

# QUANTUM MECHANICS

Wiesław Czyż

(October 22, 2016)

Kraków  
2004



# Chapter 1

## Trajectories in quantum mechanics

### 1.1 Introduction

Paul A. M. Dirac starts “The Principles of Quantum Mechanics” as follows:

*“Classical mechanics has been developed continuously from the time of Newton and applied to an ever-widening range of dynamical systems, including the electromagnetic field in interaction with matter. The underlying ideas and the laws governing their application form a simple and elegant scheme, which one would be inclined to think could not be seriously modified without having all its attractive features spoilt. Nevertheless it has been found possible to set up a new scheme, called quantum mechanics, which is more suitable for the description of phenomena on the atomic scale and which is in some respect more elegant and satisfying than the classical scheme. This possibility is due to the changes which the new scheme involves being of a very profound character and not clashing with the features of the classical theory that make it so attractive, as a result of which all these features can be incorporated in the new scheme.”*

In one of his early papers [1.1] Dirac outlined an attractive possibility of a generalization of the classical mechanics to quantum mechanics, and this idea was many years later implemented and worked out in detail by Richard P. Feynman [1.2]. Indeed, Dirac was fully aware of this new possibility of looking at quantum mechanics as the following quotation from his early Review of Modern Physics article [1.3] tells us:

*“We have here the mathematical foundation of the analogy between the classical and quantum equations of motion, and can develop it to bring out the quantum analogue of all the main features of the classical theory of dynamics”.*

This is how Feynman sees the relation of Dirac’s idea with the “standard” quantum mechanics:

*“It is a curious historical fact that modern quantum mechanics began with two quite different mathematical formulations: the differential equation of Schrödinger, and the matrix algebra of Heisenberg. The two, apparently dissimilar approaches, were proved to be mathematically equivalent. These two points of view were destined to complement one another and to be ultimately synthesized*

in Dirac's transformation theory.

*This paper will describe what is essentially a third formulation of non-relativistic quantum theory. This formulation was suggested by some of Dirac's [1.1], [1.3] remarks concerning the relation of classical action to quantum mechanics. A probability amplitude is associated with an entire motion of a particle as a function of time, rather than simply with a position of the particle at a particular time.*"

In fact it appears that quantum mechanics quickly distanced itself from classical physics, and had even some overtones of an axiomatic formulation. From the preface to the first edition of "The principles of Quantum Mechanics" by P. A. M. Dirac: "...I have chosen the symbolic method.... This necessitated a complete break from the historical line of development, but this break is an advantage through enabling the approach to the new ideas to be made as direct as possible". All this in spite of the first steps made by Bohr, Sommerfeld and Einstein [1.10] (a very important paper largely unknown!) in close touch with classical mechanics through studying of the multi-periodic trajectories.

In these lectures we will discuss this Dirac–Feynman formulation of quantum mechanics which gives an intuitively attractive transition from the classical to quantal description of the evolution in time of physical systems. Quantum mechanics "saved" classical physics long time ago from nonsensical descriptions of the microscopic world. Recently, quantum mechanics "saved" again classical mechanics from the abyss of Chaos. In this last instance understanding of the intimate relations between classical description and the limit  $\hbar \rightarrow 0$  of quantum mechanics was of primary importance. We are going to study these relations on many examples. We shall assume that the reader is familiar with the "Hamiltonian" formulation of quantum mechanics whose main tools are: Schrödinger equation and wave functions, operators corresponding to physical "observables" and their commutation relations.

Let us start with a simple case of one particle of mass  $m$  moving in a potential  $V(x)$  in one spatial dimension. In classical mechanics the position,  $x$ , is uniquely given at any time  $t$  provided the boundary conditions are specified, e.g.

$$\bar{x}(t_a) = x_a, \quad \bar{x}(t_b) = x_b \quad (1.1)$$

The trajectory  $\bar{x}(t)$  is obtained from the equations of motion

$$m \frac{d^2 x}{dt^2} = -\frac{d}{dx} V(x) \quad (1.2)$$

which follow either from the Hamiltonian,  $H = p^2/2m + V(x)$ , or the Lagrangian  $L = m(\dot{x})^2/2 - V(x)$ :

$$\text{(Hamilton)} \quad \frac{d}{dt} p = -\frac{\partial H}{\partial x}, \quad \frac{d}{dt} x = \frac{\partial H}{\partial p}, \quad (1.3)$$

$$\text{(Lagrange)} \quad \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) = \frac{\partial L}{\partial x}. \quad (1.4)$$

The boundary conditions (1.1) with the equation of motion (1.2) determine just one trajectory  $\bar{x}(t)$ .

With the help of quantum mechanics we can describe a transition of a particle from the position  $x_a$  at time  $t_a$  to the position  $x_b$  at a later time  $t_b$  but not with just one trajectory. We have to construct an amplitude for a quantal transition from the state which gives at  $t_a$  the position of particle exactly at  $x_a$ , and at  $t_b$  exactly at  $x_b$  (hence the wave functions of the initial and final states have to be  $\delta(x - x_a)$  and  $\delta(x - x_b)$ , respectively).

We accomplish it with the help of the operator of evolution in time of quantum states. From the Schrödinger equation we know the evolution in time of a state given at  $t_a$ ,  $\Psi(x, t_a)$ . Writing

$$\Psi(x, t_b) = e^{-\frac{i}{\hbar}H(t_b-t_a)}\Psi(x, t_a), \quad (1.5)$$

we see that differentiation with respect to  $t_b$  gives the Schrödinger equation for  $\Psi(x, t_b)$

$$i\hbar \frac{\partial \Psi(x, t_b)}{\partial t_b} = H\Psi(x, t_b). \quad (1.6)$$

So, indeed, the operator  $\exp(-iH(t_b - t_a)/\hbar)$  performs the evolution in time of a state given at  $t_a$ .

We denote the vector representing particle at  $x$  by  $|x\rangle$ , and the amplitude we seek is

$$K(b, a) = \langle x_b | e^{-\frac{i}{\hbar}H(t_b-t_a)} | x_a \rangle. \quad (1.7)$$

We will call  $K(b, a)$  a propagator.

## 1.2 Reminder of Dirac's notation

In quantum mechanics the quantal states are represented by vectors. The wave function is a special case of a vector: the  $x$  component of a state vector  $|\Psi\rangle$  is  $\Psi(x)$ . Thus

$$\Psi(x) = \langle x | \Psi \rangle. \quad (1.8)$$

The probability of finding the particle in the vicinity of  $x$  is  $|\langle x | \Psi \rangle|^2 dx$ .

### Example: Momentum eigenstates

the state  $|p\rangle$  which is the eigenstate of momentum belonging to the eigenvalue  $p$  has the following wave function, in other words its representation in the position space is

$$\langle x | p \rangle = N e^{\frac{i}{\hbar}px}, \quad (1.9)$$

with  $N$  being a normalization constant. The state  $\langle p |$  is conjugate to  $|p\rangle$ , hence

$$\langle p | x \rangle = N e^{-\frac{i}{\hbar}px}. \quad (1.10)$$

### End of Example

We will work with vectors of states which form complete sets of states. That is to say any state vector can be represented as a superposition of the states which belong to a complete set, for instance

$$|\Psi\rangle = \sum_p c_p |p\rangle \quad (1.11)$$

with

$$c_p = \langle p | \Psi \rangle . \quad (1.12)$$

From the above it follows that the unit operator can be represented as the sum

$$\sum_l |l\rangle \langle l| = 1 \quad (1.13)$$

where  $l$  labels any complete set of states. In particular

$$\sum_p |p\rangle \langle p| = \sum_x |x\rangle \langle x| = 1 . \quad (1.14)$$

### 1.3 Path integral representation of $K(b, a)$

Let us continue constructing an analog of the classical evolution in time ( $t_b - t_a$ ) from a given position  $x_a$  to a given position  $x_b$  (see Fig.1.1).

We compute (1.7) introducing a discretization of time:  $t_b - t_a = N\epsilon$  where  $N$  is very large, hence  $\epsilon$  very small. For the sake of simplicity we set  $\hbar = m = 1$ . Since

$$e^{-i(t_b - t_a)H} = e^{-i\epsilon NH} = e^{-i\epsilon H} e^{-i\epsilon H} \dots e^{-i\epsilon H} \quad (1.15)$$

and

$$1 = \int dx_j |x_j\rangle \langle x_j| , \quad (1.16)$$

we have

$$\begin{aligned} \langle x_b | e^{-i(t_b - t_a)H} | x_a \rangle &= \int \langle x_b | e^{-i\epsilon H} | x_{N-1} \rangle dx_{N-1} \langle x_{N-1} | e^{-i\epsilon H} | x_{N-2} \rangle \\ &\dots \langle x_2 | e^{-i\epsilon H} | x_1 \rangle dx_1 \langle x_1 | e^{-i\epsilon H} | x_a \rangle . \end{aligned} \quad (1.17)$$

Looking at Fig. 1.1 and formula (1.17) we see that the quantal analog of the classical evolution in time given by just one trajectory going from the initial spacetime point to the final spacetime point consist of *infinitely many* trajectories between the two spacetime points. These trajectories appear with different weighting factors which we will presently calculate.

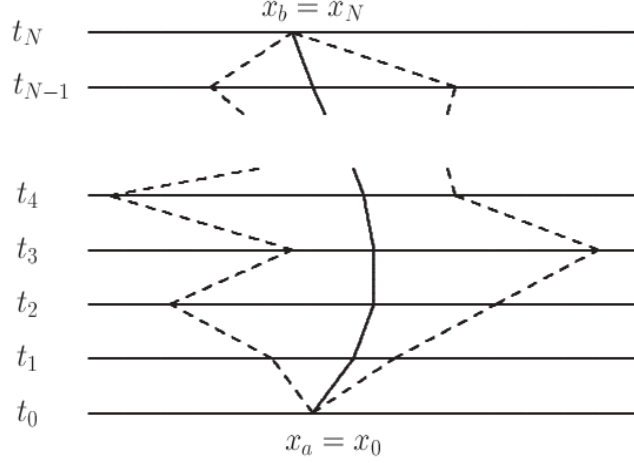


Figure 1.1: Trajectories in discretized time.

We do it for a simple hamiltonian

$$H = \frac{p^2}{2m} + V(x) = K + V. \quad (1.18)$$

Using the Campbell–Baker–Hausdorff formula, we write

$$e^{-i\epsilon H} = e^{-i\epsilon(K+V)} = e^{-i\epsilon K} e^{-i\epsilon V} + O(\epsilon^2) \quad (1.19)$$

where  $O(\epsilon^2) = -\frac{1}{2}\epsilon^2[V, K]$ , and  $[V, K] = VK - KV \neq 0$  is the commutator. The proof of the Campbell-Baker-Hausdorff formula,

$$e^A e^B = e^C \quad (1.20)$$

and

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] + \frac{1}{12}[[A, B], B] + \dots$$

for  $[A, B] \neq 0$ , is given in Appendix A.

In our amplitude (1.17) we can replace

$$\lim_{\substack{\epsilon \rightarrow 0, N \rightarrow \infty \\ N\epsilon = \text{const.}}} \left( e^{-i\epsilon(K+V)} \right)^N = \left( e^{-i\epsilon K} e^{-i\epsilon V} \right)^N. \quad (1.21)$$

Indeed, since the contents of the brackets in (1.21) differ by  $O(\epsilon^2) \sim N^{-2}$ , taking their  $N$ -th power makes that the r.h.s and the l.h.s of relation (1.21) differ by a term of  $O(N^{-1})$ . This relation, known as the Trotter product formula, is discussed in more detail in ref.[1.5].

So, we write our propagator as follows

$$\begin{aligned} K(b, a) &= \langle x_b | e^{-i(t_b - t_a)H} | x_a \rangle \\ &= \int \langle x_b | e^{-i\epsilon K} | x_{N-1} \rangle e^{-i\epsilon V(x_{N-1})} dx_{N-1} \langle x_{N-1} | e^{-i\epsilon K} | x_{N-2} \rangle \\ &\quad \times e^{-i\epsilon V(x_{N-2})} dx_{N-2} \dots dx_1 \langle x_1 | e^{-i\epsilon K} | x_a \rangle e^{-i\epsilon V(x_a)}. \end{aligned} \quad (1.22)$$

Now we calculate  $\langle x | \exp(-i\epsilon K/\hbar) | y \rangle$  inserting back  $\hbar$  and  $m$ . Since  $|p\rangle$  is the eigenvector of the operator  $K = p^2/2m$ , we insert  $1 = \int dp |p\rangle \langle p|$  and have

$$\begin{aligned} \langle x | e^{-\frac{i}{\hbar}\epsilon K} | y \rangle &= \int dp \langle x | e^{-\frac{i}{\hbar}\epsilon \frac{p^2}{2m}} | p \rangle \langle p | y \rangle \\ &= \int dp \langle x | p \rangle e^{-\frac{i\epsilon p^2}{\hbar 2m}} \langle p | y \rangle . \end{aligned} \quad (1.23)$$

But, inserting the normalization factor, we use

$$\langle p | y \rangle = \sqrt{\frac{1}{2\pi\hbar}} e^{\frac{i}{\hbar}py} . \quad (1.24)$$

Indeed, this is the correct normalization factor since

$$\langle p | p' \rangle = \int dy \langle p | y \rangle \langle y | p' \rangle = \frac{1}{2\pi\hbar} \int dy e^{\frac{i}{\hbar}(p-p')y} = \delta(p-p') .$$

So, we have finally

$$\langle x | e^{-\frac{i}{\hbar}\epsilon K} | y \rangle = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp e^{-\frac{i\epsilon p^2}{\hbar 2m}} e^{\frac{i}{\hbar}(y-x)p} = \sqrt{\frac{m}{2i\pi\hbar\epsilon}} e^{im\frac{(y-x)^2}{2\epsilon\hbar}} \quad (1.25)$$

where we employed the formula

$$\int_{-\infty}^{+\infty} dx e^{ax^2+bx} = \sqrt{\frac{\pi}{-a}} e^{-\frac{b^2}{4a}} , \quad \text{Re } a \leq 0 , \quad (1.26)$$

which will be often used in these lectures.

We insert (1.25) into (1.22) and get our final expression for the propagator

$$\begin{aligned} K(b, a) &= \lim_{\epsilon \rightarrow 0} \sqrt{\frac{m}{2i\epsilon\hbar\pi}} \int \prod_{j=1}^{N-1} dx_j \sqrt{\frac{m}{2i\epsilon\hbar\pi}} e^{\frac{i}{\hbar}\epsilon L_j} \\ &\stackrel{\text{def}}{=} \int [\mathcal{D}x(t)] e^{\frac{i}{\hbar} \int_{t_a}^{t_b} dt L[x(t), \dot{x}(t)]} = \int [\mathcal{D}x(t)] e^{\frac{i}{\hbar} S[x(t)]} \end{aligned} \quad (1.27)$$

where

$$L_j = \frac{1}{2}m \left( \frac{x_{j+1} - x_j}{\epsilon} \right)^2 - V(x_j) .$$

This is the key formula which gives the propagator in the form of a path integral. Its discretized form (the first part of (1.27)), which is a product of exponentials, can also be written as an exponential of the sum

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \int dx_1 \dots dx_{N-1} \left( \frac{m}{2i\epsilon\hbar\pi} \right)^{\frac{1}{2}N} e^{\frac{i\epsilon}{\hbar} \sum_{j=0}^{N-1} L_j} . \quad (1.28)$$

Clearly

$$\lim_{\epsilon \rightarrow 0} \sum_{j=0}^{N-1} \epsilon L_j = \int_{t_a}^{t_b} dt L(x(t), \dot{x}(t)) = S[x(t)] \quad (1.29)$$



where  $S[x(t)]$  is the functional of classical action. Hence from (1.27) and (1.28) we get an explicit expression for  $\mathcal{D}x(t)$  for a discretized form of a “path integral”:

$$[\mathcal{D}x(t)] = dx_1 \dots dx_{N-1} \left( \frac{m}{2i\epsilon\hbar\pi} \right)^{\frac{1}{2}N}. \quad (1.30)$$

From (1.7) we obtain going through the same steps as discussed above:

$$\begin{aligned} K(x_b, x_a, t_b - t_a) &= \langle x_b | e^{-\frac{i}{\hbar}(t_b-t_a)H} | x_a \rangle = \langle x_b | e^{-\frac{i}{\hbar}(t_b-t_c)H} e^{-\frac{i}{\hbar}(t_c-t_a)H} | x_a \rangle \\ &= \langle x_b | e^{-\frac{i}{\hbar}(t_b-t_c)H} \int dx_c | x_c \rangle \langle x_c | e^{-\frac{i}{\hbar}(t_c-t_a)H} | x_a \rangle \\ &= \int dx_c K(x_b, x_c, t_b - t_c) K(x_c, x_a, t_c - t_a). \end{aligned} \quad (1.31)$$

On the other hand, since  $|K(x_b, x_a, t_b - t_a)|^2$  is the probability density of finding the particle around  $x_b$  at the time  $t_b$ ,  $K$  must be a Schrödinger wave function  $\Psi(x_b, t_b)$ . Therefore,  $K$  must satisfy the Schrödinger equation

$$i\hbar \frac{\partial K(b, a)}{\partial t_b} = H_b K(b, a). \quad (1.32)$$

From (1.31) and (1.31) we see that  $K(b, a)$  propagates the wave functions in time and space:

$$\Psi(x_b, t_b) = \int dx_a K(x_b, x_a; t_b - t_a) \Psi(x_a, t_a). \quad (1.33)$$

Indeed, one can show [1.7] that the infinitely small transport of the wave function,

$$\Psi(x, t + \epsilon) = \left( \frac{m}{2i\pi\epsilon\hbar} \right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}\epsilon L[(x-y)/\epsilon, (x+y)/2]} \Psi(y, t) dy, \quad (1.34)$$

implies the Schrödinger equation for  $\Psi(x, t)$ . This is shown in the Appendix B.

A few comments are in order. First is about the role of the classical trajectories. A classical trajectory lies at the stationary point of the action  $S[x(t)]$ :

$$\delta S[\bar{x}(t)] = S[\bar{x}(t) + \delta x(t)] - S[\bar{x}(t)] = 0. \quad (1.35)$$

Therefore, around the classical trajectory the value of  $S[\bar{x}(t)]$  stays constant. So, when the dimensionless ratio

$$\frac{S[\bar{x}(t)]}{\hbar} \gg 1, \quad (1.36)$$

the contribution of the classical trajectory dominates: the out of phase contributions of the trajectories outside the stationary region of  $S[x(t)]$  cancel out in (1.27) and we can write the propagator  $K$  in the *semiclassical approximation*

$$K(b, a) = F e^{\frac{i}{\hbar} S[\bar{x}(t)]} \quad (1.37)$$

where

$$S[\bar{x}(t)] = \int_{t_a}^{t_b} dt L(\bar{x}(t), \dot{\bar{x}}(t)) = S_{cl}(t_b, t_a), \quad (1.38)$$

and  $F$  is to be determined (we shall discuss this approximation in detail later on).

The second point is that in calculations which led us to eq.(1.23) the magnitude of  $\epsilon$  was irrelevant. Hence (1.23) is valid for an arbitrary lapse of time. Since the action in this case is the one of a free particle, equation (1.23) gives the propagator for a free particle:

$$K_0(b, a) = \sqrt{\frac{m}{2i\pi\hbar(t_b - t_a)}} e^{i\frac{1}{2}m\frac{(x_b - x_a)^2}{\hbar(t_b - t_a)}}. \quad (1.39)$$

When  $t_b \rightarrow t_a$ ,  $K_0(x_b, x_a, t_b - t_a) \rightarrow \delta(x_b - x_a)$ . This is in fact true for all  $K(b, a)$ 's. We can see it by inserting twice the unity

$$1 = \sum_n |E_n\rangle\langle E_n|, \quad H|E_n\rangle = E_n|E_n\rangle \quad (1.40)$$

into (1.7)

$$K(b, a) = \langle x_b| 1 e^{-\frac{i}{\hbar}H(t_b - t_a)} 1 |x_a\rangle = \sum_n \phi_n(x_b) \phi_n^*(x_a) e^{-\frac{i}{\hbar}E_n(t_b - t_a)} \quad (1.41)$$

where  $\phi_n(x)$  are the eigenfunctions of  $H$ . When we let  $t_b \rightarrow t_a$  the propagator becomes

$$K(b, a) \rightarrow \sum_n \phi_n(x_b) \phi_n^*(x_a) = \delta(x_b - x_a). \quad (1.42)$$

The interpretation of this result is clear. Without a lapse of time,  $t_b = t_a$ , there is no change of the state of the system, thus the kernel  $K(b, a)$  which performs the evolution of the wave function  $\Psi(x, t)$ ,

$$\Psi(x_b, t_b) = \int dx_a K(x_b, x_a, t_b - t_a) \Psi(x_a, t_a), \quad (1.43)$$

must reduce to  $\delta(x_b - x_a)$ .

Before closing this Section let us illustrate the path integral formulation of quantal processes with some intuitive arguments based on diffraction experiments. First the well known two slit experiment. Let us recall that it establishes the fact that the amplitude for a particle to go from the source (at  $x_a$  and  $t_a$ ) to the detector (at  $x_b$  and  $t_b$ ) has to be the sum of two different amplitudes: the particle going along the *paths* through the slit 1, and the particle going along the *paths* through the slit 2. This implies that if we increase the numbers of, both, screens and slits, the amplitude of a prticle going from the source  $a$  to the detector  $b$  has to be the sum of all amplitudes whose paths go through all possible combinations of slits. Now, let us think of the limit of infinitely many and infinitely densely distributed screens and slits. In this limit we are getting rid of the screens: between  $a$  and  $b$  we have an empty space. But, at each step

of this limiting process we have to construct the total amplitude from the sum of contributions from all possible paths. In the limit of empty space the paths over which we have to sum cover all space between the source and the detector. This is the content of the formula (1.27).

## 1.4 Double slit diffraction

Employing (1.43) we can give an approximate description of diffraction in the double slit experiment. We do it in three dimensions postulating a form of the wave function of one particle at the initial time  $t = 0$  when the particle is at the screen. Let the screen with two slits be identified with the  $(x, y)$ -plane. The two slits are at  $x = \pm a$ , and the wave function propagates in the  $(x, y, z)$  space. We give its initial (at  $t = 0$ ) shape in the form (we shall not bother about its normalization and, for the sake of simplicity, we set  $\hbar = m = 1$ )

$$\Psi(x_0, y_0, z_0, 0) = G(x_0, y_0, z_0) \quad (1.44)$$

$$= e^{ipz_0} \left[ \sqrt{\frac{1}{2\pi\delta}} e^{-\frac{(x_0-a)^2}{2\delta}} + \sqrt{\frac{1}{2\pi\delta}} e^{-\frac{(x_0+a)^2}{2\delta}} \right] \sqrt{\frac{1}{2\pi\delta}} e^{-\frac{y_0^2}{2\delta}}.$$

There is no force acting along the  $z$ -direction, hence we describe the propagation of particles in this direction as free (a plane wave) with constant velocity  $v = p/m$ . In the  $(x, y)$ -plane the propagation is also free, but it is geometrically restricted to the two slits whose shapes must be reflected in the form of the initial wave function (1.44). The most natural form of  $G$  would be to make it zero everywhere along the  $(x, y)$ -plane and a constant around the positions of the two slits  $x = \pm a, y = 0$ , but this would lead in (1.43) to some cumbersome expressions and that is why we take  $G$  in a form of two Gaussian distributions centered at the positions of these two slits. The parameter  $\delta$  gives the size of the slits. The boundaries of such “gaussian slits” are not sharp but smeared out but, for a qualitative discussion, they are acceptable (see e.g. ref.[1.7]).

The free propagation from the screen is obtained from (1.43) by taking  $G(x_0, y_0, z_0)$  as given in (1.44) and propagating it with  $K = K_0$  given by (1.39). Elementary calculations of a few Gaussian integrals give

$$\begin{aligned} \Psi(x, y, z, t) &= \int dx_0 dy_0 dz_0 \left( \frac{1}{2\pi it} \right)^{\frac{3}{2}} e^{i\frac{[(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2]}{2t}} \quad (1.45) \\ &\times e^{ipz_0} \left[ \sqrt{\frac{1}{2\pi\delta}} e^{-\frac{(x_0-a)^2}{2\delta}} + \sqrt{\frac{1}{2\pi\delta}} e^{-\frac{(x_0+a)^2}{2\delta}} \right] \sqrt{\frac{1}{2\pi\delta}} e^{-\frac{y_0^2}{2\delta}} \\ &= e^{ipz - i\frac{1}{2}p^2 t} \sqrt{\frac{1}{2\pi(\delta + it)}} e^{-\frac{y^2}{2(\delta + it)}} \sqrt{\frac{1}{2\pi(\delta + it)}} \left[ e^{-\frac{(x-a)^2}{2(\delta + it)}} + e^{-\frac{(x+a)^2}{2(\delta + it)}} \right]. \end{aligned}$$

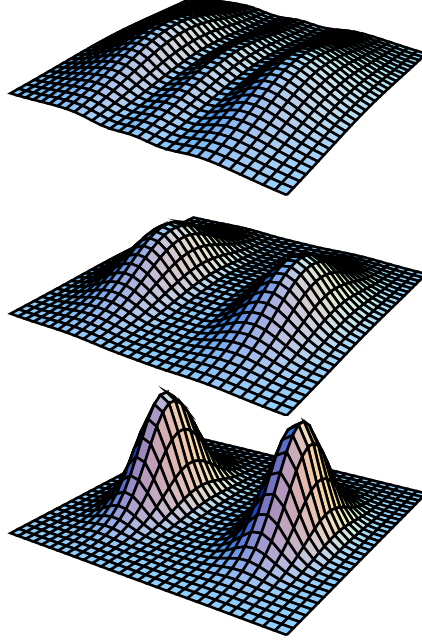


Figure 1.2: Time evolution of the two Gaussian probability (1.44). We see that initially well localized Gaussian packets gradually "melt away" and develop an interference pattern manifesting itself as a maximum in the middle.

Thus the intensity at the detector is

$$|\Psi(x, y, z, t)|^2 = \frac{1}{4\pi^2(\delta^2 + t^2)} e^{-\frac{y^2}{\delta^2 + t^2}\delta} \times \left[ e^{-\frac{(x-a)^2}{\delta^2 + t^2}\delta} + e^{-\frac{(x+a)^2}{\delta^2 + t^2}\delta} + e^{-\frac{(x^2+a^2)}{\delta^2 + t^2}\delta} 2 \cos\left(2\frac{xat}{\delta^2 + t^2}\right) \right]. \quad (1.46)$$

The diffraction pattern is in our approximation regulated by the lapse of time  $t$ , and one may identify the position of the detector as  $z = vt$ . Anyway, at  $t = 0$  we have a superposition of two Gaussians centered at  $\pm a$ , whereas at later times (1.46) develops many maxima which die out as we move to larger and larger distances from the slits.

Note that when  $\delta \rightarrow 0$ , hence the two slits become pointlike we get

$$\lim_{\delta \rightarrow 0} |\Psi|^2 = \frac{1}{2\pi^2 t^2} \left[ 1 + \cos\left(2\frac{xa}{t}\right) \right] = \frac{1}{\pi^2 t^2} \cos^2 \frac{xa}{t}. \quad (1.47)$$

In this limit we still have a pulsation of the probability distribution, however the fading as we go away from the slits disappears: the diffraction is everywhere.

Although the initial wave function (1.44) is not very realistic, the qualitative

features of diffraction come out correctly. One can certainly improve the ansatz (1.44) but then we cannot work out an analytic form of  $|\Psi|^2$ .

Path integrals have a very extensive literature. First of all there are the classic papers of Feynman [1.2],[1.6]. Then there are two textbooks by Feynman and Hibbs [1.7] and by Feynman [1.8], and very many texts by various authors. Let us quote only the one by Kleinert [1.9] which is a very comprehensive and complete account of the method with many applications – a veritable *boa constrictor* of a book. We will quote the other texts as we go along with these lectures.

## Appendix A: The Baker-Campbell-Hausdorff formula

In this Appendix we will prove the so called BCH formula which says that for two non-commuting operators  $A$  and  $B$ :

$$e^A e^B = e^C \tag{A.1}$$

and

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] + [B, [B, A]]) + \dots$$

To prove (A.1) we shall follow ref.[1.11] and introduce an auxiliary parameter  $t$

$$e^{C(t)} = e^A e^{tB}, \tag{A.2}$$

although other choices can be also used:  $e^{C(t)} = e^{tA} e^B$  or  $e^{C(t)} = e^{tA} e^{tB}$ . We encourage the reader to repeat the proof with one of these alternative choices for  $C$ .

The idea of the proof consists in solving a differential equation for  $dC/dt$  and setting  $t = 1$  in the solution. To this end let us first consider derivative of the exponent of  $C$ :

$$\frac{d}{dt} e^{C(t)} = \int_0^1 d\tau e^{\tau C(t)} \dot{C}(t) e^{(1-\tau)C(t)} = \int_0^1 d\tau e^{(1-\tau)C(t)} \dot{C}(t) e^{\tau C(t)}. \tag{A.3}$$

This equality can be easily verified by expanding in powers of  $C(t)$ .

Let us now concentrate on the  $\tau$  dependent part of eq.(A.3). We shall first define the so called adjoint operator  $\Delta_X$ , where  $X$  is some operator and the action of  $\Delta_X$  on given operator  $Y$  is given by:

$$\Delta_X Y = [X, Y]. \tag{A.4}$$

It is convenient to use this notation for the commutator, since it can be easily (formally) inverted, raised to some power, etc. For example we shall show that:

$$e^A B e^{-A} = e^{\Delta_A} B = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \dots \tag{A.5}$$

To this end one defines:

$$B(\tau) = e^{\tau A} B e^{-\tau A} \quad \text{with} \quad B(0) = B, \quad (\text{A.6})$$

and writes differential equation for  $B(\tau)$ :

$$\frac{d}{d\tau} B(\tau) = [A, B(\tau)] = \Delta_A B(\tau). \quad (\text{A.7})$$

The first equality in (A.7) comes simply from differentiation of (A.6), whereas the second equality is merely the definition of  $\Delta_A$ . However, equation (A.7) can be now formally integrated, yielding:

$$B(t) = e^{\tau \Delta_A} B, \quad (\text{A.8})$$

which just the result given in (A.5). Here we see another advantage of using  $\Delta_X$ : it is convenient to write nested commutators as powers of  $\Delta_X$ .

We can now use equation (A.8) and perform formally integration over  $d\tau$ :

$$\begin{aligned} \frac{d}{dt} e^{C(t)} &= \int_0^1 d\tau e^{(1-\tau)C(t)} \dot{C}(t) e^{\tau C(t)} = \int_0^1 d\tau e^{C(t)} e^{-\tau \Delta_{C(t)}} \dot{C}(t) \\ &= e^{C(t)} \frac{1 - e^{-\Delta_{C(t)}}}{\Delta_{C(t)}} \dot{C}(t). \end{aligned} \quad (\text{A.9})$$

After these preliminaries we can finally prove (A.1). Let us use the definition of  $C(t)$  as given by Eq.( A.2). By differentiating (A.2) with respect to  $t$  we get:

$$\frac{d}{dt} e^{C(t)} = e^{C(t)} B. \quad (\text{A.10})$$

On the other hand we can use (A.9) to derive equation for  $\dot{C}(t)$ :

$$\dot{C}(t) = \frac{\Delta_{C(t)}}{1 - e^{-\Delta_{C(t)}}} B = \frac{e^{\Delta_{C(t)}} \Delta_{C(t)}}{e^{\Delta_{C(t)}} - 1} B. \quad (\text{A.11})$$

Now we would like to integrate (A.11) over  $dt$  from  $t = 0$  to  $t = 1$ . To this end we shall prove that

$$e^{\Delta_{C(t)}} = e^{\Delta_A} e^{t \Delta_B}. \quad (\text{A.12})$$

Indeed:

$$\begin{aligned} e^{\Delta_{C(t)}} Y &= e^{C(t)} Y e^{-C(t)} = e^A (e^{tB} Y e^{-tB}) e^{-A} \\ &= e^A (e^{t \Delta_B} Y) e^{-A} = e^{\Delta_A} (e^{t \Delta_B} Y). \end{aligned} \quad (\text{A.13})$$

Therefore

$$\Delta_{C(t)} = \ln (e^{\Delta_A} e^{t \Delta_B}). \quad (\text{A.14})$$

Finally we arrive at:

$$C(1) = A + \int_0^1 dt \frac{e^{\Delta_A} e^{t \Delta_B} \ln (e^{\Delta_A} e^{t \Delta_B})}{e^{\Delta_A} e^{t \Delta_B} - 1} B. \quad (\text{A.15})$$

We can integrate (A.15) term by term by expanding in powers of variable  $z - 1 = \exp(\Delta_A) \exp(t\Delta_B) - 1$ :

$$\begin{aligned} \frac{z \ln(1 + (z - 1))}{z - 1} &= \ln(1 + (z - 1)) + \frac{\ln(1 + (z - 1))}{z - 1} \\ &= 1 + \sum_{n=1} \frac{(-1)^{n+1}}{n(n+1)} (z - 1)^n, \end{aligned}$$

where  $z$  by itself is a power series in  $t$ :

$$z = \left( 1 + \sum_{k=1} \frac{1}{k!} \Delta_A^k \right) \left( 1 + \sum_{j=1} \frac{t^j}{j!} \Delta_B^j \right) = 1 + \sum_{n=1} \sum_{m=0}^n \frac{t^m}{m!(n-m)!} \Delta_A^{(n-m)} \Delta_B^m.$$

In terms of powers of  $(z - 1)$  formula (A.15) takes the following form:

$$C(1) = A + \int_0^1 dt \left( 1 + \frac{1}{2}(z - 1) - \frac{1}{6}(z - 1)^2 + \frac{1}{12}(z - 1)^3 + \dots \right) B. \quad (\text{A.16})$$

Since we want to expand  $C$  up to some number  $n$  of nested commutators (that is up to some power  $n$  in  $\Delta_A^{n-m} \Delta_B^m$ ), we shall confine ourselves only to a few terms in  $z - 1$ . Here we shall perform calculations up to  $n = 3$ :

$$\begin{aligned} z - 1 &= \Delta_A + t \Delta_B \quad (\text{A.17}) \\ &+ \frac{1}{2} \Delta_A^2 + t \Delta_A \Delta_B + \frac{1}{2} t^2 \Delta_B^2 \\ &+ \frac{1}{6} \Delta_A^3 + \frac{1}{2} t \Delta_A^2 \Delta_B + \frac{1}{2} t^2 \Delta_A \Delta_B^2 + \frac{1}{6} t^3 \Delta_B^3 + \dots \end{aligned}$$

Note that  $\Delta_B B = 0$ . This simplifies the action on  $B$  of the first factor of  $z - 1$ :

$$(z - 1)B = \left( \Delta_A + \frac{1}{2} \Delta_A^2 + \frac{1}{6} \Delta_A^3 \right) B. \quad (\text{A.18})$$

Next we have:

$$\begin{aligned} (z - 1)^2 B &= (\Delta_A^2 + t \Delta_B \Delta_A) B \quad (\text{A.19}) \\ &+ (\Delta_A^3 + \frac{1}{2} t \Delta_B \Delta_A^2 + t \Delta_A \Delta_B \Delta_A + \frac{1}{2} t^2 \Delta_B^2 \Delta_A) B, \\ (z - 1)^3 B &= (\Delta_A^3 + t \Delta_A \Delta_B \Delta_A + t \Delta_B \Delta_A^2 + t^2 \Delta_B^2 \Delta_A) B. \end{aligned}$$

Inserting eqs. (A.18, A.19) into (A.16) and integrating over  $t$  we get finally:

$$C = A + B + \frac{1}{2} [A, B] + \frac{1}{12} \{ [A, [A, B]] - [B, [A, B]] \} - \frac{1}{24} [A, [B, [A, B]]] + \dots \quad (\text{A.20})$$

## Appendix B: Schrödinger equation

In this Appendix we shall derive the Schrödinger equation by performing an infinitely small transport of the wave function  $\Psi(x, t) \rightarrow \Psi(x, t + \epsilon)$ . This derivation can be found in ref.[1.7], however we shall go one step further to see whether this method gives consistent results up the order  $\epsilon^2$ . According to eq.(1.34)

$$\Psi(x, t + \epsilon) = \int_{-\infty}^{\infty} d\eta \exp\left(-\frac{m}{2i\hbar\epsilon}\eta^2\right) \exp\left(-\frac{i\epsilon}{\hbar}V\left(x + \frac{\eta}{2}\right)\right) \Psi(x + \eta, t). \quad (\text{B.1})$$

where  $y = \eta + x$ . Let us note, however, that other ways of discretizing the Lagrangian are possible. For example instead of  $V((x + y)/2)$  we could have taken  $(V(x) + V(y))/2$ .

The trick is to expand both sides of eq.(B.1) in  $\epsilon$ . Expansion of the left hand side is trivial

$$L = \Psi(x, t + \epsilon) = \Psi(x, t) + \epsilon \frac{d}{dt}\psi(x, t) + \frac{1}{2}\epsilon^2 \frac{d^2}{dt^2}\Psi(x, t) + \dots \quad (\text{B.2})$$

Care must be taken, however, while expanding the right hand side of eq.(B.1). Certainly we cannot expand the first exponent, since its argument is singular for  $\epsilon \rightarrow 0$ . Mathematically correct procedure would consist in rotating the integral over  $\eta$  in such a way, that the exponential would turn into a Gaussian of a width proportional to  $\sqrt{\epsilon}$ . It is clear then that, for a narrow Gaussian, only contributions from  $\eta \sim 0$  are of importance and the remainder can be safely expanded in  $\eta$ . We shall expand up to  $\epsilon^2$ , which means  $\eta^4$ . The potential has to be expanded up to  $\eta^2$  (since it is already multiplied by  $\epsilon$ ). For the two possible ways in which the potential can be discretized one obtains two different results:

$$U = V\left(\frac{x + (x + \eta)}{2}\right) = V\left(x + \frac{\eta}{2}\right) = V(x) + \frac{1}{2}\eta V'(x) + \frac{1}{8}\eta^2 V''(x) + \dots$$

or

$$U = \frac{1}{2}(V(x) + V(x + \eta)) = V(x) + \frac{1}{2}\eta V'(x) + \frac{1}{4}\eta^2 V''(x) \dots$$

We see that both choices differ by a numerical factor in front of  $V''$ . Therefore we shall use

$$U = V + \frac{1}{2}\eta V' + \frac{\alpha}{4}\eta^2 V'' \dots \quad (\text{B.3})$$

with  $\alpha = 1/2$  for the first choice and  $\alpha = 1$  for the second. In what follows we omit arguments if they refer to the point  $(x, t)$ .

The problem of a discretization of the continuous actions is of particular importance for the so called *lattice field theories*. Here we just content ourselves with an observation that two different discretizations of potential  $V(x)$  give the same result up to terms linear in  $\epsilon$  but differ at the level of  $\epsilon^2$ .

We shall also need  $U^2$  with accuracy  $\eta^0$ :

$$U^2 = V^2 + \dots$$



Finally

$$\Psi(x + \eta, t) = \Psi + \eta\Psi' + \frac{1}{2}\eta^2\Psi'' + \frac{1}{6}\eta^3\Psi''' + \frac{1}{24}\eta^4\Psi^{(4)} + \dots$$

Now, the integrand in the right hand side of eq.(B.1) reads:

$$\begin{aligned} \exp\left(-\frac{i\epsilon}{\hbar}U\right)\Psi(x + \eta, t) &= \left(1 - \frac{i\epsilon}{\hbar}U - \frac{\epsilon^2}{2\hbar^2}U^2\right)\Psi(x + \eta, t) \\ &= \Psi + \eta\Psi' + \frac{1}{2}\eta^2\Psi'' + \frac{1}{6}\eta^3\Psi''' + \frac{1}{24}\eta^4\Psi^{(4)} \\ &\quad - \frac{i\epsilon}{\hbar}U\Psi(x + \eta, t) - \frac{\epsilon^2}{2\hbar^2}U^2\Psi(x + \eta, t). \end{aligned}$$

Consider  $U\Psi(x + \eta, t)$  with accuracy  $\eta^2$ :

$$\begin{aligned} U\Psi(x + \eta, t) &= \left(V + \frac{1}{2}\eta V' + \frac{\alpha}{4}\eta^2 V''\right)\left(\Psi + \eta\Psi' + \frac{1}{2}\eta^2\Psi''\right) \\ &= V\Psi + \eta\left(\frac{1}{2}V'\Psi + V\Psi'\right) + \frac{1}{2}\eta^2\left(V\Psi'' + V'\Psi' + \frac{\alpha}{2}V''\Psi\right) \end{aligned}$$

and  $U^2\Psi(x + \eta, t)$  with accuracy  $\eta^0$ :

$$U^2\Psi(x + \eta, t) = V^2\Psi.$$

Therefore

$$\begin{aligned} \exp\left(-\frac{i\epsilon}{\hbar}U\right)\Psi(x + \eta, t) &= \Psi - \frac{i\epsilon}{\hbar}V\Psi + \frac{1}{2}\eta^2\Psi'' - \frac{\epsilon^2}{2\hbar^2}V^2\Psi + \frac{1}{24}\eta^4\Psi^{(4)} \\ &\quad - \frac{i\epsilon}{2\hbar}\eta^2\left(V\Psi'' + V'\Psi' + \frac{\alpha}{2}V''\Psi\right) \\ &\quad + \eta\Psi' + \frac{1}{6}\eta^3\Psi''' - \frac{i\epsilon}{\hbar}\eta\left(\frac{1}{2}V'\Psi + V\Psi'\right). \end{aligned} \quad (\text{B.4})$$

Note that terms odd in  $\eta$  in the last line of eq.(B.4) will vanish under integration over  $\eta$ . Using

$$\int_{-\infty}^{\infty} \frac{d\eta}{A} e^{-\beta x^2} \{1, \eta^2, \eta^4\} = \left\{1, \frac{1}{2\beta}, \frac{3}{4\beta^2}\right\}$$

for  $\beta = \frac{m}{2i\hbar\epsilon}$  and  $A = \sqrt{\beta/\pi}$  we get upon integration:

$$\{1, \eta^2, \eta^4, \} \rightarrow \left\{1, \frac{i\hbar\epsilon}{m}, -\frac{3\hbar^2\epsilon^2}{m^2}\right\}.$$

Let us compare both sides of eq.(B.1) power by power:

- $\epsilon^0$ :

$$\Psi = \Psi, \quad (\text{B.5})$$

- $\epsilon^1$ :

$$\frac{d}{dt}\Psi = \left[\frac{1}{2}\frac{i\hbar}{m}\frac{d^2}{dx^2} - \frac{i}{\hbar}V\right]\Psi, \quad (\text{B.6})$$

- $\epsilon^2$ :

$$\frac{1}{2} \frac{d^2}{dt^2} \Psi = -\frac{\hbar^2}{8m^2} \Psi^{(4)} + \frac{1}{2m} \left( V\Psi'' + V'\Psi' + \frac{\alpha}{2} V''\Psi \right) - \frac{1}{2\hbar^2} V^2\Psi \quad (\text{B.7})$$

The first equation shows that we have used proper normalization. The second is the Schrödinger equation. Indeed multiplying by  $i\hbar$  we get

$$i\hbar \frac{d}{dt} \Psi = -\frac{\hbar^2}{2m} \Psi'' + V\Psi.$$

As far as the third equation is concerned, let us calculate the left hand side using (B.6):

$$\begin{aligned} \frac{1}{2} \frac{d^2}{dt^2} \Psi &= \frac{1}{2} \left[ \frac{1}{2} \frac{i\hbar}{m} \frac{d^2}{dx^2} - \frac{i}{\hbar} V \right] \left[ \frac{1}{2} \frac{i\hbar}{m} \Psi'' - \frac{i}{\hbar} V\Psi \right] \\ &= -\frac{\hbar^2}{8m^2} \Psi^{(4)} + \frac{1}{2m} \left( V\Psi'' + V'\Psi' + \frac{1}{2} V''\Psi \right) - \frac{1}{2\hbar^2} V^2\Psi \quad (\text{B.8}) \end{aligned}$$

which is identical to (B.7) only if  $\alpha = 1$ . We see, as already remarked in the beginning of this example, that at the order  $\epsilon^2$  only one way of discretizing the potential reproduces the "square" of the Schrödinger equation. This tiny difference may improve the numerical simulations of quantum mechanical systems where one is forced to work in discrete steps in space. It is of even larger importance in quantum field theories.

## References

- [1.1] P. A. M. Dirac, *The Lagrangian in Quantum Mechanics*, Physikalische Zeitschrift der Sowjetunion, Band 3, Heft 1 (1933).
- [1.2] R. P. Feynman, *Space-time Approach to Non-relativistic Quantum Mechanics*, Rev. Mod. Phys. **20**, 267 (1948).
- [1.3] P. A. M. Dirac, *On the Analogy Between Classical and Quantum Mechanics*, Rev. Mod. Phys. **17**, 195 (1945).
- [1.4] see e.g.: M.Veltman, *Diagrammatica*, Cambridge University Press, 1994, page 8.
- [1.5] E. Nelson, *Feynman Integrals and the Schrödinger Equation*, J. Math. Phys. **5**, 332 (1964).
- [1.6] R. P. Feynman, *Mathematical Formulation of the Quantum Theory of the Electromagnetic Interactions*, Phys. Rev. **80**, 440 (1950).
- [1.7] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals*, Mc Graw-Hill, New York, 1965.

- 
- [1.8] R. P. Feynman, *Statistical Mechanics*, W. A. Benjamin, Inc, Reading, Massachusetts, 1972.
- [1.9] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics*, World Scientific, 1990.
- [1.10] A. Einstein in Verhandl. Dtsch. Phys. Ges. **19**, 82 (1917); see also J. B. Keller, *Corrected Bohr–Sommerfeld Quantum Conditions for Nonseparable Systems*, Annals of Physics **4**, 180 (1958).
- [1.11] J.M. Normand *Rotations in Quantum Mechanics*, Appendix D, North-Holland, Amsterdam 1980.