhaps it's a nice catch how Ehrenfest's theorem can be derived using unitary time evolution with an operator U instead of substituting the Schrödinger equation (of course, the two would be absolutely equivalent). Then, $\psi(t) = \mathrm{U}\psi_0$ and $\psi^*(t) = \mathrm{U}^+\psi_0^*$ with initial conditions ψ_0:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathrm{A}\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\int \mathrm{d}^3x\ \psi^*\mathrm{A}\psi = \frac{\mathrm{d}}{\mathrm{d}t}\int \mathrm{d}^3x\ \psi_0^*\mathrm{U}^+\mathrm{A}\mathrm{U}\psi_0 \tag{E.252}$$

and consequently, the time derivatives only operate on U and U^+:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathrm{A}\rangle = \int \mathrm{d}^3x\left(\psi_0^*(\partial_t\mathrm{U}^+)\mathrm{A}\mathrm{U}\psi_0 + \psi_0^*\mathrm{U}^+\mathrm{A}(\partial_t\mathrm{U})\psi_0\right) \tag{E.253}$$

As $\mathrm{U} = \exp(-\mathrm{i}\mathrm{H}t/\hbar)$ and $\mathrm{U}^+ = \exp(+\mathrm{i}\mathrm{H}t/\hbar)$ the differentiation just gives $\pm\mathrm{i}\mathrm{H}/\hbar$ as a factor, and because H and U commute, one arrives at

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathrm{A}\rangle = \frac{\mathrm{i}}{\hbar}\int \mathrm{d}^3x\ \psi_0^*\mathrm{U}^+[\mathrm{H},\mathrm{A}]\mathrm{U}\psi_0 = \frac{\mathrm{i}}{\hbar}\int \mathrm{d}^3x\ \psi^*[\mathrm{H},\mathrm{A}]\psi = \frac{\mathrm{i}}{\hbar}\langle[\mathrm{H},\mathrm{A}]\rangle \tag{E.254}$$

Here, we've used that

$$\partial_t\mathrm{U}^+ = \partial_t\exp\left(\frac{\mathrm{i}\mathrm{H}t}{\hbar}\right) = \partial_t\sum_n\frac{1}{n!}\left(\frac{\mathrm{i}\mathrm{H}t}{\hbar}\right)^n = \frac{\mathrm{i}\mathrm{H}}{\hbar}\sum_n\frac{1}{n!}\left(\frac{\mathrm{i}\mathrm{H}t}{\hbar}\right)^n = \frac{\mathrm{i}\mathrm{H}}{\hbar}\mathrm{U}^+ \tag{E.255}$$

and similarly for U.

Loosely speaking, the centres of wave packets follow the classical equation of motions: This is the central statement of the Ehrenfest-theorem. Any quantification by how much the wave packets are focused on these locations in x and p requires the computation of the uncertainties $\Delta x^2 = \langle x^2\rangle - \langle x\rangle^2$ as well as $\Delta p^2 = \langle p^2\rangle - \langle p\rangle^2$

E.4 *Dispersion of wave packets and propagation with Green-functions*

Restarting with unitary time evolution of a wave function and introducing the bra-ket-notation

$$\left|\psi(t_f)\right\rangle = \mathrm{U}(t_f,t_i)\left|\psi(t_i)\right\rangle \quad \text{with} \quad \mathrm{U}(t_f,t_i) = \exp\left(-\frac{\mathrm{i}\mathrm{H}(t_f-t_i)}{\hbar}\right) \tag{E.256}$$

with a unitary time evolution operator $\mathrm{U}(t_f, t_i)$, which is true in generality as it solves the time-dependent Schrödinger equation, asks the question whether we can find a position representation in which the Hamilton-operator H is usually written down,

essentially by setting $p^2 = -\hbar^2\Delta/(2m)$. This is in fact possible by projection

$$\psi(x_f, t_f) = \left\langle x_f|\psi(t_f)\right\rangle = \left\langle x_f|\mathrm{U}(t_f, t_i)|\psi(t_i)\right\rangle \tag{E.257}$$

Squeezing in an orthonormal basis set to write the state $|\psi(t_i)\rangle$ in position representation as well

$$\psi(x_f, t_f) = \int \mathrm{d}^3x_i \, \left\langle x_f|\mathrm{U}(t_f, t_i)|x_i\right\rangle \langle x_i|\psi(t_i)\rangle \tag{E.258}$$

shows that the final state is related to the initial one in a convolution relation

$$\psi(x_f, t_f) = \int \mathrm{d}^3x_i \, \mathrm{K}(x_i, t_i \to x_f, t_f) \, \psi(x_i, t_i) \tag{E.259}$$

with the Green-function (or propagator) $\mathrm{K}(x_i, t_i \to x_f, t_f)$ evolving the wave function by collecting up all amplitudes of the initial state and assembling the final state.

For getting a specific shape of $\mathrm{K}(x_i, t_i \to x_f, t_f)$, we would specialise the case to the propagation of a free particle with $\mathrm{H} = p^2/(2m)$ and working in momentum representation, as the eigenfunctions of p and p^2 are particularly simple:

$$\mathrm{K}(x_i, t_i \to x_f, t_f) = \int \mathrm{d}^3p_f \int \mathrm{d}^3p_i \, \left\langle x_f|p_f\right\rangle \left\langle p_f|\exp\left(-\mathrm{i}\mathrm{H}(t_f - t_i)/\hbar\right)|p_i\right\rangle \langle p_i|x_i\rangle \tag{E.260}$$

as $\left\langle x_f|p_f\right\rangle$ and $\langle p_i|x_i\rangle$ are only plane waves $\exp(+\mathrm{i}p_f x_f)$ and $\exp(-\mathrm{i}p_i x_i)$, one can substitute them and integrate the expression, essentially performing a Fourier-transform,

$$\mathrm{K}(x_i, t_i \to x_f, t_f) = \sqrt{\frac{m\hbar}{2\pi\mathrm{i}(t_f - t_i)}} \exp\left(-\frac{\mathrm{i}m}{2\hbar}\frac{(x_f - x_i)^2}{t_f - t_i}\right) \tag{E.261}$$

which can be loosely interpreted as a diffusion kernel with the typical behaviour that the width of an initially δ_{D}-shaped wave function increases $\propto \sqrt{t}$.

E.5 *Path integrals*

Path integrals are a great view on the relation between the quantum mechanical propagation of probability and the classical variational principles, and they establish $\hbar$ as a scale for the action S. But please keep R. MacKenzie's words in mind who said: *"As far as I am aware, path integrals give us no dramatic new results in quantum mechanics of a single particle. Indeed, most, if not all calculations in quantum mechanics which can be done by path integrals can be done with considerable greater ease with the standard formulations".*

Ignoring MacKenzie's advice for this section, let's introduce an intermediate time t_i in the propagation of a free particle and see how the propagators need to be linked together, i.e. whether they form a group: Time as the parameter in the unitary time evolution operator is additive, therefore

$$\mathrm{U}(t_f - t_i) = \mathrm{U}(t_f - t_1 + t_1 - t_i) = \mathrm{U}(t_f - t_1)\mathrm{U}(t_1 - t_i) \tag{E.262}$$

and therefore the Green-function $\mathrm{K}(x_i, t_i \to x_f, t_f)$ becomes

$$\left\langle x_f|\mathrm{U}(t_f, t_i)|x_i\right\rangle = \left\langle x_f|\mathrm{U}(t_f - t_1)\mathrm{U}(t_1 - t_i)|x_i\right\rangle = \int \mathrm{d}^3x_1 \left\langle x_f|\mathrm{U}(t_f - t_1)|x_1\right\rangle\langle x_1|\mathrm{U}(t_1 - t_i)|x_i\rangle \quad \text{(E.263)}$$

which implies that

$$\mathrm{K}(x_i, t_i \to x_f, t_f) = \int \mathrm{d}^3x_1\, \mathrm{K}(x_i, t_i \to x_1, t_1)\mathrm{K}(x_1, t_1 \to x_f, t_f) \quad \text{(E.264)}$$

with effectively a marginalisation over all possible stop-over points x_1. This result can be generalised to more stop-over points such that the time interval $t_f - t_i$ is subdivided into n steps, $\delta = (t_f - t_i)/n$:

$$\left\langle x_f|\mathrm{U}(t_f, t_i)|x_i\right\rangle = \left\langle x_f|(\exp(-\mathrm{i}\mathrm{H}\delta/\hbar)^n|x_i\right\rangle = \left\langle x_f|(\exp(-\mathrm{i}\mathrm{H}\delta/\hbar)\ldots\exp(-\mathrm{i}\mathrm{H}\delta/\hbar)|x_i\right\rangle \quad \text{(E.265)}$$

using $\exp(\mathrm{i}\mathrm{H}(t_f - t_i)) = \exp(\mathrm{i}\mathrm{H}n\delta) = \exp(\mathrm{i}\mathrm{H}\delta)^n$. This can be decomposed by introducing complete basis sets into all $n-1$ gaps between the individual factors of $\exp(\mathrm{i}\mathrm{H}\delta)$:

$$\mathrm{K}(x_i, t_i \to x_f, t_f) = \prod_j^{n-1} \int \mathrm{d}^3x_j\, \mathrm{K}(x_j, t_j \to x_{j+1}, t_j + \delta) \quad \text{(E.266)}$$

with $x_0 = x_i$ and $x_n = x_f$, likewise $t_0 = t_i$ and $t_n = t_f = t_i + n\delta$. Of course you're already suspecting that we should take the limit $\delta \to 0$ or $n \to \infty$, while keeping $t_f - t_i = n\delta$ fixed, and link this to the idea of generating the time evolution U with H.

E.5.1 Phase space path integral

Our view on quantum-mechanical propagation is now very abstract: There are Green-functions that depend on the Hamilton-operator, which collect up the amplitudes of ψ at t_i and assemble them at t_f. Introducing intermediate steps requires to combine the Greens-functions in a convolution relation. The unitary time evolution operator, which is equivalent to the Green-function in position representation, can be replaced by its generator H in the limit of very small time intervals δ:

$$\mathrm{K}(x_j, t_j \to x_{j+1}, t_j + \delta) = \left\langle x_j|\exp(-\mathrm{i}\mathrm{H}\delta/\hbar)|x_{j+1}\right\rangle \simeq \left\langle x_j|1 - \mathrm{i}\mathrm{H}\delta/\hbar|x_{j+1}\right\rangle \quad \text{(E.267)}$$

Let's inspect the two resulting terms separately: Firstly, the term

$$\left\langle x_j|x_{j+1}\right\rangle = \int \frac{\mathrm{d}^3p_j}{(2\pi)^3}\, \exp\left(\mathrm{i}p_j(x_j - x_{j+1})\right) = \int \frac{\mathrm{d}^3p_j}{(2\pi)^3}\, \exp\left(\mathrm{i}p_j\dot{x}_j\delta\right) \quad \text{(E.268)}$$

is effectively the δ_D-function, which we rewrite as a $\mathrm{d}p$-integral. A clever step is to extend the term by δ/δ and identify $(x_i - x_{j+1})/\delta$ as $\dot{x}_j$. Secondly, we obtain

$$\left\langle x_j|\mathrm{H}|x_{j+1}\right\rangle = \int \frac{\mathrm{d}^3p_j}{(2\pi)^3}\, \mathrm{H}\exp\left(\mathrm{i}p_j(x_j - x_{j+1})\right) \quad \text{(E.269)}$$

by substitution of the Hamilton-operator in position representation. Reconstructing the Taylor-series then gives

$$\mathrm{K}(x_j, t_j \to x_{j+1}, t_j + \delta) = \int \frac{\mathrm{d}^3 p_j}{(2\pi)^3} \exp\left(\frac{\mathrm{i}\delta}{\hbar}(p_j \dot{x}_j - \mathrm{H})\right) \tag{E.270}$$

and collecting all intermediate steps results in

$$\mathrm{K}(x_i, t_i \to x_f, t_f) = \prod_j \int \mathrm{d}^3 x_j \int \frac{\mathrm{d}^3 p_j}{(2\pi)^3} \exp\left(\frac{\mathrm{i}}{\hbar}\delta \sum_j^{n-1} p_j \dot{x}_j - \mathrm{H}\right) \tag{E.271}$$

where in the exponential a very interesting term appears: $p_j \dot{x}_j - \mathrm{H}$ is the reverse Legendre-transform of H which would result in the Lagrange-function $\mathcal{L}$, and the summation over $n-1$ time steps of size δ over $\mathcal{L}$ would correspond to the action S, which is being de-dimensionalised by the Planck-constant $\hbar$. In the continuum limit one arrives at the phase space path integral,

$$\mathrm{K}(x_i, t_i \to x_f, t_f) = \int \mathcal{D}x \int \mathcal{D}p \exp\left(\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathcal{L}\right) = \int \mathcal{D}x \int \mathcal{D}p \exp\left(\frac{\mathrm{i}}{\hbar}\mathrm{S}\right) \tag{E.272}$$

Please be careful that we did in fact carry out the derivation in a simplified case for $\mathrm{H} = p^2/(2m)$ without any potential Φ, but we generalised the expression $\dot{x}p - \mathcal{H}$ to be the Lagrange-function (or rather, operator in this case) $\mathcal{L}$.

E.5.2 Configuration-space path integral

At least half of the integrals in the phase space path integral can be solved for a standard form

$$\mathrm{H} = \frac{p^2}{2m} + \Phi \tag{E.273}$$

for the Hamilton operator H. Realising that for this form of the Hamilton-operator the phase space path integral separates in a factor involving only momenta and a factor involving only coordinates and returning to the discrete representation for a second we can write

$$\mathrm{K} = \prod_j \int \mathrm{d}^3 x_j \exp\left(\frac{\mathrm{i}}{\hbar}\delta \sum_j^{n-1} \Phi(x_j)\right) \times \int \frac{\mathrm{d}^3 p_j}{(2\pi)^3} \exp\left(\frac{\mathrm{i}}{\hbar}\delta \sum_j^{n-1} p_j \dot{x}_j - \frac{p_j^2}{2m}\right) \tag{E.274}$$

The second factor only involves Gaussian-integrals which can be solved by completion of the square in the exponent, whereas this strategy would only work for the first term for a very specific physical system: the harmonic oscillator. Carrying out all $\mathrm{d}^3 p$-integrations yields:

$$\mathrm{K} = \prod_j \int \mathrm{d}^3 x_j \left(\frac{m\hbar}{2\pi\mathrm{i}\delta}\right)^{n/2} \exp\left(\frac{\mathrm{i}}{\hbar}\delta \sum_j^{n-1} \frac{m}{2}\dot{x}_j^2 - \Phi(x_j)\right) \tag{E.275}$$

where one again recognises the Lagrange-function $\mathcal{L}$ in the exponent: The squares of $\dot{x}$ needed for kinetic energy $m\dot{x}^2$ was provided by the Gaussian integrals over

momentum space at the step of completing the square. Therefore, the final result reads:

$$\mathrm{K}(x_i, t_i \to x_f, t_f) = \int \mathcal{D}x \, \exp\left(\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t \, \mathcal{L}\right) = \int \mathcal{D}x \, \exp\left(\frac{\mathrm{i}}{\hbar}\mathrm{S}\right) \tag{E.276}$$

The interpretation of the path-integral for the propagation Green-function is highly interesting, as it joins quantum mechanics with classical mechanics. First of all, all possible paths between x_i and x_f can be taken without any energy consideration: Didn't strike you as odd that there was no boundary condition on the classical variational principles if a particle can "afford" a certain path energetically? In quantum mechanics this is not so dramatic as there is tunneling and a penetration of the wave function into energetically disallowed regions. Making the transition from quantum mechanics to classical mechanics in the limit $\hbar \to 0$ should collapse the path integral and the "tube" where the wave function propagates, onto an infinitely thin line as the classical trajectory. Introducing a variation

$$x'(t) \to x(t) + \eta(t) \tag{E.277}$$

gives a corresponding variation of the action

$$\delta\mathrm{S} = \mathrm{S}[x'] - \mathrm{S}[x] = \int \mathrm{d}t \, \left(\frac{\delta \mathrm{S}}{\delta x}\eta + \frac{\delta^2 \mathrm{S}}{\delta x^2}\frac{\eta^2}{2} + \ldots\right) \tag{E.278}$$

This difference in the action gives rise to a variation of the Green-function

$$\delta\mathrm{K} = \exp\left(\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t \, \frac{\delta \mathrm{S}}{\delta x}\eta + \frac{\delta^2 \mathrm{S}}{\delta x^2}\frac{\eta^2}{2} + \ldots\right) \tag{E.279}$$

The classical path is defined as an extremum of the action, so $\delta\mathrm{S} = 0$ and $\delta\mathrm{S}/\delta x = 0$, as required by Hamilton's principle, so the decisive term is $\propto \eta^2$: Any large deviation from the classical path, no matter if positive or negative, introduces strong oscillations into K if

$$\frac{\delta^2 \mathrm{S}}{\delta x^2}\frac{\eta^2}{2} \gg \hbar \tag{E.280}$$

and in the path-integration $\mathcal{D}x$ these oscillating terms cancel each other out. In this sense, the Planck-constant $\hbar$ is a scale for the action S, differentiating between classical motion and quantum mechanical propagation. With a little overinterpretation one could even imagine that the particle wave duality is the mechanism by which the action is extremised: A particle sends out the probability waves and could propagate along all possible paths, but the classical one is singled out as it is assigned the highest probability by constructive interference. Deviations around the classical path are of order $\hbar$ in S, and whether this matters or not depends on the magnitude of $\mathrm{S}/\hbar$. Therefore, we have identified three key properties in the transition from quantum to classical mechanics: $\hbar$ as a the action S becomes less and less important, the uncertainty $\Delta p \Delta x \geq \hbar/2$ becomes irrelevant and the averages needed for Ehrenfest's theorem become perfectly defined without any dispersion.

E.6 *Uncertainty*

All observables are represented by hermitean operators, whose spectrum of eigenvalues (which are necessarily real-valued) are possible outcomes of a measurement. Sometimes the situation arises that two observables are not measurable at arbitrary precision at the same time, and the criterion whether a simultaneous measurement is possible is the value of the commutator $[\mathrm{A}, \mathrm{B}] = \mathrm{AB} - \mathrm{BA}$ of the two operators A and B. Defining the expectation values and variances

$$\langle \mathrm{A} \rangle = \int \mathrm{d}^3x \, |\psi|^2 \mathrm{A} \quad \text{and} \quad \langle \mathrm{A}^2 \rangle = \int \mathrm{d}^3x \, |\psi|^2 \mathrm{A}^2 \tag{E.281}$$

leads to the uncertainty $\Delta\mathrm{A} = \sqrt{\langle \mathrm{A}^2 \rangle - \langle \mathrm{A} \rangle^2}$, where we'll use the simplification $\Delta\mathrm{A} = \sqrt{\langle \mathrm{A}^2 \rangle}$ because setting $\langle \mathrm{A} \rangle = 0$ is always possible by redefining the operator.

The Cauchy-Schwarz-inequality implies that

$$\left(\int \mathrm{d}^3x \, |\psi|^2 \mathrm{A}\mathrm{B}^+ \right)^2 \leq \int \mathrm{d}^3x \, |\psi|^2 \mathrm{A}^2 \times \int \mathrm{d}^3x \, |\psi|^2 \mathrm{B}^2 \tag{E.282}$$

or short, $\langle \mathrm{AB} \rangle^2 \leq \langle \mathrm{A}^2 \rangle \langle \mathrm{B}^2 \rangle$. We can use the Cauchy-Schwarz-inequality as a lower bound:

$$\Delta\mathrm{A}\Delta\mathrm{B} = \sqrt{\langle \mathrm{A}^2 \rangle} \times \sqrt{\langle \mathrm{B}^2 \rangle} \geq \left| \frac{1}{2\mathrm{i}} \left(\langle \mathrm{AB} \rangle - \langle \mathrm{AB} \rangle^* \right) \right| = \frac{1}{2} \left| \langle \mathrm{AB} \rangle - \langle \mathrm{BA} \rangle \right| = \frac{1}{2} \left| \langle [\mathrm{A}, \mathrm{B}] \rangle \right| \tag{E.283}$$

where we've used that the modulus of a complex number is always larger than its imaginary part, that the scalar product is hermitean,

$$\langle \mathrm{AB} \rangle^* = \langle \mathrm{B}^+ \mathrm{A}^+ \rangle = \langle \mathrm{BA} \rangle \tag{E.284}$$

and that the operators themselves are hermitean. Fundamental commutators between coordinates and their canonical momenta are for instance $[p, x] = \mathrm{i}\hbar$:

$$[p, x]\psi = (px - xp)\psi = \mathrm{i}\hbar \left[\partial_x (x\psi) - x\partial_x \psi \right] = \mathrm{i}\hbar \left[\psi + x\partial_x \psi - x\partial_x \psi \right] = \mathrm{i}\hbar\psi. \tag{E.285}$$

E.7 *Relativistic quantum mechanics*

The rationale behind the Schrödinger-equation is a classical dispersion relation, $\mathrm{E} = p_i p^i / (2m)$ with the canonical displacements $\mathrm{E} \to \mathrm{i}\hbar\partial_t$ and $p_i \to \mathrm{i}\hbar\partial_i$. But we know already that the classical dispersion relation is only valid for small $cp \ll mc^2$ compared to the rest mass m.

One possibility to generalise the Schrödinger-equation is to use the fully relativistic dispersion relation

$$\mathrm{E}^2 = (cp)^2 + (mc^2)^2 \tag{E.286}$$

and perform canonical replacement on this equation: This procedure leads to the Klein-Gordon-equation,

$$\partial_{ct}^2 \psi - \partial_i \partial^i \psi + \left(\frac{mc}{\hbar} \right)^2 \psi = 0 \tag{E.287}$$

or shorthand

$$\left(\Box + \lambda^{-2}\right)\psi = 0 \quad \text{with} \quad \lambda = \frac{\hbar}{mc} \tag{E.288}$$

with a fully Lorentz-covariant $\Box = \eta_{\mu\nu}\partial^\mu\partial^\nu$. The constant term is rather interesting, as it defines the de Broglie-wavelength, $\lambda = \hbar/(mc)$ pertaining to the momentum mc. And for static situations, where $\partial_{ct}\psi = 0$ and consequently $\Box \to \Delta$, we recover the Yukawa-field equation A.3

$$\left(\Delta - \lambda^{-2}\right)\psi = 0 \tag{E.289}$$

and now the de Broglie-scale $\lambda = \hbar/(mc)$ gets the interpretation of a screening length, which effectively truncates the Coulomb-potential at $\lambda r \simeq 1$. We now understand perfectly Yukawa's reasoning: By introducing a mass-term into the field equation one can deviate from $\Phi \propto 1/r$ and make the potential finite-ranged. The range is controlled by the mass of the particle that is described by the Klein-Gordon-equation, so choosing about 100 MeV as a mass gives a restriction to nuclear dimensions, exactly what has been found in the π-mesons.

Effectively, we could even take this idea one step further and define directly a canonical substitution to the relativistic momentum p^μ:

$$p^\mu = \begin{pmatrix} \mathrm{E}/c \\ p^i \end{pmatrix} \to \mathrm{i}\hbar \begin{pmatrix} \partial_{ct} \\ -\partial^i \end{pmatrix} = \mathrm{i}\hbar\partial^\mu \tag{E.290}$$

and obtain $p^\mu p_\mu = -\hbar^2\Box = (mc)^2$ directly. There is a second path which leads to the Dirac-equation and the inclusion of spin-degrees of freedom of the wave functions (so-called spinors), but this is beyond the scope of this lecture.

E.8 *Coupling to fields*

Coupling of wave functions ψ to fields $\mathrm{F}^{\mu\nu}$ is rather subtle as it proceeds over the potential A^μ with all kinds of conceptual difficulties involving the Aharonov-Bohm-experiment. Establishing a relation between the momentum p^μ and the potential A^μ is done by minimal coupling,

$$p^\mu \to p^\mu - \frac{q}{c}\mathrm{A}^\mu \tag{E.291}$$

If one tries this with the Klein-Gordon equation E.287:

$$p^\mu p_\mu \psi = \left(\mathrm{i}\hbar\partial^\mu - \frac{q}{c}\mathrm{A}^\mu\right)\left(\mathrm{i}\hbar\partial_\mu - \frac{q}{c}\mathrm{A}_\mu\right)\psi = (mc)^2\psi \tag{E.292}$$

which becomes under the assumption of Lorenz-gauge $\partial_\mu \mathrm{A}^\mu = 0$

$$\Box\psi + \left(\frac{q}{c\hbar}\right)^2 \mathrm{A}_\mu \mathrm{A}^\mu \psi = \left(\frac{mc}{\hbar}\right)^2 \psi \tag{E.293}$$

which is in this form difficult to interpret, in particular the $\mathrm{A}_\mu\mathrm{A}^\mu$-term looks weird. Let's therefore try this again in a fixed frame, where $\mathrm{A}^\mu = (\Phi, \mathrm{A}^i)^t$:

$$p^\mu p_\mu \psi = \left(\mathrm{i}\hbar\partial_{ct} - \frac{q}{c}\Phi\right)^2 \psi - \left(\mathrm{i}\hbar\partial^i - \frac{q}{c}\mathrm{A}^i\right)\left(\mathrm{i}\hbar\partial_i - \frac{q}{c}\mathrm{A}_i\right)\psi = (mc)^2\psi \tag{E.294}$$

With a very similar calculation, assuming stationary electric potentials $\partial_{ct}\Phi = 0$ and Coulomb-gauge $\partial_i A^i = 0$ for simplicity,

$$\Box\psi - \left(\frac{q}{\hbar c}\right)^2 \left(\Phi^2 + A_i A^i\right)\psi = \left(\frac{mc}{\hbar}\right)^2 \psi \tag{E.295}$$

where clearly the $A_\mu A^\mu$- and $A_i A^i$-terms are not gauge invariant. There seems to be an issue, which gets resolved by considering the action of gauging on the wave function ψ itself:

The gauge principle states that one can change the potentials $A^\mu \to A^\mu + \partial^\mu \chi$ with a gauge function χ, without changing the physical fields $F^{\mu\nu}$. The purpose of gauging is to simplify and decouple the field equations, for instance by enforcing $\partial_\mu A^\mu = 0$. Up to this point, we've shown as well, that the Lagrange-function of electrodynamics is gauge invariant *if* charges are conserved, so we've got reason to assume that gauge invariance is the symmetry principle behind charge conservation. Charge conservation is a property of the matter, though, it needs to function in a way that the charge density can only change locally if there are currents converging on that point and accumulate charge. In summary, we would want to have a gauge invariant wave equation for the matter fields, and understand why gauge-invariance implies charge conservation.

What change could one apply to a wave function without changing any of the physical observables? The answer is clearly a phase transformation,

$$\psi \to \psi \exp(+i\alpha(x)) \qquad \psi^* \to \psi^* \exp(-i\alpha(x)) \tag{E.296}$$

with a real-valued field $\alpha(x)$, and it is obvious that for instance the probability density $\rho = \psi^*\psi$ is invariant under these phase transformations. Derivatives of the wave function pick up an additional term,

$$\partial_\mu \psi \to \partial_\mu(\psi \exp(i\alpha)) = (\partial_\mu \psi)\exp(i\alpha) + i\psi \exp(i\alpha)\partial_\mu \alpha \tag{E.297}$$

so terms like $\psi^* \partial_\mu \psi$ or $\partial_\mu \psi^* \partial^\mu \psi$ are not gauge invariant. Let's try out a new derivative D_μ with this property:

$$D_\mu \psi \to \exp(i\alpha) D_\mu \psi \tag{E.298}$$

where for instance $D_\mu \psi^* D^\mu \psi$ would be perfectly invariant.

These gauge-covariant derivatives do not commute

$$[D_\mu, D_\nu]\psi = \left[\partial_\mu - i\frac{q}{c}A_\mu, \partial_\nu - i\frac{q}{c}A_\nu\right]\psi = \left(\partial_\mu - i\frac{q}{c}A_\mu\right)\left(\partial_\nu - i\frac{q}{c}A_\nu\right)\psi - \left(\partial_\nu - i\frac{q}{c}A_\nu\right)\left(\partial_\mu - i\frac{q}{c}A_\mu\right)\psi \tag{E.299}$$

where a tedious but straightforward calculation shows that

$$[D_\mu, D_\nu]\psi = \left[\partial_\mu - i\frac{q}{c}A_\mu, \partial_\nu - i\frac{q}{c}A_\nu\right]\psi = -i\frac{q}{c}\left(\partial_\mu A_\nu - \partial_\nu A_\mu\right)\psi = -i\frac{q}{c}F_{\mu\nu}\psi \tag{E.300}$$

with the gauge-invariant field tensor $F_{\mu\nu}$ appearing. This idea, that the second (gauge)-covariant differentiations do not interchange, is central to general relativity and define

the Riemann-curvature $R^{\alpha}{}_{\beta\mu\nu}$:

$$[\nabla_\mu, \nabla_\nu]v^\alpha = -R^{\alpha}{}_{\beta\mu\nu}v^\beta \tag{E.301}$$

through the non-interchangeability of the second covariant derivatives acting on the vector v^α.