Notes on Quantum Mechanics

K. Schulten
Department of Physics and Beckman Institute, University of Illinois,
405 N. Mathews Street, Urbana, IL 61801 USA

August 26, 1999

Preface

The following notes introduce *Quantum Mechanics* at an advanced level addressing students of Physics, Mathematics, Chemistry and Electrical Engineering. The aim is to put mathematical concepts and techniques like the path integral, algebraic techniques, Lie algebras and representation theory at the readers disposal. For this purpose we attempt to motivate the various physical and mathematical concepts as well as provide detailed derivations and complete sample calculations. We have made every effort to include in the derivations all assumptions and all mathematical steps implied, avoiding omission of supposedly 'trivial' information. Much of the author's writing effort went into a web of cross references accompanying the mathematical derivations such that the intelligent and diligent reader should be able to follow the text with relative ease, in particular, also when mathematically difficult material is presented. In fact, the author's driving force has been his desire to pave the reader's way into territories unchartered previously in most introductory textbooks, since few practitioners feel obliged to ease access to their field. Also the author embraced enthusiastically the potential of the TEX typesetting language to enhance the presentation of equations as to make the logical pattern behind the mathematics as transparent as possible. Any suggestion to improve the text in the respects mentioned are most welcome. It is obvious, that even though these notes attempt to serve the reader as much as was possible for the author, the main effort to follow the text and to master the material is left to the reader.

The notes start out in Section 1 with a brief review of *Classical Mechanics* in the Lagrange formulation and build on this to introduce in Section 2 *Quantum Mechanics* in the closely related *path integral formulation*. In Section 3 the *Schrödinger equation* is derived and used as an alternative description of continuous quantum systems. Section 4 is devoted to a *detailed presentation of the harmonic oscillator*, introducing algebraic techniques and comparing their use with more conventional mathematical procedures. In Section 5 we introduce the *presentation theory of the 3-dimensional rotation group and the group SU(2)* presenting Lie algebra and Lie group techniques and applying the methods to the theory of angular momentum, of the spin of single particles and of angular momenta and spins of composite systems. In Section 6 we present the *theory of many–boson and many–fermion systems* in a formulation exploiting the algebra of the associated creation and annihilation operators. Section 7 provides an introduction to *Relativistic Quantum Mechanics* which builds on the representation theory of the Lorentz group and its complex relative $Sl(2, \mathbb{C})$. This section makes a strong effort to introduce Lorentz–invariant field equations systematically, rather than relying mainly on a heuristic amalgam of Classical Special Relativity and Quantum Mechanics.

The notes are in a stage of continuing development, various sections, e.g., on the semiclassical approximation, on the Hilbert space structure of Quantum Mechanics, on scattering theory, on perturbation theory, on Stochastic Quantum Mechanics, and on the group theory of elementary particles will be added as well as the existing sections expanded. However, at the present stage the notes, for the topics covered, should be complete enough to serve the reader.

The author would like to thank Markus van Almsick and Heichi Chan for help with these notes. The author is also indebted to his department and to his University; their motivated students and their inspiring atmosphere made teaching a worthwhile effort and a great pleasure.

These notes were produced entirely on a Macintosh II computer using the TEX typesetting system, Textures, Mathematica and Adobe Illustrator.

Klaus Schulten
University of Illinois at Urbana–Champaign
August 1991

Chapter 1

Lagrangian Mechanics

Our introduction to Quantum Mechanics will be based on its correspondence to Classical Mechanics. For this purpose we will review the relevant concepts of Classical Mechanics. An important concept is that the equations of motion of Classical Mechanics can be based on a variational principle, namely, that along a path describing classical motion the action integral assumes a minimal value (Hamiltonian Principle of Least Action).

1.1 Basics of Variational Calculus

The derivation of the Principle of Least Action requires the tools of the calculus of variation which we will provide now.
Definition: A *functional* $S[\,]$ is a map

$$S[\,]\;:\;\mathcal{F}\;\to\mathbb{R}\;;\;\mathcal{F}\;=\;\{\vec{q}(t);\,\vec{q}:\,[t_0,t_1]\,\subset\,\mathbb{R}\,\to\,\mathbb{R}^M;\,\vec{q}(t)\text{ differentiable}\}\tag{1.1}$$

from a space $\mathcal{F}$ of vector-valued functions $\vec{q}(t)$ onto the real numbers. $\vec{q}(t)$ is called the *trajectory* of a system of M degrees of freedom described by the *configurational coordinates* $\vec{q}(t) = (q_1(t), q_2(t), \dots q_M(t))$.

In case of N classical particles holds $M = 3N$, i.e., there are $3N$ configurational coordinates, namely, the position coordinates of the particles in any kind of coordianate system, often in the Cartesian coordinate system. It is important to note at the outset that for the description of a classical system it will be necessary to provide information $\vec{q}(t)$ as well as $\frac{d}{dt}\vec{q}(t)$. The latter is the velocity vector of the system.
Definition: A functional $S[\,]$ is *differentiable*, if for any $\vec{q}(t) \in \mathcal{F}$ and $\delta\vec{q}(t) \in$

$\mathcal{F}_\epsilon$ where

$$\mathcal{F}_\epsilon \;=\; \{\delta\vec{q}(t);\, \delta\vec{q}(t) \,\in \mathcal{F},\, |\delta\vec{q}(t)| \,<\, \epsilon,\, |\frac{d}{dt}\delta\vec{q}(t)| \,<\, \epsilon, \forall t,\, t \,\in\, [t_0, t_1] \subset \mathbb{R}\} \tag{1.2}$$

a functional $\delta S[\,\cdot\,,\,\cdot\,]$ exists with the properties

$$\begin{array}{ll} (i) & S[\vec{q}(t) \,+\, \delta\vec{q}(t)] \;=\; S[\vec{q}(t)] \,+\, \delta S[\vec{q}(t), \delta\vec{q}(t)] \,+\, O(\epsilon^2) \\ (ii) & \delta S[\vec{q}(t), \delta\vec{q}(t)] \;\text{ is linear in } \delta\vec{q}(t). \end{array} \tag{1.3}$$

$\delta S[\,\cdot\,,\,\cdot\,]$ is called the *differential* of $S[\;]$. The linearity property above implies

$$\delta S[\vec{q}(t), \alpha_1\, \delta\vec{q}_1(t) \,+\, \alpha_2\, \delta\vec{q}_2(t)] \;=\; \alpha_1\, \delta S[\vec{q}(t), \delta\vec{q}_1(t)] \,+\, \alpha_2\, \delta S[\vec{q}(t), \delta\vec{q}_2(t)]\;. \tag{1.4}$$

Note: $\delta\vec{q}(t)$ describes small variations around the trajectory $\vec{q}(t)$, i.e. $\vec{q}(t) + \delta\vec{q}(t)$ is a 'slightly' different trajectory than $\vec{q}(t)$. We will later often assume that only variations of a trajectory $\vec{q}(t)$ are permitted for which $\delta\vec{q}(t_0) \,=\, 0$ and $\delta\vec{q}(t_1) \,=\, 0$ holds, i.e., at the ends of the time interval of the trajectories the variations vanish.

It is also important to appreciate that $\delta S[\,\cdot\,,\,\cdot\,]$ in conventional differential calculus does not correspond to a differentiated function, but rather to a differential of the function which is simply the differentiated function multiplied by the differential increment of the variable, e.g., $df \,=\, \frac{df}{dx}dx$ or, in case of a function of M variables, $df \,=\, \sum_{j=1}^{M} \frac{\partial f}{\partial x_j} dx_j$.

We will now consider a particular class of functionals $S[\;]$ which are expressed through an integral over the the interval $[t_0, t_1]$ where the integrand is a function $L(\vec{q}(t), \frac{d}{dt}\vec{q}(t), t)$ of the configuration vector $\vec{q}(t)$, the velocity vector $\frac{d}{dt}\vec{q}(t)$ and time t. We focus on such functionals because they play a central role in the so-called action integrals of Classical Mechanics.

In the following we will often use the notation for velocities and other time derivatives $\frac{d}{dt}\vec{q}(t) \,=\, \dot{\vec{q}}(t)$ and $\frac{dx_j}{dt} \,=\, \dot{x}_j$.

Theorem: Let

$$S[\vec{q}(t)] \;=\; \int_{t_0}^{t_1} dt\, L(\vec{q}(t), \dot{\vec{q}}(t), t) \tag{1.5}$$

where $L(\,\cdot\,,\,\cdot\,,\,\cdot\,)$ is a function differentiable in its three arguments. It holds

$$\delta S[\vec{q}(t), \delta\vec{q}(t)] \;=\; \int_{t_0}^{t_1} dt\, \left\{ \sum_{j=1}^{M} \left[\frac{\partial L}{\partial q_j} \;-\; \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j} \right) \right] \,\delta q_j(t) \right\} + \sum_{j=1}^{M} \frac{\partial L}{\partial \dot{q}_j} \delta q_j(t) \Bigg|_{t_0}^{t_1} \;. \tag{1.6}$$

For a proof we can use conventional differential calculus since the functional (1.6) is expressed in terms of 'normal' functions. We attempt to evaluate

$$S[\vec{q}(t) + \delta\vec{q}(t)] = \int_{t_0}^{t_1} dt\, L(\vec{q}(t) + \delta\vec{q}(t), \dot{\vec{q}}(t) + \delta\dot{\vec{q}}(t), t) \tag{1.7}$$

through Taylor expansion and identification of terms linear in $\delta q_j(t)$, equating these terms with $\delta S[\vec{q}(t), \delta\vec{q}(t)]$. For this purpose we consider

$$L(\vec{q}(t) + \delta\vec{q}(t), \dot{\vec{q}}(t) + \delta\dot{\vec{q}}(t), t) = L(\vec{q}(t), \dot{\vec{q}}(t), t) + \sum_{j=1}^{M} \left(\frac{\partial L}{\partial q_j}\delta q_j + \frac{\partial L}{\partial \dot{q}_j}\delta \dot{q}_j \right) + O(\epsilon^2) \tag{1.8}$$

We note then using $\frac{d}{dt} f(t)g(t) = \dot{f}(t)g(t) + f(t)\dot{g}(t)$

$$\frac{\partial L}{\partial \dot{q}_j}\delta \dot{q}_j = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\delta q_j \right) - \left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} \right)\delta q_j \,. \tag{1.9}$$

This yields for $S[\vec{q}(t) + \delta\vec{q}(t)]$

$$S[\vec{q}(t)] + \int_{t_0}^{t_1} dt \sum_{j=1}^{M} \left[\frac{\partial L}{\partial q_j} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j} \right) \right] \delta q_j + \int_{t_0}^{t_1} dt \sum_{j=1}^{M} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\delta q_j \right) + O(\epsilon^2) \tag{1.10}$$

From this follows (1.6) immediately.

We now consider the question for which functions the functionals of the type (1.5) assume extreme values. For this purpose we define
Definition: An extremal of a differentiable functional $S[\,]$ is a function $q_e(t)$ with the property

$$\delta S[\vec{q}_e(t), \delta\vec{q}(t)] = 0 \quad \text{for all } \delta\vec{q}(t) \in \mathcal{F}_\epsilon. \tag{1.11}$$

The extremals $\vec{q}_e(t)$ can be identified through a condition which provides a suitable differential equation for this purpose. This condition is stated in the following theorem.
Theorem: *Euler–Lagrange Condition*
For the functional defined through (1.5), it holds in case $\delta\vec{q}(t_0) = \delta\vec{q}(t_1) = 0$ that $\vec{q}_e(t)$ is an extremal, if and only if it satisfies the conditions ($j = 1, 2, \ldots, M$)

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0 \tag{1.12}$$

The proof of this theorem is based on the property
Lemma: If for a continuous function f(t)

$$f : [t_0, t_1] \subset \mathbb{R} \to \mathbb{R} \tag{1.13}$$

holds

$$\int_{t_0}^{t_1} dt\, f(t) h(t) = 0 \tag{1.14}$$

for any continuous function $h(t) \in \mathcal{F}_\epsilon$ with $h(t_0) = h(t_1) = 0$, then

$$f(t) \equiv 0 \quad \text{on } [t_0, t_1]. \tag{1.15}$$

We will not provide a proof for this Lemma.

The proof of the above theorem starts from (1.6) which reads in the present case

$$\delta S[\vec{q}(t), \delta\vec{q}(t)] = \int_{t_0}^{t_1} dt \left\{ \sum_{j=1}^{M} \left[\frac{\partial L}{\partial q_j} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j} \right) \right] \delta q_j(t) \right\} . \tag{1.16}$$

This property holds for any δq_j with $\delta\vec{q}(t) \in \mathcal{F}_\epsilon$. According to the Lemma above follows then (1.12) for $j = 1, 2, \ldots M$. On the other side, from (1.12) for $j = 1, 2, \ldots M$ and $\delta q_j(t_0) = \delta q_j(t_1) = 0$ follows according to (1.16) the property $\delta S[\vec{q}_e(t), \cdot] \equiv 0$ and, hence, the above theorem.

An Example

As an application of the above rules of the variational calculus we like to prove the well-known result that a straight line in $\mathbb{R}^2$ is the shortest connection (geodesics) between two points (x_1, y_1) and (x_2, y_2). Let us assume that the two points are connected by the path $y(x)$, $y(x_1) = y_1$, $y(x_2) = y_2$. The length of such path can be determined starting from the fact that the incremental length ds in going from point $(x, y(x))$ to $(x + dx, y(x + dx))$ is

$$ds = \sqrt{(dx)^2 + (\frac{dy}{dx}dx)^2} = dx\sqrt{1 + (\frac{dy}{dx})^2} . \tag{1.17}$$

The total path length is then given by the integral

$$s = \int_{x_0}^{x_1} dx \sqrt{1 + (\frac{dy}{dx})^2} . \tag{1.18}$$

s is a functional of $y(x)$ of the type (1.5) with $L(y(x), \frac{dy}{dx}) = \sqrt{1 + (dy/dx)^2}$. The shortest path is an extremal of $s[y(x)]$ which must, according to the theorems above, obey the Euler–Lagrange condition. Using $y' = \frac{dy}{dx}$ the condition reads

$$\frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right) = \frac{d}{dx}\left(\frac{y'}{\sqrt{1 + (y')^2}}\right) = 0 \,. \tag{1.19}$$

From this follows $y'/\sqrt{1 + (y')^2} = const$ and, hence, $y' = const$. This in turn yields $y(x) = ax + b$. The constants a and b are readily identified through the conditons $y(x_1) = y_1$ and $y(x_2) = y_2$. One obtains

$$y(x) = \frac{y_1 - y_2}{x_1 - x_2}(x - x_2) + y_2 \,. \tag{1.20}$$

Exercise 1.1.1: Show that the shortest path between two points on a sphere are great circles, i.e., circles whose centers lie at the center of the sphere.

1.2 Lagrangian Mechanics

The results of variational calculus derived above allow us now to formulate the Hamiltonian Principle of Least Action of Classical Mechanics and study its equivalence to the Newtonian equations of motion.
Threorem: *Hamiltonian Principle of Least Action*
The trajectories $\vec{q}(t)$ of systems of particles described through the Newtonian equations of motion

$$\frac{d}{dt}(m_j \dot{q}_j) + \frac{\partial U}{\partial q_j} = 0 \quad ; \; j = 1, 2, \ldots M \tag{1.21}$$

are extremals of the functional, the so-called *action integral*,

$$S[\vec{q}(t)] = \int_{t_0}^{t_1} dt \, L(\vec{q}(t), \dot{\vec{q}}(t), t) \tag{1.22}$$

where $L(\vec{q}(t), \dot{\vec{q}}(t), t)$ is the so-called *Lagrangian*

$$L(\vec{q}(t), \dot{\vec{q}}(t), t) = \sum_{j=1}^{M} \frac{1}{2} m_j \dot{q}_j^2 - U(q_1, q_2, \ldots, q_M) \,. \tag{1.23}$$

Presently we consider only velocity–independent potentials. Velocity–dependent potentials which describe particles moving in electromagnetic fields will be considered below.

For a proof of the Hamiltonian Principle of Least Action we inspect the Euler–Lagrange conditions associated with the action integral defined through (1.22, 1.23). These conditions read in the present case

$$\frac{\partial L}{\partial q_j} \;-\; \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) \;=\; 0 \;\rightarrow\; -\frac{\partial U}{\partial q_j} \;-\; \frac{d}{dt}(m_j \dot{q}_j) \;=\; 0 \tag{1.24}$$

which are obviously equivalent to the Newtonian equations of motion.

Particle Moving in an Electromagnetic Field

We will now consider the Newtonian equations of motion for a single particle of charge q with a trajectory $\vec{r}(t) \;=\; (x_1(t), x_2(t), x_3(t))$ moving in an electromagnetic field described through the electrical and magnetic field components $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$, respectively. The equations of motion for such a particle are

$$\frac{d}{dt}(m\dot{\vec{r}}) \;=\; \vec{F}(\vec{r},t)\;;\; \vec{F}(\vec{r},t) \;=\; q\,\vec{E}(\vec{r},t) \;+\; \frac{q}{c}\,\vec{v}\times\vec{B}(\vec{r},t) \tag{1.25}$$

where $\frac{d\vec{r}}{dt} \;=\; \vec{v}$ and where $\vec{F}(\vec{r},t)$ is the Lorentz force.

The fields $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$ obey the Maxwell equations

$$\nabla\times\vec{E} \;+\; \tfrac{1}{c}\tfrac{\partial}{\partial t}\vec{B} \;=\; 0 \tag{1.26}$$

$$\nabla\cdot\vec{B} \;=\; 0 \tag{1.27}$$

$$\nabla\times\vec{B} \;-\; \tfrac{1}{c}\tfrac{\partial}{\partial t}\vec{E} \;=\; \frac{4\pi\vec{J}}{c} \tag{1.28}$$

$$\nabla\cdot\vec{E} \;=\; 4\pi\rho \tag{1.29}$$

where $\rho(\vec{r},t)$ describes the charge density present in the field and $\vec{J}(\vec{r},t)$ describes the charge current density. Equations (1.27) and (1.28) can be satisfied implicitly if one represents the fields through a scalar potential $V(\vec{r},t)$ and a vector potential $\vec{A}(\vec{r},t)$ as follows

$$\vec{B} \;=\; \nabla\times\vec{A} \tag{1.30}$$

$$\vec{E} \;=\; -\nabla V \;-\; \frac{1}{c}\frac{\partial\vec{A}}{\partial t}\,. \tag{1.31}$$

Gauge Symmetry of the Electromagnetic Field

It is well known that the relationship between fields and potentials (1.30, 1.31) allows one to transform the potentials without affecting the fields and without affecting the equations of motion (1.25) of a particle moving in the field. The transformation which leaves the fields invariant is

$$\vec{A}'(\vec{r},t) \;=\; \vec{A}(\vec{r},t) \;+\; \nabla K(\vec{r},t) \tag{1.32}$$

$$V'(\vec{r},t) \;=\; V(\vec{r},t) \;-\; \frac{1}{c}\frac{\partial}{\partial t}K(\vec{r},t) \tag{1.33}$$

Lagrangian of Particle Moving in Electromagnetic Field

We want to show now that the equation of motion (1.25) follows from the Hamiltonian Principle of Least Action, if one assumes for a particle the Lagrangian

$$L(\vec{r},\dot{\vec{r}},t) \;=\; \frac{1}{2}m\vec{v}^2 \;-\; q\,V(\vec{r},t) \;+\; \frac{q}{c}\,\vec{A}(\vec{r},t)\cdot\vec{v}\,. \tag{1.34}$$

For this purpose we consider only one component of the equation of motion (1.25), namely,

$$\frac{d}{dt}(mv_1) \;=\; F_1 \;=\; -q\,\frac{\partial V}{\partial x_1} \;+\; \frac{q}{c}\,[\vec{v}\times\vec{B}]_1\,. \tag{1.35}$$

We notice using (1.30), e.g., $B_3 = \frac{\partial A_2}{\partial x_1} - \frac{\partial A_1}{\partial x_2}$

$$[\vec{v}\times\vec{B}]_1 \;=\; \dot{x}_2 B_3 \;-\; \dot{x}_3 B_2 \;=\; \dot{x}_2\left(\frac{\partial A_2}{\partial x_1} - \frac{\partial A_1}{\partial x_2}\right) \;-\; \dot{x}_3\left(\frac{\partial A_1}{\partial x_3} - \frac{\partial A_3}{\partial x_1}\right)\,. \tag{1.36}$$

This expression allows us to show that (1.35) is equivalent to the Euler–Lagrange condition

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_1}\right) \;-\; \frac{\partial L}{\partial x_1} \;=\; 0\,. \tag{1.37}$$

The second term in (1.37) is

$$\frac{\partial L}{\partial x_1} \;=\; -q\,\frac{\partial V}{\partial x_1} \;+\; \frac{q}{c}\left(\frac{\partial A_1}{\partial x_1}\,\dot{x}_1 \;+\; \frac{\partial A_2}{\partial x_1}\,\dot{x}_2 \;+\; \frac{\partial A_3}{\partial x_1}\,\dot{x}_3\right)\,. \tag{1.38}$$

The first term in (1.37) is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_1}\right) \;=\; \frac{d}{dt}(m\dot{x}_1) + \frac{q}{c}\,\frac{dA_1}{dt} \;=\; \frac{d}{dt}(m\dot{x}_1) + \frac{q}{c}\left(\frac{\partial A_1}{\partial x_1}\,\dot{x}_1 \;+\; \frac{\partial A_1}{\partial x_2}\,\dot{x}_2 \;+\; \frac{\partial A_1}{\partial x_3}\,\dot{x}_3\right)\,. \tag{1.39}$$

The results (1.38, 1.39) together yield

$$\frac{d}{dt}(m\dot{x}_1) \;=\; -q\,\frac{\partial V}{\partial x_1} \;+\; \frac{q}{c}\,O \tag{1.40}$$

where

$$\begin{aligned} O \;&=\; \frac{\partial A_1}{\partial x_1}\,\dot{x}_1 \;+\; \frac{\partial A_2}{\partial x_1}\,\dot{x}_2 \;+\; \frac{\partial A_3}{\partial x_1}\,\dot{x}_3 \;-\; \frac{\partial A_1}{\partial x_1}\,\dot{x}_1 \;-\; \frac{\partial A_1}{\partial x_2}\,\dot{x}_2 \;-\; \frac{\partial A_1}{\partial x_3}\,\dot{x}_3 \\ &=\; \dot{x}_2\left(\frac{\partial A_2}{\partial x_1} \;-\; \frac{\partial A_1}{\partial x_2}\right) \;-\; \dot{x}_3\left(\frac{\partial A_1}{\partial x_3} \;-\; \frac{\partial A_3}{\partial x_1}\right) \end{aligned} \tag{1.41}$$

which is identical to the term (1.36) in the Newtonian equation of motion. Comparing then (1.40, 1.41) with (1.35) shows that the Newtonian equations of motion and the Euler–Lagrange conditions are, in fact, equivalent.

1.3 Symmetry Properties in Lagrangian Mechanics

Symmetry properties play an eminent role in Quantum Mechanics since they reflect the properties of the elementary constituents of physical systems, and since these properties allow one often to simplify mathematical descriptions.

We will consider in the following two symmetries, gauge symmetry and symmetries with respect to spatial transformations.

The gauge symmetry, encountered above in connection with the transformations (1.32, 1.33) of electromagnetic potentials, appear in a different, surprisingly simple fashion in Lagrangian Mechanics. They are the subject of the following theorem.

Theorem: *Gauge Transformation of Lagrangian*

The equation of motion (Euler–Lagrange conditions) of a classical mechanical system are unaffected by the following transformation of its Lagrangian

$$L'(\vec{q}, \dot{\vec{q}}, t) \;=\; L(\vec{q}, \dot{\vec{q}}, t) \;+\; \frac{d}{dt}\frac{q}{c}\,K(\vec{q}, t) \tag{1.42}$$

This transformation is termed gauge transformation. The factor $\frac{q}{c}$ has been introduced to make this transformation equivalent to the gauge transformation (1.32, 1.33) of electyromagnetic potentials. Note that one adds the *total* time derivative of a function $K(\vec{r}, t)$ the Lagrangian. This term is

$$\frac{d}{dt}K(\vec{r}, t) \;=\; \frac{\partial K}{\partial x_1}\,\dot{x}_1 \;+\; \frac{\partial K}{\partial x_2}\,\dot{x}_2 \;+\; \frac{\partial K}{\partial x_3}\,\dot{x}_3 \;+\; \frac{\partial K}{\partial t} \;=\; (\nabla K)\cdot\vec{v} \;+\; \frac{\partial K}{\partial t}\,. \tag{1.43}$$

To prove this theorem we determine the action integral corresponding to the transformed Lagrangian

$$S'[\vec{q}(t)] = \int_{t_0}^{t_1} dt L'(\vec{q}, \dot{\vec{q}}, t) = \int_{t_0}^{t_1} dt L(\vec{q}, \dot{\vec{q}}, t) + \frac{q}{c} K(\vec{q}, t)\Big|_{t_0}^{t_1}$$
$$= S[\vec{q}(t)] + \frac{q}{c} K(\vec{q}, t)\Big|_{t_0}^{t_1} \qquad (1.44)$$

Since the condition $\delta\vec{q}(t_0) = \delta\vec{q}(t_1) = 0$ holds for the variational functions of Lagrangian Mechanics, Eq. (1.44) implies that the gauge transformation amounts to adding a constant term to the action integral, i.e., a term not affected by the variations allowed. One can conclude then immediately that any extremal of $S'[\vec{q}(t)]$ is also an extremal of $S[\vec{q}(t)]$.

We want to demonstrate now that the transformation (1.42) is, in fact, equivalent to the gauge transformation (1.32, 1.33) of electromagnetic potentials. For this purpose we consider the transformation of the single particle Lagrangian (1.34)

$$L'(\vec{r}, \dot{\vec{r}}, t) = \frac{1}{2} m\vec{v}^2 - q V(\vec{r}, t) + \frac{q}{c} \vec{A}(\vec{r}, t) \cdot \vec{v} + \frac{q}{c} \frac{d}{dt} K(\vec{r}, t) \,. \qquad (1.45)$$

Inserting (1.43) into (1.45) and reordering terms yields using (1.32, 1.33)

$$L'(\vec{r}, \dot{\vec{r}}, t) = \frac{1}{2} m\vec{v}^2 - q \left(V(\vec{r}, t) - \frac{1}{c} \frac{\partial K}{\partial t} \right) + \frac{q}{c} \left(\vec{A}(\vec{r}, t) + \nabla K \right) \cdot \vec{v}$$
$$= \frac{1}{2} m\vec{v}^2 - q V'(\vec{r}, t) + \frac{q}{c} \vec{A}'(\vec{r}, t) \cdot \vec{v} \,. \qquad (1.46)$$

Obviously, the transformation (1.42) corresponds to replacing in the Lagrangian potentials $V(\vec{r}, t)$, $\vec{A}(\vec{r}, t)$ by gauge transformed potentials $V'(\vec{r}, t)$, $\vec{A}'(\vec{r}, t)$. We have proven, therefore, the equivalence of (1.42) and (1.32, 1.33).

We consider now invariance properties connected with coordinate transformations. Such invariance properties are very familiar, for example, in the case of central force fields which are invariant with respect to rotations of coordinates around the center.

The following description of spatial symmetry is important in two respects, for the connection between invariance properties and constants of motion, which has an important analogy in Quantum Mechanics, and for the introduction of infinitesimal transformations which will provide a crucial method for the study of symmetry in Quantum Mechanics. The transformations we consider are the most simple kind, the reason being that our interest

lies in achieving familiarity with the principles (just mentioned above) of symmetry properties rather than in providing a general tool in the context of Classical Mechanics. The transformations considered are specified in the following definition.
Definition: Infinitesimal One-Parameter Coordinate Transformations
A *one-parameter coordinate transformation* is decribed through

$$\vec{r}\,' \;=\; \vec{r}\,'(\vec{r},\epsilon)\;,\;\vec{r},\,\vec{r}\,' \,\in\, \mathbb{R}^3\;,\;\epsilon\,\in\,\mathbb{R} \tag{1.47}$$

where the origin of ϵ is chosen such that

$$\vec{r}\,'(\vec{r},0) \;=\; \vec{r}\;. \tag{1.48}$$

The corresponding *infinitesimal transformation* is defined for small ϵ through

$$\vec{r}\,'(\vec{r},\epsilon) \;=\; \vec{r} \,+\, \epsilon\,\vec{R}(\vec{r}) \,+\, O(\epsilon^2)\;;\quad \vec{R}(\vec{r}) \;=\; \left.\frac{\partial\vec{r}\,'}{\partial\epsilon}\right|_{\epsilon=0} \tag{1.49}$$

In the following we will denote *unit vectors* as $\hat{a}$, i.e., for such vectors holds $\hat{a}\cdot\hat{a} \,=\, 1$.

Examples of Infinitesimal Transformations

The beauty of infinitesimal transformations is that they can be stated in a very simple manner. In case of a *translation transformation* in the direction $\hat{e}$ nothing new is gained. However, we like to provide the transformation here anyway for later reference

$$\vec{r}\,' \;=\; \vec{r} \,+\, \epsilon\,\hat{e}\;. \tag{1.50}$$

A non-trivial example is furnished by the infinitesimal rotation around axis $\hat{e}$

$$\vec{r}\,' \;=\; \vec{r} \,+\, \epsilon\,\hat{e}\times\vec{r}\;. \tag{1.51}$$

We would like to derive this transformation in a somewhat complicated, but nevertheless instructive way considering rotations around the x_3–axis. In this case the transformation can be written in matrix form

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} \;=\; \begin{pmatrix} \cos\epsilon & -\sin\epsilon & 0 \\ \sin\epsilon & \cos\epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \tag{1.52}$$

In case of small ϵ this transformation can be written neglecting terms $O(\epsilon^2)$ using $\cos\epsilon = 1 + O(\epsilon^2)$, $\sin\epsilon = \epsilon + O(\epsilon^2)$

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} 0 & -\epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + O(\epsilon^2) \,. \tag{1.53}$$

One can readily verify that in case $\hat{e} = \hat{e}_3$ ($\hat{e}_j$ denoting the unit vector in the direction of the x_j–axis) (1.51) reads

$$\vec{r}\,' = \vec{r} - x_2\,\hat{e}_1 + x_1\,\hat{e}_2 \tag{1.54}$$

which is equivalent to (1.53).

Anytime, a classical mechanical system is invariant with respect to a coordinate transformation a constant of motion exists, i.e., a quantity $C(\vec{r}, \dot{\vec{r}})$ which is constant along the classical path of the system. We have used here the notation corresponding to single particle motion, however, the property holds for any system.

The property has been shown to hold in a more general context, namely for fields rather than only for particle motion, by Noether. We consider here only the 'particle version' of the theorem. Before the embark on this theorem we will comment on what is meant by the statement that a classical mechanical system is invariant under a coordinate transformation. In the context of Lagrangian Mechanics this implies that such transformation leaves the Lagrangian of the system unchanged.

Theorem: *Noether's Theorem*

If $L(\vec{q}, \dot{\vec{q}}, t)$ is invariant with respect to an infinitesimal transformation $\vec{q}\,' = \vec{q} + \epsilon\,\vec{Q}(\vec{q})$, then $\sum_{j=1}^{M} Q_j \frac{\partial L}{\partial \dot{x}_j}$ is a constant of motion.

We have generalized in this theorem the definition of infinitesimal coordinate transformation to M–dimensional vectors $\vec{q}$.

In order to prove Noether's theorem we note

$$q_j' = q_j + \epsilon\,Q_j(\vec{q}) \tag{1.55}$$

$$\dot{q}_j' = \dot{q}_j + \epsilon \sum_{k=1}^{M} \frac{\partial Q_j}{\partial q_k}\,\dot{q}_k \,. \tag{1.56}$$

Inserting these infinitesimal changes of q_j and $\dot{q}_j$ into the Lagrangian $L(\vec{q}, \dot{\vec{q}}, t)$ yields after Taylor expansion, neglecting terms of order $O(\epsilon^2)$,

$$L'(\vec{q}, \dot{\vec{q}}, t) = L(\vec{q}, \dot{\vec{q}}, t) + \epsilon \sum_{j=1}^{M} \frac{\partial L}{\partial q_j} Q_j + \epsilon \sum_{j,k=1}^{M} \frac{\partial L}{\partial \dot{q}_j} \frac{\partial Q_j}{\partial q_k} \dot{q}_k \tag{1.57}$$

where we used $\frac{d}{dt}Q_j = \sum_{k=1}^{M}(\frac{\partial}{\partial q_k}Q_j)\dot{q}_k$. Invariance implies $L' = L$, i.e., the second and third term in (1.57) must cancel each other or both vanish. Using the fact, that *along the classical path* holds the Euler-Lagrange condition $\frac{\partial L}{\partial q_j} = \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}_j})$ one can rewrite the sum of the second and third term in (1.57)

$$\sum_{j=1}^{M}\left(Q_j \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) + \frac{\partial L}{\partial \dot{q}_j}\frac{d}{dt}Q_j \right) = \frac{d}{dt}\left(\sum_{j=1}^{M} Q_j \frac{\partial L}{\partial \dot{q}_j} \right) = 0 \tag{1.58}$$

From this follows the statement of the theorem.

Application of Noether's Theorem

We consider briefly two examples of invariances with respect to coordinate transformations for the Lagrangian $L(\vec{r},\vec{v}) = \frac{1}{2}m\vec{v}^{\,2} - U(\vec{r})$.

We first determine the constant of motion in case of invariance with respect to translations as defined in (1.50). In this case we have $Q_j = \hat{e}_j \cdot \hat{e}$, $j = 1, 2, 3$ and, hence, Noether's theorem yields the constant of motion ($q_j = x_j$, $j = 1, 2, 3$)

$$\sum_{j=1}^{3} Q_j \frac{\partial L}{\partial \dot{x}_j} = \hat{e} \cdot \sum_{j=1}^{3} \hat{e}_j m \dot{x}_j = \hat{e} \cdot m\vec{v}\,. \tag{1.59}$$

We obtain the well known result that in this case the momentum in the direction, for which translational invariance holds, is conserved.

We will now investigate the consequence of rotational invariance as described according to the infinitesimal transformation (1.51). In this case we will use the same notation as in (1.59), except using now $Q_j = \hat{e}_j \cdot (\hat{e} \times \vec{r})$. A calculation similar to that in (1.59) yields the constant of motion $(\hat{e} \times \vec{r}) \cdot m\vec{v}$. Using the cyclic property $(\vec{a} \times \vec{b}) \cdot \vec{c} = (\vec{b} \times \vec{c}) \cdot \vec{a} = (\vec{c} \times \vec{a}) \cdot \vec{b}$ allows one to rewrite the constant of motion $\hat{e} \cdot (\vec{r} \times m\vec{v})$ which can be identified as the component of the angular momentum $m\vec{r} \times \vec{v}$ in the $\hat{e}$ direction. It was, of course, to be expected that this is the constant of motion.

The important result to be remembered for later considerations of symmetry transformations in the context of Quantum Mechanics is that it is sufficient to know the consequences of infinitesimal transformations to predict the symmetry properties of Classical Mechanics. It is not necessary to investigate the consequences of global. i.e, not infinitesimal transformations.

Chapter 2

Quantum Mechanical Path Integral

2.1 The Double Slit Experiment

Will be supplied at later date

2.2 Axioms for Quantum Mechanical Description of Single Particle

Let us consider a particle which is described by a Lagrangian $L(\vec{r}, \dot{\vec{r}}, t)$. We provide now a set of formal rules which state how the probability to observe such a particle at some space–time point $\vec{r}$, t is described in Quantum Mechanics.

1. The particle is described by a wave function $\psi(\vec{r}, t)$
$$\psi : \mathbb{R}^3 \otimes \mathbb{R} \rightarrow \mathbb{C}. \tag{2.1}$$

2. The probability that the particle is detected at space–time point $\vec{r}, t$ is
$$|\psi(\vec{r}, t)|^2 = \overline{\psi(\vec{r}, t)}\psi(\vec{r}, t) \tag{2.2}$$
where $\overline{z}$ is the conjugate complex of z.

3. The probability to detect the particle with a detector of sensitivity $f(\vec{r})$ is
$$\int_\Omega d^3r\, f(\vec{r})\, |\psi(\vec{r}, t)|^2 \tag{2.3}$$

where Ω is the space volume in which the particle can exist. At present one may think of $f(\vec{r})$ as a sum over δ–functions which represent a multi–slit screen, placed into the space at some particular time and with a detector behind each slit.

4. The wave function $\psi(\vec{r}, t)$ is normalized

$$\int_\Omega d^3r \, |\psi(\vec{r}, t)|^2 \;=\; 1 \qquad \forall t,\, t \,\in\, [t_0, t_1]\,, \tag{2.4}$$

a condition which enforces that the probability of finding the particle somewhere in Ω at any particular time t in an interval $[t_0, t_1]$ in which the particle is known to exist, is unity.

5. The time evolution of $\psi(\vec{r}, t)$ is described by a linear map of the type

$$\psi(\vec{r}, t) \;=\; \int_\Omega d^3r' \, \phi(\vec{r}, t|\vec{r}', t') \, \psi(\vec{r}', t') \qquad t \,>\, t',\; t, t' \,\in\, [t_0, t_1] \tag{2.5}$$

6. Since (2.4) holds for all times, the propagator is unitary, i.e., ($t \,>\, t',\; t, t' \,\in\, [t_0, t_1]$)

$$\begin{aligned} &\textstyle\int_\Omega d^3r \, |\psi(\vec{r}, t)|^2 \;= \\ &\textstyle\int_\Omega d^3r \int_\Omega d^3r' \int_\Omega d^3r'' \; \phi(\vec{r}, t|\vec{r}', t') \; \overline{\phi(\vec{r}, t|\vec{r}'', t')} \; \psi(\vec{r}', t') \; \overline{\psi(\vec{r}'', t')} \\ &\;=\; \textstyle\int_\Omega d^3r \, |\psi(\vec{r}, t')|^2 \;=\; 1 \,. \end{aligned} \tag{2.6}$$

This must hold for any $\psi(\vec{r}', t')$ which requires

$$\int_\Omega d^3r' \, \phi(\vec{r}, t|\vec{r}', t') \overline{\phi(\vec{r}, t|\vec{r}'', t')} \;=\; \delta(\vec{r}' \,-\, \vec{r}'') \tag{2.7}$$

7. The following so-called completeness relationship holds for the propagator ($t \,>\, t' \quad t, t' \,\in\, [t_0, t_1]$)

$$\int_\Omega d^3r \, \phi(\vec{r}, t|\vec{r}', t') \; \phi(\vec{r}', t'|\vec{r}_0, t_0) \;=\; \phi(\vec{r}, t|\vec{r}_0, t_0) \tag{2.8}$$

This relationship has the following interpretation: Assume that at time t_0 a particle is generated by a source at one point $\vec{r}_0$ in space, i.e., $\psi(\vec{r}_0, t_0) \;=\; \delta(\vec{r} \,-\, \vec{r}_0)$. The state of a system at time t, described by $\psi(\vec{r}, t)$, requires then according to (2.8) a knowledge of the state at all space points $\vec{r}' \,\in \Omega$ at some intermediate time t'. This is different from the classical situation where the particle follows a discrete path and, hence, at any intermediate time the particle needs only be known at one space point, namely the point on the classical path at time t'.

8. The generalization of the completeness property to $N-1$ intermediate points $t > t_{N-1} > t_{N-2} > \ldots > t_1 > t_0$ is

$$\phi(\vec{r},t|\vec{r}_0,t_0) = \int_\Omega d^3r_{N-1} \int_\Omega d^3r_{N-2} \cdots \int_\Omega d^3r_1$$
$$\phi(\vec{r},t_|\vec{r}_{N-1},t_{N-1})\, \phi(\vec{r}_{N-1},t_{N-1}|\vec{r}_{N-2},t_{N-2}) \cdots \phi(\vec{r}_1,t_1|\vec{r}_0,t_0) \quad (2.9)$$

Employing a continuum of intermediate times $t' \in [t_0, t_1]$ yields an expression of the form

$$\phi(\vec{r},t|\vec{r}_0,t_0) = \iint_{\vec{r}(t_0)=\vec{r}_0}^{\vec{r}(t_N)=\vec{r}_N} d[\vec{r}(t)]\; \Phi[\vec{r}(t)]\ . \quad (2.10)$$

We have introduced here a new symbol, the path integral

$$\iint_{\vec{r}(t_0)=\vec{r}_0}^{\vec{r}(t_N)=\vec{r}_N} d[\vec{r}(t)]\ \cdots \quad (2.11)$$

which denotes an integral over all paths $\vec{r}(t)$ with end points $\vec{r}(t_0) = \vec{r}_0$ and $\vec{r}(t_N) = \vec{r}_N$. This symbol will be defined further below. The definition will actually assume an infinite number of intermediate times and express the path integral through integrals of the type (2.9) for $N \to \infty$.

9. The functional $\Phi[\vec{r}(t)]$ in (2.11) is

$$\Phi[\vec{r}(t)] = \exp\left\{ \frac{i}{\hbar} S[\vec{r}(t)] \right\} \quad (2.12)$$

where $S[\vec{r}(t)]$ is the classical action integral

$$S[\vec{r}(t)] = \int_{t_0}^{t_N} dt\, L(\vec{r},\dot{\vec{r}},t) \quad (2.13)$$

and

$$\hbar = 1.0545 \cdot 10^{-27}\, \text{erg s}\ . \quad (2.14)$$

In (2.13) $L(\vec{r},\dot{\vec{r}},t)$ is the Lagrangian of the classical particle. However, in complete distinction from Classical Mechanics, expressions (2.12, 2.13) are built on action integrals for all possible paths, not only for the classical path. Situations which are well described classically will be distinguished through the property that the classical path gives the dominant, actually often essentially exclusive, contribution to the path integral (2.12, 2.13). However, for microscopic particles like the electron this is by no means the case, i.e., for the electron many paths contribute and the action integrals for non-classical paths need to be known.

The constant $\hbar$ given in (2.14) has the same dimension as the action integral $S[\vec{r}(t)]$. Its value is extremely small in comparision with typical values for action integrals of macroscopic particles. However, it is comparable to action integrals as they arise for microscopic particles under typical circumstances. To show this we consider the value of the action integral for a particle of mass $m = 1$ g moving over a distance of 1 cm/s in a time period of 1 s. The value of $S[\vec{r}(t)]$ is then

$$S_{cl} \;=\; \frac{1}{2}\, m\, v^2\, t \;=\; \frac{1}{2} \mathrm{erg\,s}\,. \tag{2.15}$$

The exponent of (2.12) is then $S_{cl}/\hbar \approx 0.5 \cdot 10^{27}$, i.e., a very large number. Since this number is multiplied by 'i', the exponent is a very large imaginary number. Any variations of S_{cl} would then lead to strong oscillations of the contributions $\exp(\frac{i}{\hbar}S)$ to the path integral and one can expect destructive interference betwen these contributions. Only for paths close to the classical path is such interference ruled out, namely due to the property of the classical path to be an extremal of the action integral. This implies that small variations of the path near the classical path alter the value of the action integral by very little, such that destructive interference of the contributions of such paths does not occur.

The situation is very different for microscopic particles. In case of a proton with mass $m = 1.6725 \cdot 10^{-24}$ g moving over a distance of 1 Å in a time period of 10^{-14} s the value of $S[\vec{r}(t)]$ is $S_{cl} \approx 10^{-26}$ erg s and, accordingly, $S_{cl}/\hbar \approx 8$. This number is much smaller than the one for the macroscopic particle considered above and one expects that variations of the exponent of $\Phi[\vec{r}(t)]$ are of the order of unity for protons. One would still expect significant descructive interference between contributions of different paths since the value calculated is comparable to 2π. However, interferences should be much less dramatic than in case of the macroscopic particle.

2.3 How to Evaluate the Path Integral

In this section we will provide an explicit algorithm which defines the path integral (2.12, 2.13) and, at the same time, provides an avenue to evaluate path integrals. For the sake of simplicity we will consider the case of particles moving in one dimension labelled by the position coordinate x. The particles have associated with them a Lagrangian

$$L(x, \dot{x}, t) \;=\; \frac{1}{2} m \dot{x}^2 \;-\; U(x)\,. \tag{2.16}$$

In order to define the path integral we assume, as in (2.9), a series of times $t_N > t_{N-1} > t_{N-2} > \ldots > t_1 > t_0$ letting N go to infinity later. The spacings between the times t_{j+1} and t_j will all be identical, namely

$$t_{j+1} - t_j = (t_N - t_0)/N = \epsilon_N . \tag{2.17}$$

The discretization in time leads to a discretization of the paths $x(t)$ which will be represented through the series of space–time points

$$\{(x_0, t_0), (x_1, t_1), \ldots (x_{N-1}, t_{N-1}), (x_N, t_N)\} . \tag{2.18}$$

The time instances are fixed, however, the x_j values are not. They can be anywhere in the allowed volume which we will choose to be the interval $]-\infty, \infty[$. In passing from one space–time instance (x_j, t_j) to the next (x_{j+1}, t_{j+1}) we assume that kinetic energy and potential energy are constant, namely $\frac{1}{2}m(x_{j+1} - x_j)^2/\epsilon_N^2$ and $U(x_j)$, respectively. These assumptions lead then to the following Riemann form for the action integral

$$S[x(t)] = \lim_{N\to\infty} \epsilon_N \sum_{j=0}^{N-1} \left(\frac{1}{2} m \frac{(x_{j+1} - x_j)^2}{\epsilon_N^2} - U(x_j) \right) . \tag{2.19}$$

The main idea is that one can replace the path integral now by a multiple integral over x_1, x_2, etc. This allows us to write the evolution operator using (2.10) and (2.12)

$$\begin{aligned} \phi(x_N, t_N | x_0, t_0) = \; & \lim_{N\to\infty} C_N \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2 \ldots \int_{-\infty}^{+\infty} dx_{N-1} \\ & \exp\left\{ \tfrac{i}{\hbar}\, \epsilon_N \sum_{j=0}^{N-1} \left[\tfrac{1}{2} m \tfrac{(x_{j+1}-x_j)^2}{\epsilon_N^2} - U(x_j) \right] \right\} . \end{aligned} \tag{2.20}$$

Here, C_N is a constant which depends on N (actually also on other constant in the exponent) which needs to be chosen to ascertain that the limit in (2.20) can be properly taken. Its value is

$$C_N = \left[\frac{m}{2\pi i \hbar \epsilon_N} \right]^{\frac{N}{2}} \tag{2.21}$$

2.4 Propagator for a Free Particle

As a first example we will evaluate the path integral for a free particle following the algorithm introduced above.

Rather then using the integration variables x_j, it is more suitable to define new integration variables y_j, the origin of which coincides with the classical path of the particle. To see the benifit of such approach we define a path $y(t)$ as follows

$$x(t) \;=\; x_{cl}(t) \;+\; y(t) \tag{2.22}$$

where $x_{cl}(t)$ is the classical path which connects the space–time points (x_0, t_0) and (x_N, t_N), namely,

$$x_{cl}(t) \;=\; x_0 \;+\; \frac{x_N \;-\; x_0}{t_N \;-\; t_0}(\, t \;-\; t_0)\;. \tag{2.23}$$

It is essential for the following to note that, since $x(t_0) \;=\; x_{cl}(t_0) \;=\; x_0$ and $x(t_N) \;=\; x_{cl}(t_N) \;=\; x_N$, it holds

$$y(t_0) \;=\; y(t_N) \;=\; 0\;. \tag{2.24}$$

Also we use the fact that the velocity of the classical path $\dot{x}_{cl} \;=\; (x_N \;-\; x_0)/(t_n - t_0)$ is constant. The action integral[1] $S[x(t)|x(t_0) = x_0,\, x(t_N) = x_N]$ for any path $x(t)$ can then be expressed through an action integral over the path $y(t)$ relative to the classical path. One obtains

$$\begin{aligned} S[x(t)|x(t_0) = x_0,\, x(t_N) = x_N] \;&=\; \textstyle\int_{t_0}^{t_N} dt \frac{1}{2} m(\dot{x}_{cl}^2 \;+\; 2\dot{x}_{cl}\dot{y} \;+\; \dot{y}^2) \;=\; \\ &\textstyle\int_{t_0}^{t_N} dt \frac{1}{2} m\dot{x}_{cl}^2 \;+\; m\dot{x}_{cl} \int_{t_0}^{t_N} dt\dot{y} \;+\; \int_{t_0}^{t_N} dt \frac{1}{2} m\dot{y}^2\;. \end{aligned} \tag{2.25}$$

The condition (2.24) implies for the second term on the r.h.s.

$$\int_{t_0}^{t_N} dt\, \dot{y} \;=\; y(t_N) \;-\; y(t_0) \;=\; 0\;. \tag{2.26}$$

The first term on the r.h.s. of (2.25) is, using (2.23),

$$\int_{t_0}^{t_N} dt\, \frac{1}{2}\, m\, \dot{x}_{cl}^2 \;=\; \frac{1}{2} m \frac{(x_N \;-\; x_0)^2}{t_N \;-\; t_0}\;. \tag{2.27}$$

The third term can be written in the notation introduced

$$\int_{t_0}^{t_N} dt\, \frac{1}{2} m\dot{y}^2 \;=\; S[x(t)|x(t_0) = 0,\, x(t_N) = 0]\;, \tag{2.28}$$

[1] We have denoted explicitly that the action integral for a path connecting the space–time points (x_0, t_0) and (x_N, t_N) is to be evaluated.

i.e., due to (2.24), can be expressed through a path integral with end-points $x(t_0) = 0$, $x(t_N) = 0$. The resulting expression for $S[x(t)|x(t_0) = x_0, \, x(t_N) = x_N]$ is

$$\begin{aligned} S[x(t)|x(t_0) = x_0, \, x(t_N) = x_N] \; &= \frac{1}{2} m \frac{(x_N - x_0)^2}{t_N - t_0} + 0 + \\ &+ S[x(t)|x(t_0) = 0, \, x(t_N) = 0] \, . \end{aligned} \tag{2.29}$$

This expression corresponds to the action integral in (2.13). Inserting the result into (2.10, 2.12) yields

$$\phi(x_N, t_N | x_0, t_0) \; = \; \exp\left[\frac{im}{2\hbar} \frac{(x_N - x_0)^2}{t_N - t_0} \right] \int_{x(t_0)=0}^{x(t_N)=0} d[x(t)] \, \exp\left\{ \frac{i}{\hbar} \, S[x(t)] \right\} \tag{2.30}$$

a result, which can also be written

$$\phi(x_N, t_N | x_0, t_0) \; = \; \exp\left[\frac{im}{2\hbar} \frac{(x_N - x_0)^2}{t_N - t_0} \right] \, \phi(0, t_N | 0, t_0) \tag{2.31}$$

Evaluation of the necessary path integral

To determine the propagator (2.31) for a free particle one needs to evaluate the following path integral

$$\begin{aligned} \phi(0, t_N | 0, t_0) \; &= \; lim_{N \to \infty} \left[\tfrac{m}{2\pi i \hbar \epsilon_N} \right]^{\frac{N}{2}} \times \\ \times \int_{-\infty}^{+\infty} dy_1 \cdots \int_{-\infty}^{+\infty} dy_{N-1} \, &\exp\left[\tfrac{i}{\hbar} \, \epsilon_N \, \textstyle\sum_{j=0}^{N-1} \, \tfrac{1}{2} m \tfrac{(y_{j+1} - y_j)^2}{\epsilon_N^2} \right] \end{aligned} \tag{2.32}$$

The exponent E can be written, noting $y_0 = y_N = 0$, as the quadratic form

$$\begin{aligned} E \; &= \; \frac{im}{2\hbar\epsilon_N} \, (\, 2y_1^2 - y_1 y_2 - y_2 y_1 + 2y_2^2 - y_2 y_3 - y_3 y_2 \\ &+ 2y_3^2 - \cdots - y_{N-2} y_{N-1} - y_{N-1} y_{N-2} + 2y_{N-1}^2 \,) \\ &= \; i \sum_{j,k=1}^{N-1} y_j \, a_{jk} \, y_k \end{aligned} \tag{2.33}$$

where a_{jk} are the elements of the following symmetric $(N-1) \times (N-1)$ matrix

$$\left(a_{jk} \right) = \frac{m}{2\hbar\epsilon_N} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & & -1 & 2 \end{pmatrix} \tag{2.34}$$

The following integral

$$\int_{-\infty}^{+\infty} dy_1 \cdots \int_{-\infty}^{+\infty} dy_{N-1} \exp \left(i \sum_{j,k=1}^{N-1} y_j a_{jk} y_k \right) \tag{2.35}$$

must be determined. In the appendix we prove

$$\int_{-\infty}^{+\infty} dy_1 \cdots \int_{-\infty}^{+\infty} dy_{N-1} \exp \left(i \sum_{j,k=1}^{d} y_j b_{jk} y_k \right) = \left[\frac{(i\pi)^d}{\det(b_{jk})} \right]^{\frac{1}{2}} . \tag{2.36}$$

which holds for a d-dimensional, real, symmetric matrix (b_{jk}) and $\det(b_{jk}) \neq 0$.

In order to complete the evaluation of (2.32) we split off the factor $\frac{m}{2\hbar\epsilon_N}$ in the definition (2.34) of (a_{jk}) defining a new matrix (A_{jk}) through

$$a_{jk} = \frac{m}{2\hbar\epsilon_N} A_{jk} . \tag{2.37}$$

Using

$$\det(a_{jk}) = \left[\frac{m}{2\hbar\epsilon_N} \right]^{N-1} \det(A_{jk}) , \tag{2.38}$$

a property which follows from $\det(c\mathbf{B}) = c^n \det\mathbf{B}$ for any $n \times n$ matrix $\mathbf{B}$, we obtain

$$\phi(0, t_N | 0, t_0) = lim_{N\to\infty} \left[\frac{m}{2\pi i\hbar\epsilon_N} \right]^{\frac{N}{2}} \left[\frac{2\pi i\hbar\epsilon_N}{m} \right]^{\frac{N-1}{2}} \frac{1}{\sqrt{\det(A_{jk})}} . \tag{2.39}$$

In order to determine $\det(A_{jk})$ we consider the dimension n of (A_{jk}), presently $N-1$, variable, let say n, $n = 1, 2, \dots$. We seek then to evaluate the determinant of the $n \times n$ matrix

$$D_n = \left| \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & & -1 & 2 \end{pmatrix} \right| . \tag{2.40}$$

For this purpose we expand (2.40) in terms of subdeterminants along the last column. One can readily verify that this procedure leads to the following recursion equation for the determinants

$$D_n = 2\,D_{n-1} - D_{n-2} \, . \tag{2.41}$$

To solve this three term recursion relationship one needs two starting values. Using

$$D_1 = |(2)| = 2 \, ; \quad D_2 = \left| \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \right| = 3 \tag{2.42}$$

one can readily verify

$$D_n = n + 1 \, . \tag{2.43}$$

We like to note here for further use below that one might as well employ the 'artificial' starting values $D_0 = 1$, $D_1 = 2$ and obtain from (2.41) the same result for D_2, $D_3, \dots$.

Our derivation has provided us with the value $\det(A_{jk}) = N$. Inserting this into (2.39) yields

$$\phi(0, t_N|0, t_0) = lim_{N\to\infty} \left[\frac{m}{2\pi i\hbar \epsilon_N N} \right]^{\frac{1}{2}} \tag{2.44}$$

and with $\epsilon_N N = t_N - t_0$, which follows from (2.18) we obtain

$$\phi(0, t_N|0, t_0) = \left[\frac{m}{2\pi i\hbar (t_N - t_0)} \right]^{\frac{1}{2}} . \tag{2.45}$$

Expressions for Free Particle Propagator

We have now collected all pieces for the final expression of the propagator (2.31) and obtain, defining $t = t_N$, $x = x_N$

$$\phi(x, t|x_0, t_0) = \left[\frac{m}{2\pi i\hbar (t - t_0)} \right]^{\frac{1}{2}} \exp \left[\frac{im}{2\hbar} \frac{(x - x_0)^2}{t - t_0} \right] . \tag{2.46}$$

This propagator, according to (2.5) allows us to predict the time evolution of any state function $\psi(x,t)$ of a free particle. Below we will apply this to a particle at rest and a particle forming a so-called wave packet.

The result (2.46) can be generalized to three dimensions in a rather obvious way. One obtains then for the propagator (2.10)

$$\phi(\vec{r},t|\vec{r}_0,t_0) \; = \; \left[\frac{m}{2\pi i\hbar(t-t_0)}\right]^{\frac{3}{2}} \exp\left[\frac{im}{2\hbar}\frac{(\vec{r}-\vec{r}_0)^2}{t-t_0}\right] \; . \tag{2.47}$$

One-Dimensional Free Particle Described by Wave Packet

We assume a particle at time $t = t_o = 0$ is described by the wave function

$$\psi(x_0,t_0) \; = \; \left[\frac{1}{\pi\delta^2}\right]^{\frac{1}{4}} \exp\left(-\frac{x_0^2}{2\delta^2} + i\frac{p_o}{\hbar}\,x\right) \tag{2.48}$$

Obviously, the associated probability distribution

$$|\psi(x_0,t_0)|^2 \; = \; \left[\frac{1}{\pi\delta^2}\right]^{\frac{1}{2}} \exp\left(-\frac{x_0^2}{\delta^2}\right) \tag{2.49}$$

is Gaussian of width δ, centered around $x_0 = 0$, and describes a single particle since

$$\left[\frac{1}{\pi\delta^2}\right]^{\frac{1}{2}} \int_{-\infty}^{+\infty} dx_0 \exp\left(-\frac{x_0^2}{\delta^2}\right) \; = \; 1 \; . \tag{2.50}$$

One refers to such states as *wave packets*. We want to apply axiom (2.5) to (2.48) as the initial state using the propagator (2.46).

We will obtain, thereby, the wave function of the particle at later times. We need to evaluate for this purpose the integral

$$\begin{aligned}\psi(x,t) \; &= \; \left[\frac{1}{\pi\delta^2}\right]^{\frac{1}{4}} \left[\frac{m}{2\pi i\hbar t}\right]^{\frac{1}{2}} \\ &\qquad \int_{-\infty}^{+\infty} dx_0 \exp \underbrace{\left[\frac{im}{2\hbar}\frac{(x-x_0)^2}{t} - \frac{x_0^2}{2\delta^2} + i\frac{p_o}{\hbar}\,x_o\right]}_{E_o(x_o,x) \; + \; E(x)}\end{aligned} \tag{2.51}$$

For this evaluation we adopt the strategy of combining in the exponential the terms quadratic ($\sim x_0^2$) and linear ($\sim x_0$) in the integration variable to a complete square

$$a x_0^2 + 2 b x_0 \; = \; a\left(x_0 + \frac{b}{a}\right)^2 - \frac{b^2}{a} \tag{2.52}$$

and applying (2.247).

We devide the contributions to the exponent $E_o(x_o, x) + E(x)$ in (2.51) as follows

$$E_o(x_o, x) = \frac{im}{2\hbar t} \left[x_o^2 \left(1 + i\frac{\hbar t}{m\delta^2} \right) - 2x_o \left(x - \frac{p_o}{m} t \right) + f(x) \right] \tag{2.53}$$

$$E(x) = \frac{im}{2\hbar t} \left[x^2 - f(x) \right] . \tag{2.54}$$

One chooses then $f(x)$ to complete, according to (2.52), the square in (2.53)

$$f(x) = \left(\frac{x - \frac{p_o}{m} t}{\sqrt{1 + i\frac{\hbar t}{m\delta^2}}} \right)^2 . \tag{2.55}$$

This yields

$$E_o(x_o, x) = \frac{im}{2\hbar t} \left(x_o \sqrt{1 + i\frac{\hbar t}{m\delta^2}} - \frac{x - \frac{p_o}{m} t}{\sqrt{1 + i\frac{\hbar t}{m\delta^2}}} \right)^2 . \tag{2.56}$$

One can write then (2.51)

$$\psi(x, t) = \left[\frac{1}{\pi\delta^2} \right]^{\frac{1}{4}} \left[\frac{m}{2\pi i\hbar t} \right]^{\frac{1}{2}} e^{E(x)} \int_{-\infty}^{+\infty} dx_0 \, e^{E_o(x_o, x)} \tag{2.57}$$

and needs to determine the integral

$$\begin{aligned} I &= \int_{-\infty}^{+\infty} dx_0 \, e^{E_o(x_o, x)} \\ &= \int_{-\infty}^{+\infty} dx_0 \exp \left[\frac{im}{2\hbar t} \left(x_o \sqrt{1 + i\frac{\hbar t}{m\delta^2}} - \frac{x - \frac{p_o}{m} t}{\sqrt{1 + i\frac{\hbar t}{m\delta^2}}} \right)^2 \right] \\ &= \int_{-\infty}^{+\infty} dx_0 \exp \left[\frac{im}{2\hbar t} \left(1 + i\frac{\hbar t}{m\delta^2} \right) \left(x_o - \frac{x - \frac{p_o}{m} t}{1 + i\frac{\hbar t}{m\delta^2}} \right)^2 \right] . \end{aligned} \tag{2.58}$$

The integrand is an analytical function everywhere in the complex plane and we can alter the integration path, making certain, however, that the new path does not lead to additional contributions to the integral.

We proceed as follows. We consider a transformation to a new integration variable ρ defined through

$$\sqrt{i\left(1 - i\frac{\hbar t}{m\delta^2}\right)}\,\rho \;=\; x_0 \;-\; \frac{x \;-\; \frac{p_o}{m}\,t}{1 + i\frac{\hbar t}{m\delta^2}}\;. \tag{2.59}$$

An integration path in the complex x_0–plane along the direction

$$\sqrt{i\left(1 - i\frac{\hbar t}{m\delta^2}\right)} \tag{2.60}$$

is then represented by real ρ values. The beginning and the end of such path are the points

$$z_1' \;=\; -\infty \,\times\, \sqrt{i\left(1 - i\frac{\hbar t}{m\delta^2}\right)}\;,\quad z_2' \;=\; +\infty \,\times\, \sqrt{i\left(1 - i\frac{\hbar t}{m\delta^2}\right)} \tag{2.61}$$

whereas the original path in (2.58) has the end points

$$z_1 \;=\; -\infty\;,\quad z_2 \;=\; +\infty\;. \tag{2.62}$$

If one can show that an integration of (2.58) along the path $z_1 \rightarrow z_1'$ and along the path $z_2 \rightarrow z_2'$ gives only vanishing contributions one can replace (2.58) by

$$I \;=\; \sqrt{i\left(1 - i\frac{\hbar t}{m\delta^2}\right)}\int_{-\infty}^{+\infty} d\rho \exp\left[-\frac{m}{2\hbar t}\left(1 \,+\, \left(\frac{\hbar t}{m\delta^2}\right)^2\right)\rho^2\right] \tag{2.63}$$

which can be readily evaluated. In fact, one can show that z_1' lies at $-\infty - i \times \infty$ and z_2' at $+\infty + i \times \infty$. Hence, the paths between $z_1 \rightarrow z_1'$ and $z_2 \rightarrow z_2'$ have a real part of x_0 of $\pm\infty$. Since the exponent in (2.58) has a leading contribution in x_0 of $-x_0^2/\delta^2$ the integrand of (2.58) vanishes for $Re\, x_0 \rightarrow \pm\infty$. We can conclude then that (2.63) holds and, accordingly,

$$I \;=\; \sqrt{\frac{2\pi i\hbar t}{m(1 \,+\, i\frac{\hbar t}{m\delta^2})}}\;. \tag{2.64}$$

Equation (2.57) reads then

$$\psi(x,t) \;=\; \left[\frac{1}{\pi\delta^2}\right]^{\frac{1}{4}}\left[\frac{1}{1 \,+\, i\frac{\hbar t}{m\delta^2}}\right]^{\frac{1}{2}} \exp\left[\,E(x)\,\right]\;. \tag{2.65}$$

Seperating the phase factor

$$\left[\frac{1 \,-\, i \frac{\hbar t}{m \delta^2}}{1 \,+\, i \frac{\hbar t}{m \delta^2}} \right]^{\frac{1}{4}} \,, \tag{2.66}$$

yields

$$\psi(x,t) \;=\; \left[\frac{1 \,-\, i \frac{\hbar t}{m \delta^2}}{1 \,+\, i \frac{\hbar t}{m \delta^2}} \right]^{\frac{1}{4}} \left[\frac{1}{\pi \delta^2 \,(1 \,+\, \frac{\hbar^2 t^2}{m^2 \delta^4})} \right]^{\frac{1}{4}} \exp\left[\, E(x) \,\right] \,. \tag{2.67}$$

We need to determine finally (2.54) using (2.55). One obtains

$$E(x) \;=\; -\,\frac{x^2}{2\delta^2 (1 + i \frac{\hbar t}{m \delta^2})} \;+\; \frac{i \frac{p_o}{\hbar} x}{1 + i \frac{\hbar t}{m \delta^2}} \;-\; \frac{\frac{i}{\hbar} \frac{p_o^2}{2m} t}{1 + i \frac{\hbar t}{m \delta^2}} \tag{2.68}$$

and, using

$$\frac{a}{1 \,+\, b} \;=\; a \;-\; \frac{a\, b}{1 \,+\, b} \,, \tag{2.69}$$

finally

$$E(x) \;=\; -\frac{(x \,-\, \frac{p_o}{m}\, t)^2}{2\delta^2 (1 + i \frac{\hbar t}{m \delta^2})} \;+\; i \frac{p_o}{\hbar} x \;-\; \frac{i}{\hbar} \frac{p_o^2}{2m} t \tag{2.70}$$

which inserted in (2.67) provides the complete expression of the wave function at all times t

$$\psi(x,t) \;=\; \left[\frac{1 \,-\, i \frac{\hbar t}{m \delta^2}}{1 \,+\, i \frac{\hbar t}{m \delta^2}} \right]^{\frac{1}{4}} \left[\frac{1}{\pi \delta^2 \,(1 \,+\, \frac{\hbar^2 t^2}{m^2 \delta^4})} \right]^{\frac{1}{4}} \times \tag{2.71}$$

$$\times \exp\left[-\frac{(x \,-\, \frac{p_o}{m}\, t)^2}{2\delta^2 (1 \,+\, \frac{\hbar^2 t^2}{m^2 \delta^4})} (1 \,-\, i \frac{\hbar t}{m \delta^2}) \;+\; i \frac{p_o}{\hbar} x \;-\; \frac{i}{\hbar} \frac{p_o^2}{2m} t \right] \,.$$

The corresponding probability distribution is

$$|\psi(x,t)|^2 \;=\; \left[\frac{1}{\pi \delta^2 \,(1 \,+\, \frac{\hbar^2 t^2}{m^2 \delta^4})} \right]^{\frac{1}{2}} \exp\left[-\, \frac{(x \,-\, \frac{p_o}{m}\, t)^2}{\delta^2 (1 \,+\, \frac{\hbar^2 t^2}{m^2 \delta^4})} \right] \,. \tag{2.72}$$

Comparision of Moving Wave Packet with Classical Motion

It is revealing to compare the probability distributions (2.49), (2.72) for the initial state (2.48) and for the final state (2.71), respectively. The center of the distribution (2.72) moves in the direction of the positive x-axis with velocity $v_o = p_o/m$ which identifies p_o as the momentum of the particle. The width of the distribution (2.72)

$$\delta \sqrt{1 + \frac{\hbar^2 t^2}{m^2 \delta^4}} \tag{2.73}$$

increases with time, coinciding at $t = 0$ with the width of the initial distribution (2.49). This 'spreading' of the wave function is a genuine quantum phenomenon. Another interesting observation is that the wave function (2.71) conserves the phase factor $\exp[i(p_o/\hbar)x]$ of the original wave function (2.48) and that the respective phase factor is related with the velocity of the classical particle and of the center of the distribution (2.72). The conservation of this factor is particularly striking for the (unnormalized) initial wave function

$$\psi(x_0, t_0) \; = \; \exp\left(i \frac{p_o}{m} x_o \right) \; , \tag{2.74}$$

which corresponds to (2.48) for $\delta \to \infty$. In this case holds

$$\psi(x, t) \; = \; \exp\left(i \frac{p_o}{m} x \; - \; \frac{i}{\hbar} \frac{p_o^2}{2m} t \right) \; . \tag{2.75}$$

i.e., the spatial dependence of the initial state (2.74) remains invariant in time. However, a time-dependent phase factor $\exp[-\frac{i}{\hbar}(p_o^2/2m)\, t]$ arises which is related to the energy $\epsilon = p_o^2/2m$ of a particle with momentum p_o. We had assumed above [c.f. (2.48)] $t_o = 0$. the case of arbitrary t_o is recovered iby replacing $t \to t_o$ in (2.71, 2.72). This yields, instead of (2.75)

$$\psi(x, t) \; = \; \exp\left(i \frac{p_o}{m} x \; - \; \frac{i}{\hbar} \frac{p_o^2}{2m} (t \, - \, t_o) \right) \; . \tag{2.76}$$

From this we conclude that an initial wave function

$$\psi(x_o, t_0) \; = \; \exp\left(i \frac{p_o}{m} x_o \; - \; \frac{i}{\hbar} \frac{p_o^2}{2m} t_o \right) \; . \tag{2.77}$$

becomes at $t > t_o$

$$\psi(x,t) \;=\; \exp\left(i\frac{p_o}{m}\,x \;-\; \frac{i}{\hbar}\frac{p_o^2}{2m}t \right)\;, \tag{2.78}$$

i.e., the spatial as well as the temporal dependence of the wave function remains invariant in this case. One refers to the respective states as *stationary states*. Such states play a cardinal role in quantum mechanics.

2.5 Propagator for a Quadratic Lagrangian

We will now determine the propagator (2.10, 2.12, 2.13)

$$\phi(x_N, t_N|x_0, t_0) \;=\; \iint_{x(t_0)=x_0}^{x(t_N)=x_N} d[x(t)]\,\exp\left\{ \frac{i}{\hbar}\,S[x(t)] \right\} \tag{2.79}$$

for a quadratic Lagrangian

$$L(x,\dot{x},t) \;=\; \frac{1}{2}m\dot{x}^2 \;-\; \frac{1}{2}c(t)x^2 \;-\; e(t)x\;. \tag{2.80}$$

For this purpose we need to determine the action integral

$$S[x(t)] \;=\; \int_{t_0}^{t_N} dt'\,L(x,\dot{x},t) \tag{2.81}$$

for an arbitrary path $x(t)$ with end points $x(t_0) = x_0$ and $x(t_N) = x_N$. In order to simplify this task we define again a new path $y(t)$

$$x(t) \;=\; x_{cl}(t) \;+\; y(t) \tag{2.82}$$

which describes the deviation from the classical path $x_{cl}(t)$ with end points $x_{cl}(t_0) = x_0$ and $x_{cl}(t_N) = x_N$. Obviously, the end points of $y(t)$ are

$$y(t_0) \;=\; 0 \quad ; \quad y(t_N) \;=\; 0\;. \tag{2.83}$$

Inserting (2.80) into (2.82) one obtains

$$L(x_{cl}+y, \dot{x}_{cl}+\dot{y}(t), t) \;=\; L(x_{cl}, \dot{x}_{cl}, t) \;+\; L'(y, \dot{y}(t), t) \;+\; \delta L \tag{2.84}$$

where

$$\begin{aligned} L(x_{cl}, \dot{x}_{cl}, t) \;&=\; \frac{1}{2}m\dot{x}_{cl}^2 \;-\; \frac{1}{2}c(t)x_{cl}^2 \;-\; e(t)x_{cl} \\ L'(y, \dot{y}(t), t) \;&=\; \frac{1}{2}m\dot{y}^2 \;-\; \frac{1}{2}c(t)y^2 \\ \delta L \;&=\; m\dot{x}_{cl}\dot{y}(t) \;-\; c(t)x_{cl}y \;-\; e(t)y\;. \end{aligned} \tag{2.85}$$

We want to show now that the contribution of δL to the action integral (2.81) vanishes[2]. For this purpose we use

$$\dot{x}_{cl}\dot{y} \;=\; \frac{d}{dt}\,(\dot{x}_{cl}\,y) \;-\; \ddot{x}_{cl}\,y \tag{2.86}$$

and obtain

$$\int_{t_0}^{t_N} dt\,\delta L \;=\; m\;\left[\dot{x}_{cl}\,y\right]\Big|_{t_0}^{t_N} \;-\; \int_{t_0}^{t_N} dt\;\left[\,m\ddot{x}_{cl}(t) \,+\, c(t)\,x_{cl}(t) \,+\, e(t)\,\right]\,y(t)\;. \tag{2.87}$$

According to (2.83) the first term on the r.h.s. vanishes. Applying the Euler–Lagrange conditions (1.24) to the Lagrangian (2.80) yields for the classical path

$$m\ddot{x}_{cl} \;+\; c(t)\,x_{cl} \;+\; e(t) \;=\; 0 \tag{2.88}$$

and, hence, also the second contribution on the r.h.s. of (2.88) vanishes. One can then express the propagator (2.79)

$$\phi(x_N, t_N|x_0, t_0) \;=\; \exp\left\{\,\frac{i}{\hbar}\,S[x_{cl}(t)]\,\right\}\tilde{\phi}(0, t_N|0, t_0) \tag{2.89}$$

where

$$\tilde{\phi}(0, t_N|0, t_0) \;=\; \int_{y(t_0)=0}^{y(t_N)=0} d[y(t)]\;\exp\left\{\,\frac{i}{\hbar}\int_{t_0}^{t_N} dt\,L'(y, \dot{y}, t)\,\right\}\;. \tag{2.90}$$

Evaluation of the Necessary Path Integral

We have achieved for the quadratic Lagrangian a separation in terms of a classical action integral and a propagator connecting the end points $y(t_0) = 0$ and $y(t_N) = 0$ which is analogue to the result (2.31) for the free particle propagator. For the evaluation of $\tilde{\phi}(0, t_N|0, t_0)$ we will adopt a strategy which is similar to that used for the evaluation of (2.32). The discretization scheme adopted above yields in the present case

$$\tilde{\phi}(0, t_N|0, t_0) \;=\; lim_{N\to\infty}\left[\tfrac{m}{2\pi i\hbar\epsilon_N}\right]^{\frac{N}{2}} \;\times \tag{2.91}$$
$$\times\;\int_{-\infty}^{+\infty} dy_1 \cdots \int_{-\infty}^{+\infty} dy_{N-1}\,\exp\left[\tfrac{i}{\hbar}\,\epsilon_N\,\sum_{j=0}^{N-1}\left(\tfrac{1}{2}m\tfrac{(y_{j+1}-y_j)^2}{\epsilon_N^2} \;-\; \tfrac{1}{2}\,c_j\,y_j^2\right)\right]$$

---

[2]The reader may want to verify that the contribution of δL to the action integral is actually equal to the differential $\delta S[x_{cl}, y(t)]$ which vanishes according to the Hamiltonian principle as discussed in Sect. 1.

where $c_j = c(t_j)$, $t_j = t_0 + \epsilon_N\, j$. One can express the exponent E in (2.91) through the quadratic form

$$E \;=\; i \sum_{j,k=1}^{N-1} y_j\, a_{jk}\, y_k \tag{2.92}$$

where a_{jk} are the elements of the following $(N-1) \times (N-1)$ matrix

$$\begin{aligned}
\left(a_{jk} \right) \;&=\; \frac{m}{2\hbar\epsilon_N} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & & -1 & 2 \end{pmatrix} \\
&\quad - \frac{\epsilon_N}{2\hbar} \begin{pmatrix} c_1 & 0 & 0 & \dots & 0 & 0 \\ 0 & c_2 & 0 & \dots & 0 & 0 \\ 0 & 0 & c_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & c_{N-2} & 0 \\ 0 & 0 & 0 & & 0 & c_{N-1} \end{pmatrix}
\end{aligned} \tag{2.93}$$

In case $\det(a_{jk}) \neq 0$ one can express the multiple integral in (2.91) according to (2.36) as follows

$$\begin{aligned}
\tilde{\phi}(0, t_N | 0, t_0) \;&=\; lim_{N\to\infty} \left[\frac{m}{2\pi i \hbar \epsilon_N} \right]^{\frac{N}{2}} \left[\frac{(i\pi)^{N-1}}{\det(\mathbf{a})} \right]^{\frac{1}{2}} \\
&=\; lim_{N\to\infty} \left[\frac{m}{2\pi i \hbar} \frac{1}{\epsilon_N \left(\frac{2\hbar\epsilon_N}{m} \right)^{N-1} \det(\mathbf{a})} \right]^{\frac{1}{2}} .
\end{aligned} \tag{2.94}$$

In order to determine $\tilde{\phi}(0, t_N | 0, t_0)$ we need to evaluate the function

$$f(t_0, t_N) \;=\; lim_{N\to\infty} \left[\epsilon_N \left(\frac{2\hbar\epsilon_N}{m} \right)^{N-1} \det(\mathbf{a}) \right] . \tag{2.95}$$

According to (2.93) holds

$$D_{N-1} \;\stackrel{\text{def}}{=}\; \left[\frac{2\hbar\epsilon_N}{m} \right]^{N-1} \det(\mathbf{a}) \tag{2.96}$$

$$= \left| \begin{pmatrix} 2 - \frac{\epsilon_N^2}{m} c_1 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 - \frac{\epsilon_N^2}{m} c_2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 - \frac{\epsilon_N^2}{m} c_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 - \frac{\epsilon_N^2}{m} c_{N-2} & -1 \\ 0 & 0 & 0 & & -1 & 2 - \frac{\epsilon_N^2}{m} c_{N-1} \end{pmatrix} \right|$$

In the following we will asume that the dimension $n = N - 1$ of the matrix in (2.97) is variable. One can derive then for D_n the recursion relationship

$$D_n = \left(2 - \frac{\epsilon_N^2}{m} c_n \right) D_{n-1} - D_{n-2} \tag{2.97}$$

using the well-known method of expanding a determinant in terms of the determinants of lower dimensional submatrices. Using the starting values [c.f. the comment below Eq. (2.43)]

$$D_0 = 1 \, ; \quad D_1 = 2 - \frac{\epsilon_N^2}{m} c_1 \tag{2.98}$$

this recursion relationship can be employed to determine D_{N-1}. One can express (2.97) through the 2nd order difference equation

$$\frac{D_{n+1} - 2D_n + D_{n-1}}{\epsilon_N^2} = - \frac{c_{n+1} D_n}{m} \, . \tag{2.99}$$

Since we are interested in the solution of this equation in the limit of vanishing ϵ_N we may interpret (2.99) as a 2nd order differential equation in the continuous variable $t = n\epsilon_N + t_0$

$$\frac{d^2 f(t_0, t)}{dt^2} = - \frac{c(t)}{m} f(t_0, t) \, . \tag{2.100}$$

The boundary conditions at $t = t_0$, according to (2.98), are

$$\begin{aligned} f(t_0, t_0) &= \epsilon_N D_0 = 0 \, ; \\ \frac{df(t_0,t)}{dt}\Big|_{t=t_0} &= \epsilon_N \frac{D_1 - D_0}{\epsilon_N} = 2 - \frac{\epsilon_N^2}{m} c_1 - 1 = 1 \, . \end{aligned} \tag{2.101}$$

We have then finally for the propagator (2.79)

$$\phi(x, t | x_0, t_0) = \left[\frac{m}{2\pi i \hbar f(t_o, t)} \right]^{\frac{1}{2}} \exp \left\{ \frac{i}{\hbar} S[x_{cl}(t)] \right\} \tag{2.102}$$

where $f(t_0, t)$ is the solution of (2.100, 2.101) and where $S[x_{cl}(t)]$ is determined by solving first the Euler–Lagrange equations for the Lagrangian (2.80) to obtain the classical path $x_{cl}(t)$ with end points $x_{cl}(t_0) = x_0$ and $x_{cl}(t_N) = x_N$ and then evaluating (2.81) for this path. Note that the required solution $x_{cl}(t)$ involves a solution of the Euler–Lagrange equations for boundary conditions which are different from those conventionally encountered in Classical Mechanics where usually a solution for initial conditions $x_{cl}(t_0) = x_0$ and $\dot{x}_{cl}(t_0) = v_0$ are determined.

2.6 Wave Packet Moving in Homogeneous Force Field

We want to consider now the motion of a quantum mechanical particle, decribed at time $t = t_o$ by a wave packet (2.48), in the presence of a homogeneous force due to a potential $V(x) = -f\,x$. As we have learnt from the study of the time-development of (2.48) in case of free particles the wave packet (2.48) corresponds to a classical particle with momentum p_o and position $x_o = 0$. We expect then that the classical particle assumes the following position and momentum at times $t > t_o$

$$y(t) = \frac{p_o}{m}\,(t - t_o) + \frac{1}{2}\,\frac{f}{m}\,(t - t_o)^2 \tag{2.103}$$

$$p(t) = p_o + f\,(t - t_o) \tag{2.104}$$

The Lagrangian for the present case is

$$L(x, \dot{x}, t) = \frac{1}{2} m\,\dot{x}^2 + f\,x\,. \tag{2.105}$$

This corresponds to the Lagrangian in (2.80) for $c(t) \equiv 0$, $e(t) \equiv -f$. Accordingly, we can employ the expression (2.89, 2.90) for the propagator where, in the present case, holds $L'(y, \dot{y}, t) = \frac{1}{2} m \dot{y}^2$ such that $\tilde{\phi}(0, t_N|0, t_0)$ is the free particle propagator (2.45). One can write then the propagator for a particle moving subject to a homogeneous force

$$\phi(x, t|x_0, t_0) = \left[\frac{m}{2\pi i\hbar(t - t_0)}\right]^{\frac{1}{2}} \exp\left[\frac{i}{\hbar} S[x_{cl}(\tau)]\right]\,. \tag{2.106}$$

Here $S[x_{cl}(\tau)]$ is the action integral over the classical path with end points

$$x_{cl}(t_o) = x_o \quad , \qquad x_{cl}(t) = x\,. \tag{2.107}$$

The classical path obeys

$$m\,\ddot{x}_{cl} \;=\; f\;. \tag{2.108}$$

The solution of (2.107, 2.108) is

$$x_{cl}(\tau) \;=\; x_o \;+\; \left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)\tau \;+\; \frac{1}{2}\frac{f}{m}\,\tau^2 \tag{2.109}$$

as can be readily verified. The velocity along this path is

$$\dot{x}_{cl}(\tau) \;=\; \frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \;+\; \frac{f}{m}\,\tau \tag{2.110}$$

and the Lagrangian along the path, considered as a function of τ, is

$$\begin{aligned}
g(\tau) \;=&\; \frac{1}{2}m\dot{x}_{cl}^2\,(\tau) \;+\; f\,x_{cl}\,(\tau) \\
=&\; \frac{1}{2}m\left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)^2 \;+\; f\left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)\tau \\
&\;+\; \frac{1}{2}\frac{f^2}{m}\,\tau^2 + \;f\,x_o \;+\; f\left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)\tau \;+\; \frac{1}{2}\frac{f^2}{m}\,\tau^2 \\
=&\; \frac{1}{2}m\left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)^2 \;+\; 2f\left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)\tau \\
&\;+\; \frac{f^2}{m}\,\tau^2 \;+\; f\,x_o
\end{aligned} \tag{2.111}$$

One obtains for the action integral along the classical path

$$\begin{aligned}
S[x_{cl}\,(\tau)] \;=&\; \int_{t_o}^{t} d\tau\; g(\tau) \\
=&\; \frac{1}{2}m\left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)^2 (t\,-\,t_o) \\
&\;+ f\left(\frac{x\,-\,x_o}{t\,-\,t_o} \;-\; \frac{1}{2}\frac{f}{m}\,(t\,-\,t_o) \right)(t\,-\,t_o)^2 \\
&\;+ \frac{1}{3}\frac{f^2}{m}\,(t\,-\,t_o)^3 \;+\; x_o\,f\,(t\,-\,t_o) \\
=&\; \frac{1}{2}\,m\,\frac{(x\,-\,x_o)^2}{t\,-\,t_o} \;+\; \frac{1}{2}\,(x\,+\,x_o)\,f\,(t\,-\,t_o) \;-\; \frac{1}{24}\frac{f^2}{m}\,(t\,-\,t_o)^3
\end{aligned} \tag{2.112}$$

and, finally, for the propagator

$$\phi(x,t|x_o,t_o) = \left[\frac{m}{2\pi i\hbar(t-t_o)}\right]^{\frac{1}{2}} \times \tag{2.113}$$
$$\times \exp\left[\frac{im}{2\hbar}\frac{(x-x_o)^2}{t-t_o} + \frac{i}{2\hbar}(x+x_o)\,f\,(t-t_o) - \frac{i}{24}\frac{f^2}{\hbar m}(t-t_o)^3\right]$$

The propagator (2.113) allows one to determine the time-evolution of the initial state (2.48) using (2.5). Since the propagator depends only on the time-difference $t - t_o$ we can assume, withoult loss of generality, $t_o = 0$ and are lead to the integral

$$\psi(x,t) = \left[\frac{1}{\pi\delta^2}\right]^{\frac{1}{4}}\left[\frac{m}{2\pi i\hbar t}\right]^{\frac{1}{2}}\int_{-\infty}^{+\infty} dx_0 \tag{2.114}$$
$$\exp\underbrace{\left[\frac{im}{2\hbar}\frac{(x-x_0)^2}{t} - \frac{x_0^2}{2\delta^2} + i\frac{p_o}{\hbar}x_o + \frac{i}{2\hbar}(x+x_o)\,f\,t - \frac{i}{24}\frac{f^2}{m\hbar}t^3\right]}_{E_o(x_o,x)\;+\;E(x)}$$

To evaluate the integral we adopt the same computational strategy as used for (2.51) and divide the exponent in (2.114) as follows [c.f. (2.54)]

$$E_o(x_o,x) = \frac{im}{2\hbar t}\left[x_o^2\left(1 + i\frac{\hbar t}{m\delta^2}\right) - 2x_o\left(x - \frac{p_o}{m}t - \frac{f\,t^2}{2m}\right) + f(x)\right] \tag{2.115}$$

$$E(x) = \frac{im}{2\hbar t}\left[x^2 + \frac{f\,t^2}{m}x - f(x)\right] - \frac{1}{24}\frac{f^2t^3}{\hbar m}\,. \tag{2.116}$$

One chooses then $f(x)$ to complete, according to (2.52), the square in (2.115)

$$f(x) = \left(\frac{x - \frac{p_o}{m}t - \frac{f\,t^2}{2m}}{\sqrt{1 + i\frac{\hbar t}{m\delta^2}}}\right)^2\,. \tag{2.117}$$

This yields

$$E_o(x_o,x) = \frac{im}{2\hbar t}\left(x_o\sqrt{1 + i\frac{\hbar t}{m\delta^2}} - \frac{x - \frac{p_o}{m}t - \frac{f\,t^2}{2m}}{\sqrt{1 + i\frac{\hbar t}{m\delta^2}}}\right)^2\,. \tag{2.118}$$

Following in the footsteps of the calculation on page 23 ff. one can state again

$$\psi(x,t) \;=\; \left[\frac{1 - i\frac{\hbar t}{m\delta^2}}{1 + i\frac{\hbar t}{m\delta^2}}\right]^{\frac{1}{4}} \left[\frac{1}{\pi\delta^2\,(1 + \frac{\hbar^2 t^2}{m^2\delta^4})}\right]^{\frac{1}{4}} \exp\left[\,E(x)\,\right] \tag{2.119}$$

and is lead to the exponential (2.116)

$$E(x) \;=\; -\,\frac{1}{24}\,\frac{f^2 t^3}{\hbar m} \;+\; \frac{im}{2\hbar t(1 + i\frac{\hbar t}{m\delta^2})}\,S(x) \tag{2.120}$$

where

$$\begin{aligned} S(x) \;&=\; x^2\left(1 + i\frac{\hbar t}{m\delta^2}\right) + x\,\frac{f t^2}{m}\left(1 + i\frac{\hbar t}{m\delta^2}\right) - \left(x - \frac{p_o}{m}\,t - \frac{f t^2}{2m}\right)^2 \\ &=\; \left(x - \frac{p_o}{m}\,t - \frac{f t^2}{2m}\right)^2\left(1 + i\frac{\hbar t}{m\delta^2}\right) - \left(x - \frac{p_o}{m}\,t - \frac{f t^2}{2m}\right)^2 \\ &\quad + \left[x\,\frac{f t^2}{m} + 2x\left(\frac{p_o}{m}\,t + \frac{f t^2}{2m}\right) - \left(\frac{p_o}{m}\,t + \frac{f t^2}{2m}\right)^2\right]\left(1 + i\frac{\hbar t}{m\delta^2}\right) \end{aligned} \tag{2.121}$$

Inserting this into (2.120) yields

$$\begin{aligned} E(x) \;&=\; -\,\frac{\left(x - \frac{p_o}{m}\,t - \frac{f t^2}{2m}\right)^2}{2\delta^2\left(1 + i\,\frac{\hbar t}{m\delta^2}\right)} \\ &\quad + \frac{i}{\hbar}\,(p_o + f\,t)\,x - \frac{i}{2m\hbar}\left(p_o t + p_o f t^2 + \frac{f^2 t^3}{4} + \frac{f^2 t^3}{12}\right) \end{aligned} \tag{2.122}$$

The last term can be written

$$-\,\frac{i}{2m\hbar}\left(p_o t + p_o f t^2 + \frac{f^2 t^3}{3}\right) \;=\; -\,\frac{i}{2m\hbar}\int_0^t d\tau\,(p_o + f\tau)^2\,. \tag{2.123}$$

Altogether, (2.119, 2.122, 2.123) provide the state of the particle at time $t > 0$

$$\psi(x,t) \;=\; \left[\frac{1 - i\frac{\hbar t}{m\delta^2}}{1 + i\frac{\hbar t}{m\delta^2}}\right]^{\frac{1}{4}} \left[\frac{1}{\pi\delta^2\,(1 + \frac{\hbar^2 t^2}{m^2\delta^4})}\right]^{\frac{1}{4}} \times$$

$$\times \exp\left[- \frac{\left(x - \frac{p_o}{m}\,t - \frac{f t^2}{2m}\right)^2}{2\delta^2 \left(1 + \frac{\hbar^2 t^2}{m^2\delta^4}\right)} \left(1 - i\,\frac{\hbar t}{m\delta^2}\right) \right] \times$$

$$\times \exp\left[\frac{i}{\hbar}\,(p_o + f\,t)\,x - \frac{i}{\hbar}\int_0^t d\tau\, \frac{(p_o + f\tau)^2}{2m} \right] . \quad (2.124)$$

The corresponding probablity distribution is

$$|\psi(x,t)|^2 = \left[\frac{1}{\pi\delta^2\,(1 + \frac{\hbar^2 t^2}{m^2\delta^4})} \right]^{\frac{1}{2}} \exp\left[- \frac{\left(x - \frac{p_o}{m}\,t - \frac{f t^2}{2m}\right)^2}{\delta^2\left(1 + \frac{\hbar^2 t^2}{m^2\delta^4}\right)} \right] . \quad (2.125)$$

Comparision of Moving Wave Packet with Classical Motion

It is again [c.f. (1)] revealing to compare the probability distributions for the initial state (2.48) and for the states at time t, i.e., (2.125). Both distributions are Gaussians. Distribution (2.125) moves along the x-axis with distribution centers positioned at $y(t)$ given by (2.103), i.e., as expected for a classical particle. The states (2.124), in analogy to the states (2.71) for free particles, exhibit a phase factor $\exp[ip(t)x/\hbar]$, for which $p(t)$ agrees with the classical momentum (2.104). While these properties show a close correspondence between classical and quantum mechanical behaviour, the distribution shows also a pure quantum effect, in that it increases its width . This increase, for the homogeneous force case, is identical to the increase (2.73) determined for a free particle. Such increase of the width of a distribution is not a necessity in quantum mechanics. In fact, in case of so-called bound states, i.e., states in which the classical and quantum mechanical motion is confined to a finite spatial volume, states can exist which do not alter their spatial distribution in time. Such states are called stationary states. In case of a harmonic potential there exists furthermore the possibility that the center of a wave packet follows the classical behaviour and the width remains constant in time. Such states are referred to as coherent states, or Glauber states, and will be studied below. It should be pointed out that in case of vanishing, linear and quadratic potentials quantum mechanical wave packets exhibit a particularly simple evolution; in case of other type of potential functions and, in particular, in case of higher-dimensional motion, the quantum behaviour can show features which are much more distinctive from classical behaviour, e.g., tunneling and interference effects.

2.7 Propagator of a Harmonic Oscillator

In order to illustrate the evaluation of (2.102) we consider the case of a harmonic oscillator. In this case holds for the coefficents in the Lagrangian (2.80) $c(t) = m\omega^2$ and $e(t) = 0$, i.e., the Lagrangian is

$$L(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 . \tag{2.126}$$

.We determine first $f(t_0, t)$. In the present case holds

$$\ddot{f} = -\omega^2 f \; ; \quad f(t_0, t_0) = 0 \; ; \quad \dot{f}(t_o, t_o) = 1 . \tag{2.127}$$

The solution which obeys the stated boundary conditions is

$$f(t_0, t) = \frac{\sin\omega(t - t_0)}{\omega} . \tag{2.128}$$

We determine now $S[x_{cl}(\tau)]$. For this purpose we seek first the path $x_{cl}(\tau)$ which obeys $x_{cl}(t_0) = x_0$ and $x_{cl}(t) = x$ and satisfies the Euler–Lagrange equation for the harmonic oscillator

$$m\ddot{x}_{cl} + m\omega^2 x_{cl} = 0 . \tag{2.129}$$

This equation can be written

$$\ddot{x}_{cl} = -\omega^2 x_{cl} . \tag{2.130}$$

the general solution of which is

$$x_{cl}(\tau') = A \sin\omega(\tau - t_0) + B \cos\omega(\tau - t_0) . \tag{2.131}$$

The boundary conditions $x_{cl}(t_0) = x_0$ and $x_{cl}(t) = x$ are satisfied for

$$B = x_0 \; ; \quad A = \frac{x - x_0 \cos\omega(t - t_o)}{\sin\omega(t - t_0)} , \tag{2.132}$$

and the desired path is

$$x_{cl}(\tau) = \frac{x - x_0\, c}{s} \sin\omega(\tau - t_0) + x_0 \cos\omega(\tau - t_0) \tag{2.133}$$

where we introduced

$$c = \cos\omega(t - t_o) , \quad s = \sin\omega(t - t_o) \tag{2.134}$$

We want to determine now the action integral associated with the path (2.133, 2.134)

$$S[x_{cl}(\tau)] \;=\; \int_{t_0}^{t} d\tau \left(\frac{1}{2} m \dot{x}_{cl}^2(\tau) \;-\; \frac{1}{2} m\omega^2 x_{cl}^2(\tau) \right) \tag{2.135}$$

For this purpose we assume presently $t_o = 0$. From (2.133) follows for the velocity along the classical path

$$\dot{x}_{cl}(\tau) \;=\; \omega \, \frac{x - x_0\, c}{s} \cos\omega\tau \;-\; \omega\, x_0 \sin\omega\tau \tag{2.136}$$

and for the kinetic energy

$$\begin{aligned} \frac{1}{2} m \dot{x}_{cl}^2(\tau) \;&=\; \frac{1}{2} m\omega^2 \, \frac{(x - x_0\, c)^2}{s^2} \cos^2\omega\tau \\ &\quad - m\omega^2 x_o \, \frac{x - x_0\, c}{s} \cos\omega\tau \sin\omega\tau \\ &\quad + \frac{1}{2} m\omega^2 \, x_o^2 \sin^2\omega\tau \end{aligned} \tag{2.137}$$

Similarly, one obtains from (2.133) for the potential energy

$$\begin{aligned} \frac{1}{2} m\omega^2 x_{cl}^2(\tau) \;&=\; \frac{1}{2} m\omega^2 \, \frac{(x - x_0\, c)^2}{s^2} \sin^2\omega\tau \\ &\quad + m\omega^2 x_o \, \frac{x - x_0\, c}{s} \cos\omega\tau \sin\omega\tau \\ &\quad + \frac{1}{2} m\omega^2 \, x_o^2 \cos^2\omega\tau \end{aligned} \tag{2.138}$$

Using

$$\cos^2\omega\tau \;=\; \frac{1}{2} \;+\; \frac{1}{2} \cos 2\omega\tau \tag{2.139}$$

$$\sin^2\omega\tau \;=\; \frac{1}{2} \;-\; \frac{1}{2} \cos 2\omega\tau \tag{2.140}$$

$$\cos\omega\tau \sin\omega\tau \;=\; \frac{1}{2} \sin 2\omega\tau \tag{2.141}$$

the Lagrangian, considered as a function of τ, reads

$$\begin{aligned} g(\tau) \;=\; \frac{1}{2} m \dot{x}_{cl}^2(\tau) \;-\; \frac{1}{2} m\omega^2 x_{cl}^2(\tau) \;&=\; \frac{1}{2} m\omega^2 \, \frac{(x - x_0\, c)^2}{s^2} \cos 2\omega\tau \\ &\quad - m\omega^2 x_o \, \frac{x - x_0\, c}{s} \sin 2\omega\tau \\ &\quad - \frac{1}{2} m\omega^2 \, x_o^2 \cos 2\omega\tau \end{aligned} \tag{2.142}$$

Evaluation of the action integral (2.135), i.e., of $S[x_{cl}(\tau)] = \int_0^t d\tau g(\tau)$ requires the integrals

$$\int_0^t d\tau \cos 2\omega\tau = \frac{1}{2\omega} \sin 2\omega t = \frac{1}{\omega} s\, c \tag{2.143}$$

$$\int_0^t d\tau \sin 2\omega\tau = \frac{1}{2\omega} [\, 1 - \cos 2\omega t\,] = \frac{1}{\omega} s^2 \tag{2.144}$$

where we employed the definition (2.134) Hence, (2.135) is, using $s^2 + c^2 = 1$,

$$\begin{aligned} S[x_{cl}(\tau)] &= \frac{1}{2} m\omega \frac{(x - x_0\, c)^2}{s^2}\, s\, c - m\omega x_o \frac{x - x_0\, c}{s}\, s^2 - \frac{1}{2} m\omega^2 x_o^2\, s\, c \\ &= \frac{m\omega}{2s} \left[(x^2 - 2x x_o c + x_o^2 c^2)\, c - 2x_o x s^2 + 2x_o^2 c s^2 - x_o^2 s^2 c \right] \\ &= \frac{m\omega}{2s} \left[(x^2 + x_o^2)\, c - 2x_o x \right] \end{aligned} \tag{2.145}$$

and, with the definitions (2.134),

$$S[x_{cl}(\tau)] = \frac{m\omega}{2 \sin\omega(t - t_0)} \left[(x_0^2 + x^2) \cos\omega(t - t_0) - 2x_0 x \right] . \tag{2.146}$$

For the propagator of the harmonic oscillator holds then

$$\begin{aligned} \phi(x, t | x_0, t_0) &= \left[\tfrac{m\omega}{2\pi i \hbar \sin\omega(t - t_0)} \right]^{\frac{1}{2}} \times \\ \times \exp \Big\{ & \tfrac{i\, m\, \omega}{2\hbar \sin\omega(t - t_0)} \left[(x_0^2 + x^2) \cos\omega(t - t_0) - 2x_0 x \right] \Big\} \end{aligned} . \tag{2.147}$$

Quantum Pendulum or Coherent States

As a demonstration of the application of the propagator (2.147) we use it to describe the time development of the wave function for a particle in an initial state

$$\psi(x_0, t_0) = \left[\frac{m\omega}{\pi\hbar} \right]^{\frac{1}{4}} \exp \left(- \frac{m\omega(x_0 - b_o)^2}{2\hbar} + \frac{i}{\hbar} p_o\, x_o \right) . \tag{2.148}$$

The initial state is decribed by a Gaussian wave packet centered around the position $x = b_o$ and corresponds to a particle with initial momentum p_o. The latter property follows from the role of such factor for the initial state (2.48) when applied to the case of a free particle [c.f. (2.71)] or to the case of a particle moving in a homogeneous force [c.f. (2.124, 2.125)] and will be borne out of the following analysis; at present one may regard it as an assumption.

If one identifies the center of the wave packet with a classical particle, the following holds for the time development of the position (displacement), momentum, and energy of the particle

$$\begin{aligned} b(t) &= b_o \cos\omega(t-t_o) + \frac{p_o}{m\omega}\sin\omega(t-t_o) && \text{displacement} \\ p(t) &= -m\omega b_o \sin\omega(t-t_o) + p_o \cos\omega(t-t_o) && \text{momentum} \\ \epsilon_o &= \frac{p_o^2}{2m} + \tfrac{1}{2}m\omega^2 b_o^2 && \text{energy} \end{aligned} \tag{2.149}$$

We want to explore, using (2.5), how the probability distribution $|\psi(x,t)|^2$ of the quantum particle propagates in time.

The wave function at times $t > t_0$ is

$$\psi(x,t) = \int_{-\infty}^{\infty} dx_0\, \phi(x,t|x_0,t_0)\, \psi(x_0,t_0)\ . \tag{2.150}$$

Expressing the exponent in (2.148)

$$\frac{i\,m\,\omega}{2\hbar \sin\omega(t-t_o)}\left[i\,(x_o-b_o)^2 \sin\omega(t-t_o) + \frac{2p_o}{m\omega}\,x_o\,\sin\omega(t-t_o)\right] \tag{2.151}$$

(2.147, 2.150, 2.151) can be written

$$\psi(x,t) = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} \left[\frac{m}{2\pi i\omega\hbar\sin\omega(t-t_0)}\right]^{\frac{1}{2}} \int_{-\infty}^{\infty} dx_0 \exp\left[E_0 + E\right] \tag{2.152}$$

where

$$E_0(x_o,x) = \frac{i\,m\,\omega}{2\hbar s}\left[x_o^2 c - 2x_o x + isx_o^2 - 2isx_o b_o + \frac{2p_o}{m\omega}\,x_o s + f(x)\right] \tag{2.153}$$

$$E(x) = \frac{im\omega}{2\hbar s}\left[x^2 c + isb_o^2 - f(x)\right]\ . \tag{2.154}$$

$$c = \cos\omega(t-t_o)\ ,\quad s = \sin\omega(t-t_o)\ . \tag{2.155}$$

Here $f(x)$ is a function which is introduced to complete the square in (2.153) for simplification of the Gaussian integral in x_0. Since $E(x)$ is independent of x_o (2.152) becomes

$$\psi(x,t) = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} \left[\frac{m}{2\pi i\omega\hbar\sin\omega(t-t_0)}\right]^{\frac{1}{2}} e^{E(x)} \int_{-\infty}^{\infty} dx_0 \exp\left[E_0(x_o,x)\right] \tag{2.156}$$

We want to determine now $E_o(x_o, x)$ as given in (2.153). It holds

$$E_o \;=\; \frac{i\,m\,\omega}{2\hbar s}\left[x_o^2\,e^{i\omega(t-t_o)} \;-\; 2x_o(x+isb_o-\frac{p_o}{m\omega}\,s) \;+\; f(x)\right] \tag{2.157}$$

For $f(x)$ to complete the square we choose

$$f(x) \;=\; (x \;+\; isb_o \;-\; \frac{p_o}{m\omega}\,s)^2\,e^{-i\omega(t-t_o)}\;. \tag{2.158}$$

One obtains for (2.157)

$$E_0(x_o,x) \;=\; \frac{im\omega}{2\hbar s}\exp\left[i\omega(t-t_0)\right]\left[x_0 \;-\; (x+isb_o-\frac{p_o}{m\omega}\,s)\exp\left(-i\omega(t-t_0)\right)\right]^2\;. \tag{2.159}$$

To determine the integral in (2.156) we employ the integration formula (2.247) and obtain

$$\int_{-\infty}^{+\infty} dx_0\,e^{E_0(x_0)} \;=\; \left[\frac{2\pi i\hbar\,\sin\omega(t-t_0)}{m\omega\,\exp[i\omega(t-t_0)]}\right]^{\frac{1}{2}} \tag{2.160}$$

Inserting this into (2.156) yields

$$\psi(x,t) \;=\; \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}}\;e^{E(x)} \tag{2.161}$$

For $E(x)$ as defined in (2.154) one obtains, using $\exp[\pm i\omega(t-t_o)] = c \pm is$,

$$\begin{aligned}
E(x) \;&=\; \tfrac{im\omega}{2\hbar s}\Big[x^2c \,+\, isb_o^2 \,-\, x^2c \,+\, isx^2 \,-\, 2isxb_oc \,-\, 2s^2xb_o \\
&\qquad +s^2b_o^2c \,-\, is^3b_o^2 \,+\, 2\,\tfrac{p_o}{m\omega}\,xsc \,+\, 2i\,\tfrac{p_o}{m\omega}\,b_os^2c \\
&\qquad -2i\,\tfrac{p_o}{m\omega}\,xs^2 \,+\, 2\,\tfrac{p_o}{m\omega}\,b_os^3 \,-\, \tfrac{p_o^2}{m^2\omega^2}\,s^2c \,+\, i\,\tfrac{p_o^2}{m^2\omega^2}\,s^3\Big] \\
&=\; -\,\tfrac{m\omega}{2\hbar}\Big[x^2 \,+\, c^2b_o^2 \,-\, 2xb_oc \,+\, 2ixsb_o \,-\, ib_o^2sc \\
&\qquad -2\,\tfrac{p_o}{m\omega}\,xs \,+\, 2\,\tfrac{p_o}{m\omega}\,b_osc \,+\, \tfrac{p_o^2}{m^2\omega^2}\,s^2 \,-\, 2i\,\tfrac{p_o}{m\omega}\,xc \\
&\qquad -2i\,\tfrac{p_o}{m\omega}\,b_os^2 \,+\, i\,\tfrac{p_o^2}{m^2\omega^2}\,sc\Big] \\
&=\; -\,\tfrac{m\omega}{2\hbar}\,(x \,-\, cb_o \,-\, \tfrac{p_o}{m\omega}\,s)^2 \,+\, \frac{i}{\hbar}\,(-\,m\omega b_os \,+\, p_oc)\,x \\
&\qquad -\,\frac{i}{\hbar}\,(\tfrac{p_o^2}{2m\omega} \,-\, \tfrac{1}{2}m\omega b_o^2)sc \,+\, \frac{i}{\hbar}\,p_ob_os^2
\end{aligned} \tag{2.162}$$

We note the following identities

$$\int_{t_o}^{t} d\tau \, \frac{p^2(\tau)}{2m}$$
$$= \frac{1}{2}\,\epsilon_o(t-t_o) \;+\; \frac{1}{2}\left(\frac{p_o^2}{2m\omega} \;-\; \frac{m\omega b_o^2}{2}\right)\, sc \;-\; \frac{1}{2}\, b_o p_o s^2 \qquad (2.163)$$
$$\int_{t_o}^{t} d\tau \, \frac{m\omega^2 b^2(\tau)}{2}$$
$$= \frac{1}{2}\,\epsilon_o(t-t_o) \;-\; \frac{1}{2}\left(\frac{p_o^2}{2m\omega} \;-\; \frac{m\omega b_o^2}{2}\right)\, sc \;+\; \frac{1}{2}\, b_o p_o s^2 \qquad (2.164)$$

where we employed $b(\tau)$ and $p(\tau)$ as defined in (2.149). From this follows, using $p(\tau) = m\dot{b}(\tau)$ and the Lagrangian (2.126),

$$\int_{t_o}^{t} d\tau \, L[b(\tau), \dot{b}(\tau)] \;=\; \left(\frac{p_o^2}{2m\omega} \;-\; \frac{m\omega b_o^2}{2}\right)\, sc \;-\; b_o p_o s \qquad (2.165)$$

such that $E(x)$ in (2.162) can be written, using again (2.149)),

$$E(x) \;=\; -\,\frac{m\omega}{2\hbar}\,[x-b(t)]^2 \;+\; \frac{i}{\hbar}\,p(t)\,x \;-\; i\,\frac{1}{2}\,\omega\,(t-t_o) \;-\; \frac{i}{\hbar}\int_{t_o}^{t} d\tau\, L[b(\tau),\dot{b}(\tau)] \qquad (2.166)$$

Inserting this into (2.161) yields,

$$\psi(x,t) \;=\; \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} \;\times\; \exp\left\{-\,\frac{m\omega}{2\hbar}\,[x-b(t)]^2\right\} \;\times \qquad (2.167)$$
$$\times\; \exp\left\{\frac{i}{\hbar}\,p(t)\,x \;-\; i\,\frac{1}{2}\,\omega\,(t-t_o) \;-\; \frac{i}{\hbar}\int_{t_o}^{t} d\tau\, L[b(\tau),\dot{b}(\tau)]\right\}$$

where $b(t)$, $p(t)$, and ϵ_o are the classical displacement, momentum and energy, respectively, defined in (2.149).

Comparision of Moving Wave Packet with Classical Motion

The probability distribution associated with (2.167)

$$|\psi(x,t)|^2 \;=\; \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{2}} \;\exp\left\{-\frac{m\omega}{\hbar}\,[x \;-\; b(t)]^2\right\} \qquad (2.168)$$

is a Gaussian of time-independent width, the center of which moves as described by $b(t)$ given in (2.148) , i.e., the center follows the motion of a classical oscillator (pendulum) with initial position b_o and initial momentum p_o. It is of interest to recall that propagating wave packets in the case of vanishing [c.f. (2.72)] or linear [c.f. (2.125)] potentials exhibit an increase of their width in time; in case of the quantum oscillator for the particular width chosen for the initial state (2.148) the width, actually, is conserved. One can explain this behaviour as arising from constructive interference due to the restoring forces of the harmonic oscillator. We will show in Chapter **??** [c.f. (**??**, **??**) and Fig. **??**] that an initial state of arbitrary width propagates as a Gaussian with oscillating width.

In case of the free particle wave packet (2.48, 2.71) the factor $\exp(ip_o x)$ gives rise to the translational motion of the wave packet described by $p_o t/m$, i.e., p_o also corresponds to initial classical momentum. In case of a homogeneous force field the phase factor $\exp(ip_o x)$ for the initial state (2.48) gives rise to a motion of the center of the propagating wave packet [c.f. (2.125)] described by $(p_o/m)t + \frac{1}{2}ft^2$ such that again p_o corresponds to the classical momentum. Similarly, one observes for all three cases (free particle, linear and quadratic potential) a phase factor $\exp[ip(t)x/\hbar]$ for the propagating wave packet where f$p(t)$ corresponds to the initial classical momentum at time t. One can, hence, summarize that for the three cases studied (free particle, linear and quadratic potential) propagating wave packets show remarkably close analogies to classical motion.

We like to consider finally the propagation of an initial state as in (2.148), but with $b_o = 0$ and $p_o = 0$. Such state is given by the wave function

$$\psi(x_0, t_0) \;=\; \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} \exp\left(-\,\frac{m\omega x_0^2}{2\hbar} \;-\; \frac{i\omega}{2}\, t_o \right) . \tag{2.169}$$

where we added a phase factor $\exp(-i\omega t_o/2)$. According to (2.167) the state (2.169) reproduces itself at later times t and the probablity distribution remains at all times equal to

$$\left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{2}} \exp\left(-\,\frac{m\omega x_0^2}{\hbar} \right) , \tag{2.170}$$

i.e., the state (2.169) is a stationary state of the system. The question arises if the quantum oscillator posesses further stationary states. In fact, there exist an infinite number of such states which will be determined now.

2.8 Stationary States of the Harmonic Oscillator

In order to find the stationary states of the quantum oscillator we consider the function

$$W(x,t) \;=\; \exp\left(2\sqrt{\frac{m\omega}{\hbar}}\, x\, e^{-i\omega t} \;-\; e^{-2i\omega t} \;-\; \frac{m\omega}{2\hbar}\, x^2 \;-\; \frac{i\omega t}{2} \right) . \tag{2.171}$$

We want to demonstrate that $w(x,t)$ is invariant in time, i.e., for the propagator (2.147) of the harmonic oscillator holds

$$W(x,t) \;=\; \int_{-\infty}^{+\infty} dx_o\, \phi(x,t|x_o,t_o)\, W(x_o,t_o)\, . \tag{2.172}$$

We will demonstrate further below that (2.172) provides us in a nutshell with all the stationary states of the harmonic oscillator, i.e., with all the states with time-independent probability distribution.

In order to prove (2.172) we express the propagator, using (2.147) and the notation $T = t - t_o$

$$\begin{aligned} \phi(x,t|x_o,t_o) \;&=\; e^{-\frac{1}{2}i\omega T}\left[\frac{m\omega}{\pi\hbar(1-e^{-2i\omega T})} \right]^{\frac{1}{2}} \;\times \\ &\times\, \exp\left[-\frac{m\omega}{2\hbar}\,(x_o^2 \,+\, x^2)\, \frac{1\,+\,e^{-2i\omega T}}{1\,-\,e^{-2i\omega T}} \;-\; \frac{m\omega}{\hbar\omega}\, \frac{2x\,x_o e^{-i\omega T}}{1\,-\,e^{-2i\omega T}} \right] \end{aligned} \tag{2.173}$$

One can write then the r.h.s. of (2.172)

$$I \;=\; e^{-\frac{1}{2}i\omega t}\left[\frac{m\omega}{\pi\hbar(1-e^{-2i\omega T})} \right]^{\frac{1}{2}} \int_{-\infty}^{+\infty} dx_o \exp[\, E_o(x_o,x) \;+\; E(x)\,] \tag{2.174}$$

where

$$\begin{aligned} E_o(x_o,x) \;&=\; -\frac{m\omega}{2\hbar}\left[x_o^2 \left(\frac{1+e^{-2i\omega T}}{1-e^{-2i\omega T}} + 1 \right) \right. \\ &\qquad \left. +\; 2x_o \left(\frac{2xe^{-i\omega T}}{1-e^{-2i\omega T}} \;+\; 2\sqrt{\frac{\hbar}{m\omega}}\, e^{-i\omega t_o} \right) \;+\; f(x) \right] \end{aligned} \tag{2.175}$$

$$E(x) \;=\; -\frac{m\omega}{2\hbar}\left[x^2\, \frac{1+e^{-2i\omega T}}{1-e^{-2i\omega T}} \;+\; \frac{2\hbar}{m\omega}\, e^{-2i\omega t_o} \;-\; f(x) \right] \tag{2.176}$$

Following the by now familiar strategy one choses $f(x)$ to complete the square in (2.175), namely,

$$f(x) \;=\; \frac{1}{2}\,(1 \,-\, e^{-2i\omega T}) \left(\frac{2xe^{-i\omega T}}{1-e^{-2i\omega T}} \;+\; 2\sqrt{\frac{\hbar}{m\omega}}\, e^{-i\omega t_o} \right)^2 . \tag{2.177}$$

This choice of $f(x)$ results in

$$\begin{aligned} E_o(x_o, x) &= -\frac{m\omega}{2\hbar}\left[x_o\sqrt{\frac{2}{1-e^{-2i\omega T}}}\right. \\ &\qquad \left. + \sqrt{\frac{1-e^{-2i\omega T}}{2}}\left(\frac{2xe^{-i\omega T}}{1-e^{-2i\omega T}} + 2\sqrt{\frac{\hbar}{m\omega}}\,e^{-i\omega t_o}\right)\right]^2 \\ &= i\,\frac{m\,\omega}{i\hbar(e^{-2i\omega T}-1)}\,(x_o + z_o)^2 \end{aligned} \tag{2.178}$$

for some constant $z_o \in \mathbb{C}$. Using (2.247) one obtains

$$\int_{-\infty}^{+\infty} dx_o\, e^{E_o(x_o,x)} = \left[\frac{\pi\hbar(1 - e^{-2i\omega T}}{m\omega}\right]^{\frac{1}{2}} \tag{2.179}$$

and, therefore, one obtains for (2.174)

$$I = e^{-\frac{1}{2}i\omega t}\, e^{E(x)}\,. \tag{2.180}$$

For $E(x)$, as given in (2.176, 2.177), holds

$$\begin{aligned} E(x) &= -\frac{m\omega}{2\hbar}\left[x^2\,\frac{1+e^{-2i\omega T}}{1-e^{-2i\omega T}} + \frac{2\hbar}{m\omega}\,e^{-2i\omega t_o} - \frac{2x^2e^{-2i\omega T}}{1-e^{-2i\omega T}}\right. \\ &\qquad \left. -4\sqrt{\frac{\hbar}{m\omega}}\,x\,e^{-i\omega T} - 2\,(1-e^{-2i\omega T})\,\frac{\hbar}{m\omega}\,e^{-2i\omega t_o}\right] \\ &= -\frac{m\omega}{2\hbar}\left[x^2 - 4\sqrt{\frac{\hbar}{m\omega}}\,x\,e^{-i\omega t} + \frac{2\hbar}{m\omega}\,e^{-2i\omega t}\right] \\ &= -\frac{m\omega}{2\hbar}\,x^2 + 2\sqrt{\frac{m\omega}{\hbar}}\,x\,e^{-i\omega t} - e^{-2i\omega t} \end{aligned} \tag{2.181}$$

Altogether, one obtains for the r.h.s. of (2.172)

$$I = \exp\left(2\sqrt{\frac{m\omega}{\hbar}}\,x\,e^{-i\omega t} - e^{-2i\omega t} - \frac{m\omega}{2\hbar}\,x^2 - \frac{1}{2}i\omega t\right)\,. \tag{2.182}$$

Comparision with (2.171) concludes the proof of (2.172).

We want to inspect the consequences of the invariance property (2.171, 2.172). We note that the factor $\exp(2\sqrt{m\omega/\hbar}\,xe^{-i\omega t} - e^{-2i\omega t})$ in (2.171) can be expanded in terms of $e^{-in\omega t}$, $n = 1, 2, \ldots$. Accoordingly, one can expand (2.171)

$$W(x,t) \;=\; \sum_{n=0}^{\infty} \frac{1}{n!} \exp[\,-i\omega(n+\tfrac{1}{2})\,t\,]\;\tilde{\phi}_n(x) \tag{2.183}$$

where the expansion coefficients are functions of x, but not of t. Noting that the propagator (2.147) in (2.172) is a function of $t - t_o$ and defining accordingly

$$\Phi(x, x_o; t - t_o) \;=\; \phi(x, t|x_o, t_o) \tag{2.184}$$

we express (2.172) in the form

$$\begin{aligned}&\sum_{n=0}^{\infty} \frac{1}{n!} \exp[-i\omega(n+\tfrac{1}{2})\,t]\;\tilde{\phi}_n(x)\\ &\quad = \sum_{m=0}^{\infty} \int_{-\infty}^{+\infty} dx_o\, \Phi(x, x_o; t - t_o)\; \frac{1}{m!} \exp[-i\omega(m+\tfrac{1}{2})\,t_o]\;\tilde{\phi}_m(x_o)\end{aligned} \tag{2.185}$$

Replacing $t \to t + t_o$ yields

$$\begin{aligned}&\sum_{n=0}^{\infty} \frac{1}{n!} \exp[-i\omega(n+\tfrac{1}{2})\,(t+t_o)]\;\tilde{\phi}_n(x)\\ &\quad = \sum_{m=0}^{\infty} \int_{-\infty}^{+\infty} dx_o\, \Phi(x, x_o; t)\; \frac{1}{m!} \exp[-i\omega(m+\tfrac{1}{2})\,t_o]\;\tilde{\phi}_m(x_o)\end{aligned} \tag{2.186}$$

Fourier transform, i.e., $\int_{-\infty}^{+\infty} dt_o\, \exp[i\omega(n+\tfrac{1}{2})\,t_o]\cdots$, results in

$$\begin{aligned}&\frac{1}{n!} \exp[-i\omega(n+\tfrac{1}{2})\,t]\;\tilde{\phi}_n(x)\\ &\quad = \int_{-\infty}^{+\infty} dx_o\, \Phi(x, x_o; t - t_o)\; \frac{1}{n!}\;\tilde{\phi}_n(x_o)\end{aligned} \tag{2.187}$$

or

$$\begin{aligned}&\exp[-i\omega(n+\tfrac{1}{2})\,t]\;\tilde{\phi}_n(x)\\ &\quad = \int_{-\infty}^{+\infty} dx_o\, \phi(x, t|x_o, t_o)\; \exp[-i\omega(n+\tfrac{1}{2})\,t_o]\;\tilde{\phi}_n(x_o)\,.\end{aligned} \tag{2.188}$$

Equation (2.188) identifies the functions $\tilde{\psi}_n(x,t) \;=\; \exp[-i\omega(n+\tfrac{1}{2})\,t]\;\tilde{\phi}_n(x)$ as invariants under the action of the propagator $\phi(x,t|x_o,t_o)$. In contrast to $W(x,t)$, which also exhibits such invariance, the functions $\tilde{\psi}_n(x,t)$ are associated with a time-independent probablity density $|\tilde{\psi}_n(x,t)|^2 \;=\; |\tilde{\phi}_n(x)|^2$.

Actually, we have identified then, through the expansion coefficients $\tilde{\phi}_n(x)$ in (2.183), stationary wave functions $\psi_n(x,t)$ of the quantum mechanical harmonic oscillator

$$\psi_n(x,t) \;=\; \exp[-i\omega(n+\tfrac{1}{2})\,t]\;N_n\,\tilde{\phi}_n(x)\;, \quad n \;=\; 0,1,2,\ldots \tag{2.189}$$

Here N_n are constants which normalize $\psi_n(x,t)$ such that

$$\int_{-\infty}^{+\infty} dx\,|\psi(x,t)|^2 \;=\; N_n^2 \int_{-\infty}^{+\infty} dx\,\tilde{\phi}_n^2(x) \;=\; 1 \tag{2.190}$$

is obeyed. In the following we will characterize the functions $\tilde{\phi}_n(x)$ and determine the normalization constants N_n. We will also argue that the functions $\psi_n(x,t)$ provide all stationary states of the quantum mechanical harmonic oscillator.

The Hermite Polynomials

The function (2.171), through expansion (2.183), characterizes the wave functions $\tilde{\phi}_n(x)$. To obtain closed expressions for $\tilde{\phi}_n(x)$ we simplify the expansion (2.183). For this purpose we introduce first the new variables

$$y \;=\; \sqrt{\frac{m\omega}{\hbar}}\,x \tag{2.191}$$

$$z \;=\; e^{-i\omega t} \tag{2.192}$$

and write (2.171)

$$W(x,t) \;=\; z^{\frac{1}{2}}\,e^{-y^2/2}\,w(y,z) \tag{2.193}$$

where

$$w(y,z) \;=\; \exp(2yz \;-\; z^2)\;. \tag{2.194}$$

Expansion (2.183) reads then

$$w(y,z)\,z^{\frac{1}{2}}\,e^{-y^2/2} \;=\; z^{\frac{1}{2}} \sum_{n=0}^{\infty} \frac{z^n}{n!}\,\tilde{\phi}_n(y) \tag{2.195}$$

or

$$w(y,z) \;=\; \sum_{n=0}^{\infty} \frac{z^n}{n!}\,H_n(y) \tag{2.196}$$

where

$$H_n(y) \;=\; e^{y^2/2}\,\tilde{\phi}_n(y)\;. \tag{2.197}$$

The expansion coefficients $H_n(y)$ in (2.197) are called *Hermite polynomials* which are polynomials of degree n which will be evaluated below. Expression (2.194) plays a central role for the *Hermite* polynomials since it contains, according to (2.194), in a 'nutshell' all information on the *Hermite* polynomials. This follows from

$$\frac{\partial^n}{\partial z^n} w(y,z)\bigg|_{z=0} = H_n(y) \tag{2.198}$$

which is a direct consequence of (2.196). One calls $w(y,z)$ the *generating function* for the *Hermite* polynomials. As will become evident in the present case generating functions provide an extremely elegant access to the special functions of Mathematical Physics[3]. We will employ (2.194, 2.196) to derive, among other properties, closed expressions for $H_n(y)$, normalization factors for $\tilde{\phi}(y)$, and recursion equations for the efficient evaluation of $H_n(y)$.

The identity (2.198) for the Hermite polynomials can be expressed in a more convenient form employing definition (2.196)

$$\begin{aligned}\frac{\partial^n}{\partial z^n} w(y,z)\bigg|_{z=0} &= \frac{\partial^n}{\partial z^n} e^{2\,y\,z\,-\,z^2}\bigg|_{z=0} \quad e^{y^2}\; \frac{\partial^n}{\partial z^n} e^{-(y-z)^2}\bigg|_{z=0} \\ &= (-1)^n\, e^{y^2}\; \frac{\partial^n}{\partial y^n} e^{-(y-z)^2}\bigg|_{z=0} = (-1)^n\, e^{y^2}\; \frac{\partial^n}{\partial y^n} e^{-y^2} \end{aligned} \tag{2.199}$$

Comparision with (2.196) results in the so-called Rodrigues formula for the *Hermite* polynomials

$$H_n(y) = (-1)^n\, e^{y^2}\; \frac{\partial^n}{\partial y^n} e^{-y^2}\;. \tag{2.200}$$

One can deduce from this expression the polynomial character of $H_n(y)$, i.e., that $H_n(y)$ is a polynomial of degree n. (2.200) yields for the first *Hermite* polynomials

$$H_0(y) = 1, \quad H_1(y) = 2y, \quad H_2(y) = 4y^2 - 2, \quad H_3(y) = 8y^3 - 12y, \ldots \tag{2.201}$$

We want to derive now explicit expressions for the *Hermite* polynomials. For this purpose we expand the generating function (2.194) in a Taylor

[3] *generatingfunctionology* by H.S.Wilf (Academic Press, Inc., Boston, 1990) is a useful introduction to this tool as is a chapter in the eminently useful *Concrete Mathematics* by R.L.Graham, D.E.Knuth, and O.Patashnik (Addison-Wesley, Reading, Massachusetts, 1989).

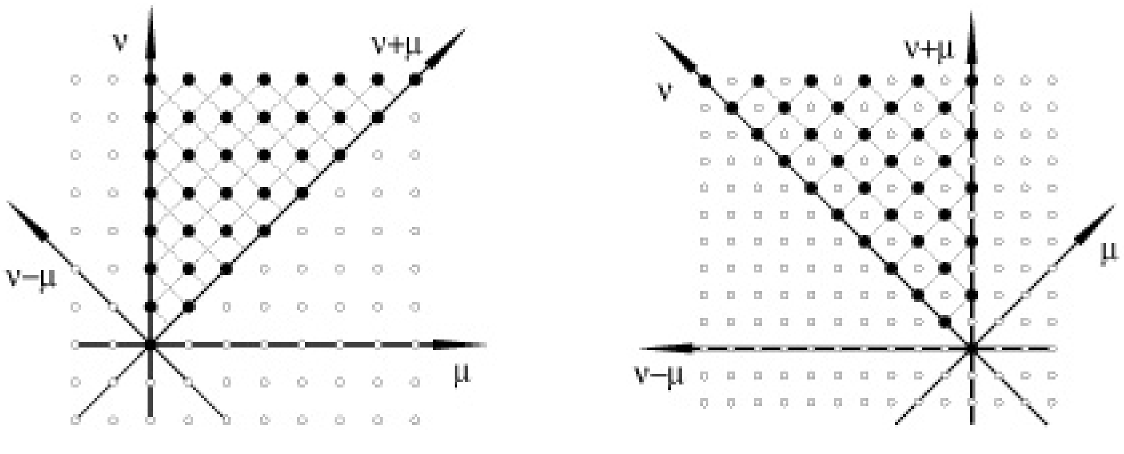

Figure 2.1: Schematic representation of change of summation variables ν and μ to $n = \nu + \mu$ and $m = \nu - \mu$. The diagrams illustrate that a summation over all points in a ν, μ lattice (left diagram) corresponds to a summation over only every other point in an n, m lattice (right diagram). The diagrams also identify the areas over which the summation is to be carried out.

series in terms of $y^p\, z^q$ and identify the corresponding coefficient c_{pq} with the coefficient of the p–th power of y in $H_q(y)$. We start from

$$\begin{aligned} e^{2yz\,-\,z^2} &= \sum_{\nu=0}^{\infty}\sum_{\mu=0}^{\nu}\frac{1}{\nu!}\begin{pmatrix}\nu\\ \mu\end{pmatrix} z^{2\mu}(-1)^{\mu}(2y)^{\nu-\mu}z^{\nu-\mu} \\ &= \sum_{\nu=0}^{\infty}\sum_{\mu=0}^{\nu}\frac{1}{\nu}\begin{pmatrix}\nu\\ \mu\end{pmatrix}(-1)^{\mu}(2y)^{\nu-\mu}z^{\nu+\mu} \end{aligned} \tag{2.202}$$

and introduce now new summation variables

$$n \;=\; \nu \,+\, \mu\,, \quad m \;=\; \nu \,-\, \mu \quad 0 \leq n \,<\, \infty\,,\; 0 \,\leq\, m \,\leq\, n\,. \tag{2.203}$$

The old summation variables ν, μ expressend in terms of n, m are

$$\nu \;=\; \frac{n\,+\,m}{2}\,, \quad \mu \;=\; \frac{n\,-\,m}{2}\,. \tag{2.204}$$

Since ν, μ are integers the summation over n, m must be restricted such that either both n and m are even or both n and m are odd. The lattices representing the summation terms are shown in Fig. **??**. *With this restriction* *in mind* one can express (2.202)

$$e^{2yz - z^2} = \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{m \geq 0}^{\leq n} \frac{n!\,(-1)^{\frac{n-m}{2}}}{(\frac{n-m}{2})!\,m!}\,(2y)^m\,. \tag{2.205}$$

Since $(n-m)/2$ is an integer we can introduce now the summation variable $k = (n-m)/2\,,\ 0 \leq k \leq [n/2]$ where $[x]$ denotes the largest integer p, $p \leq x$. One can write then using $m = n - 2k$

$$e^{2yz - z^2} = \sum_{n=0}^{\infty} \frac{z^n}{n!} \underbrace{\sum_{k=0}^{[n/2]} \frac{n!\,(-1)^k}{k!\,(n-2k)!}\,(2y)^{n-2k}}_{= H_n(y)}\,. \tag{2.206}$$

From this expansion we can identify $H_n(y)$

$$H_n(y) = \sum_{k=0}^{[n/2]} \frac{(-1)^k\,n!}{k!\,(n-2k)!}\,(2y)^{n-2k}\,. \tag{2.207}$$

This expression yields for the first four *Hermite* polynomials

$$H_0(y) = 1, \quad H_1(y) = 2y, \quad H_2(y) = 4y^2 - 2, \quad H_3(y) = 8y^3 - 12y, \ldots \tag{2.208}$$

which agrees with the expressions in (2.201).

From (2.207) one can deduce that $H_n(y)$, in fact, is a polynomial of degree n. In case of even n , the sum in (2.207) contains only even powers, otherwise, i.e., for odd n, it contains only odd powers. Hence, it holds

$$H_n(-y) = (-1)^n\,H_n(y)\,. \tag{2.209}$$

This property follows also from the generating function. According to (2.194) holds $w(-y,z) = w(y,-z)$ and, hence, according to 2.197)

$$\sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(-y) = \sum_{n=0}^{\infty} \frac{(-z)^n}{n!} H_n(y) = \sum_{n=0}^{\infty} \frac{z^n}{n!}\,(-1)^n\,H_n(y) \tag{2.210}$$

from which one can conclude the property (2.209).

The generating function allows one to determine the values of $H_n(y)$ at $y = 0$. For this purpose one considers $w(0,z) = \exp(-z^2)$ and carries out the Taylor expansion on both sides of this expression resulting in

$$\sum_{m=0}^{\infty} \frac{(-1)^m\,z^{2m}}{m!} = \sum_{n=0}^{\infty} H_n(0)\,\frac{z^n}{n!}\,. \tag{2.211}$$

Comparing terms on both sides of the equation yields

$$H_{2n}(0) \;=\; (-1)^n \frac{(2n)!}{n!}\,, \quad H_{2n+1}(0) \;=\; 0\,, \quad n \;=\; 0,1,2,\ldots \tag{2.212}$$

This implies that stationary states of the harmonic oscillator $\phi_{2n+1}(x)$, as defined through (2.188, 2.197) above and given by (2.233) below, have a node at $y = 0$, a property which is consistent with (2.209) since odd functions have a node at the origin.

Recursion Relationships

A useful set of properties for special functions are the so-called recursion relationships. For *Hermite* polynomials holds, for example,

$$H_{n+1}(y) \;-\; 2y\, H_n(y) \;+\; 2n\, H_{n-1}(y) \;=\; 0\,, \quad n \;=\; 1,2,\ldots \tag{2.213}$$

which allow one to evaluate $H_n(y)$ from $H_0(y)$ and $H_1(y)$ given by (2.208). Another relationship is

$$\frac{d}{dy} H_n(y) \;=\; 2n\, H_{n-1}(y), \quad n \;=\; 1,2,\ldots \tag{2.214}$$

We want to derive (**??**) using the *generating function*. Starting point of the derivation is the property of $w(y,z)$

$$\frac{\partial}{\partial z}\, w(y,z) \;-\; (2y \;-\; 2z)\, w(y,z) \;=\; 0 \tag{2.215}$$

which can be readily verified using (2.194). Substituting expansion (2.196) into the differential equation (2.215) yields

$$\sum_{n=1}^{\infty} \frac{z^{n-1}}{(n-1)!} H_n(y) \;-\; 2y \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(y) \;+\; 2 \sum_{n=0}^{\infty} \frac{z^{n+1}}{n!} H_n(y) \;=\; 0\,. \tag{2.216}$$

Combining the sums and collecting terms with identical powers of z

$$\sum_{n=1}^{\infty} \frac{z^n}{n!} \Big[H_{n+1}(y) \;-\; 2y\, H_n(y) \;+\; 2n\, H_{n-1}(y) \Big] \;+\; H_1(y) \;-\; 2y H_0(y) \;=\; 0 \tag{2.217}$$

gives

$$H_1(y) - 2y\, H_0(y) \;=\; 0,\;\; H_{n+1}(y) - 2y\, H_n(y) + 2n\, H_{n-1}(y) \;=\; 0,\; n = 1,2,\ldots \tag{2.218}$$

The reader should recognize the connection between the pattern of the differential equation (**??**) and the pattern of the recursion equation (**??**): a differential operator d/dz increases the order n of H_n by one, a factor z reduces the order of H_n by one and introduces also a factor n. One can then readily state which differential equation of $w(y,z)$ should be equivalent to the relationship (**??**), namely, $dw/dy - 2zw = 0$. The reader may verify that $w(y,z)$, as given in (2.194), indeed satisfies the latter relationship.

Integral Representation of Hermite Polynomials

An integral representation of the *Hermite polynomials* can be derived starting from the integral

$$I(y) = \int_{-\infty}^{+\infty} dt\, e^{2iy\,t - t^2}\,. \tag{2.219}$$

which can be written

$$I(y) = e^{-y^2} \int_{-\infty}^{+\infty} dt e^{-(t-iy)^2} = e^{-y^2} \int_{-\infty}^{+\infty} dz e^{-z^2}\,. \tag{2.220}$$

Using (2.247) for $a = i$ one obtains

$$I(y) = \sqrt{\pi}\, e^{-y^2} \tag{2.221}$$

and, acording to the definition (2.226a),

$$e^{-y^2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dt\, e^{2iyt - t^2}\,. \tag{2.222}$$

Employing this expression now on the r.h.s. of the *Rodrigues* formula (2.200) yields

$$H_n(y) = \frac{(-1)^n}{\sqrt{\pi}}\, e^{y^2} \int_{-\infty}^{+\infty} dt\, \frac{d^n}{dy^n}\, e^{2iyt - t^2}\,. \tag{2.223}$$

The identity

$$\frac{d^n}{dy^n} e^{2iy\,t - t^2} = (2\,i\,t)^n\, e^{2iy\,t - t^2} \tag{2.224}$$

results, finally, in the integral representation of the *Hermite* polynomials

$$H_n(y) = \frac{2^n\,(-i)^n e^{y^2}}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dt\, t^n\, e^{2iy\,t - t^2}\,, \quad n = 0, 1, 2, \ldots \tag{2.225}$$

Orthonormality Properties

We want to derive from the generating function (2.194, 2.196) the orthogonality properties of the *Hermite* polynomials. For this purpose we consider the integral

$$\begin{aligned} \textstyle\int_{-\infty}^{+\infty} dy\, w(y,z)\, w(y,z')\, e^{-y^2} &= e^{2\,z\,z'} \int_{-\infty}^{+\infty} dy\, e^{-(y-z-z')^2} = \sqrt{\pi}\, e^{2\,z\,z'} \\ &= \sqrt{\pi} \sum_{n=0}^{\infty} \frac{2^n\, z^n\, z'^n}{n!} \;. \end{aligned} \tag{2.226}$$

Expressing the l.h.s. through a double series over *Hermite* polynomials using (2.194, 2.196) yields

$$\sum_{n,n'=0}^{\infty} \int_{-\infty}^{+\infty} dy\, H_n(y)\, H_{n'}(y)\, e^{-y^2} \frac{z^n\, z'^{n'}}{n!\, n'!} = \sum_{n=0}^{\infty} 2^n n!\, \sqrt{\pi}\, \frac{z^n\, z'^n}{n!\, n!} \tag{2.227}$$

Comparing the terms of the expansions allows one to conclude the orthonormality conditions

$$\int_{-\infty}^{+\infty} dy\, H_n(y)\, H_{n'}(y)\, e^{-y^2} = 2^n\, n!\, \sqrt{\pi}\;\; \delta_{n\,n'} \;. \tag{2.228}$$

Normalized Stationary States

The orthonormality conditions (2.228) allow us to construct normalized stationary states of the harmonic oscillator. According to (2.197) holds

$$\tilde{\phi}_n(y) = e^{-y^2/2}\, H_n(y) \;. \tag{2.229}$$

The normalized states are [c.f. (2.189, 2.190)]

$$\phi_n(y) = N_n\, e^{-y^2/2}\, H_n(y) \;. \tag{2.230}$$

and for the normalization constants N_n follows from (2.228)

$$N_n^2 \int_{-\infty}^{+\infty} dy\, e^{-y^2}\, H_n^2(y) = N_n^2\, 2^n\, n!\, \sqrt{\pi} = 1 \tag{2.231}$$

We conclude

$$N_n = \frac{1}{\sqrt{2^n\, n!\, \sqrt{\pi}}} \tag{2.232}$$

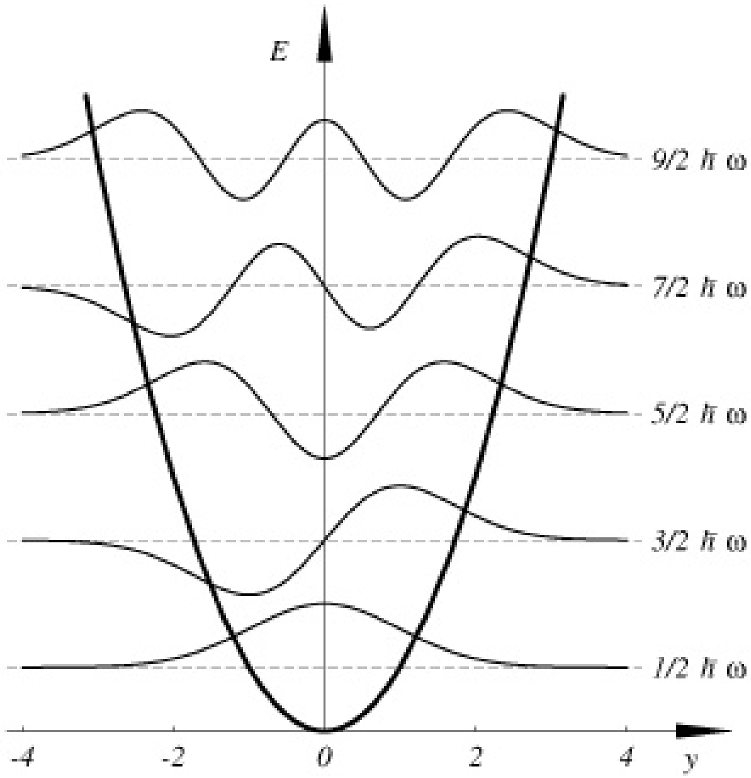

Figure 2.2: Stationary states $\phi_n(y)$ of the harmonic oscillator for $n = 0, 1, 2, 3, 4$.

and can finally state the explicit form of the normalized stationary states

$$\phi_n(y) \;=\; \frac{1}{\sqrt{2^n\, n!\, \sqrt{\pi}}}\; e^{-y^2/2}\, H_n(y)\;. \tag{2.233}$$

The stationary states (2.233) are presented for $n = 0, 1, 2, 3, 4$ in Fig. **??**. One can recognize, in agreement with our above discussions, that the wave functions are even for $n = 0, 2, 4$ and odd for $n = 1, 3$. One can also recognize that n is equal to the number of nodes of the wave function. Furthermore, the value of the wave function at $y = 0$ is positive for $n = 0, 4$, negative for $n = 2$ and vanishes for $n = 1, 3$, in harmony with (**??**).

The normalization condition (2.231) of the wave functions differs from that postulated in (2.189) by the Jacobian dx/dy, i.e., by

$$\sqrt{\left|\frac{dx}{dy}\right|} \;=\; \left[\frac{m\omega}{\hbar}\right]^{\frac{1}{4}}\;. \tag{2.234}$$

The explicit form of the stationary states of the harmonic oscillator in terms of the position variable x is then, using (2.233) and (2.189)

$$\phi_n(x) \;=\; \frac{1}{\sqrt{2^n\, n!}}\left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}\, H_n(\sqrt{\frac{m\omega}{\hbar}}x)\;. \tag{2.235}$$

Completeness of the Hermite Polynomials

The *Hermite* polynomials are the first members of a large class of *special functions* which one encounters in the course of describing stationary quantum states for various potentials and in spaces of different dimensions. The *Hermite* polynomials are so-called orthonogal polynomials since they obey the conditions (2.228). The various orthonogal polynomials differ in the spaces $\Omega \subset \mathbb{R}$ over which they are defined and differ in a weight function $w(y)$ which enter in their orthonogality conditions. The latter are written for polynomials $p_n(x)$ in the general form

$$\int_\Omega dx\; p_n(x)\, p_m(x)\, w(x) \;=\; I_n\, \delta_{nm} \tag{2.236}$$

where $w(x)$ is a so-called weight function with the property

$$w(x) \,\geq\, 0,\;\; w(x) \,=\, 0 \quad \text{only at a discrete set of points } x_k \in \Omega \tag{2.237}$$

and where I_n denotes some constants. Comparision with (2.228) shows that the orthonogality condition of the *Hermite* polynomials is in complience with (2.236 , 2.237) for $\Omega = \mathbb{R}$, $w(x) = \exp(-x^2)$, and $I_n = 2^n n! \sqrt{\pi}$.

Other examples of orthogonal polynomials are the *Legendre* and *Jacobi* polynomials which arise in solving three-dimensional stationary Schrödinger equations, the *ultra-spherical harmonics* which arise in n–dimensional Schrödinger equations and the associated *Laguerre* polynomials which arise for the stationary quantum states of particles moving in a Coulomb potential. In case of the Legendre polynomials, denoted by $P_\ell(x)$ and introduced in Sect. **??** below [c.f. (**??** , **??**, **??**, **??**] holds $\Omega = [-1, 1]$, $w(x) \equiv 1$, and $I_\ell = 2/(2\ell + 1)$. In case of the associated *Laguerre* polynomials, denoted by $L_n^{(\alpha)}(x)$ and encountered in case of the stationary states of the non-relativistic [see Sect. ??? and eq. ???] and relativistic [see Sect. **??** and eq. (**??**] hydrogen atom, holds $\Omega = [0, +\infty[$, $w(x) = x^\alpha e^{-x}$, $I_n = \Gamma(n + \alpha + 1)/n!$ where $\Gamma(z)$ is the so-called *Gamma function*.

The orthogonal polynomials p_n mentioned above have the important property that they form a *complete* basis in the space $\mathcal{F}$ of normalizable functions, i.e., of functions which obey

$$\int_\Omega dx \; f^2(x) \; w(x) \;\; = < \infty \; , \tag{2.238}$$

where the space is endowed with the scalar product

$$(f|g) \;=\; \int_\Omega dx \; f(x) \, g(x) \; w(x) \;\; = < \infty \; , \quad f, \, g \;\in\; \mathcal{F} \; . \tag{2.239}$$

As a result holds for any $f \in \mathcal{F}$

$$f(x) \;=\; \sum_n c_n \, p_n(x) \tag{2.240}$$

where

$$c_n \;=\; \frac{1}{I_n} \int_\Omega dx \; w(x) \, f(x) \, p_n(x) \; . \tag{2.241}$$

The latter identity follows from (2.236). If one replaces for all $f \in \mathcal{F}$: $f(x) \to \sqrt{w(x)}\, f(x)$ and, in particular, $p_n(x) \to \sqrt{w(x)}\, p_n(x)$ the scalar product (2.239) becomes the conventional scalar product of quantum mechanics

$$\langle f|g\rangle \;=\; \int_\Omega dx \; f(x) \, g(x) \; . \tag{2.242}$$

Let us assume now the case of a function space governed by the norm (2.242) and the existence of a normalizable state $\psi(y,t)$ which is stationary under the action of the harmonic oscillator propagator (2.147), i.e., a state for which (2.172) holds. Since the *Hermite* polynomials form a complete basis for such states we can expand

$$\psi(y,t) \;=\; \sum_{n=0}^{\infty} c_n(t)\, e^{-y^2/2}\, H_n(y)\;. \tag{2.243}$$

To be consistent with(2.188, 2.197) it must hold $c_n(t) \;=\; d_n\, \exp[-i\omega(n+\frac{1}{2})t]$ and, hence, the stationary state $\psi(y,t)$ is

$$\psi(y,t) \;=\; \sum_{n=0}^{\infty} d_n\, \exp[-i\omega(n+\frac{1}{2})t]\, e^{-y^2/2}\, H_n(y)\;. \tag{2.244}$$

For the state to be stationary $|\psi(x,t)|^2$, i.e.,

$$\sum_{n,m=0}^{\infty} d_n^* d_m\, \exp[i\omega(m-n)t]\, e^{-y^2}\, H_n(y) H_m(y)\;, \tag{2.245}$$

must be time-independent. The only possibility for this to be true is $d_n \;=\; 0$, except for a single $n \;=\; n_o$, i.e., $\psi(y,t)$ must be identical to one of the stationary states (2.233). Therefore, the states (2.233) exhaust all stationary states of the harmonic oscillator.

Appendix: Exponential Integral

We want to prove

$$I \;=\; \int_{-\infty}^{+\infty} dy_1 \ldots \int_{-\infty}^{+\infty} dy_n \;\; e^{i\sum_{j,k}^{n} y_j a_{jk} y_k} \;=\; \sqrt{\frac{(i\pi)^n}{det(\mathbf{a})}}\;, \tag{2.246}$$

for $det(\mathbf{a}) \neq 0$ and real, symmetric $\mathbf{a}$, i.e. $\mathbf{a}^T \;=\; \mathbf{a}$. In case of $n \;=\; 1$ this reads

$$\int_{-\infty}^{+\infty} dx\, e^{i\,a\,x^2} \;=\; \sqrt{\frac{i\,\pi}{a}}\;, \tag{2.247}$$

which holds for $a \in \mathbb{C}$ as long as $a \neq 0$.

The proof of (2.246) exploits that for any real, symmetric matrix exists a similarity transformation such that

$$\mathbf{S}^{-1}\mathbf{a}\,\mathbf{S} \;=\; \tilde{\mathbf{a}} \;=\; \begin{pmatrix} \tilde{a}_{11} & 0 & \dots & 0 \\ 0 & \tilde{a}_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \tilde{a}_{nn} \end{pmatrix} . \tag{2.248}$$

where $\mathbf{S}$ can be chosen as an orthonormal transformation, i.e.,

$$\mathbf{S}^T\mathbf{S} \;=\; 1\!\!1 \qquad \text{or} \qquad \mathbf{S} \;=\; \mathbf{S}^{-1} . \tag{2.249}$$

The $\tilde{a}_{kk}$ are the eigenvalues of $\mathbf{a}$ and are real. This property allows one to simplify the bilinear form $\sum_{j,k}^n y_j a_{jk} y_k$ by introducing new integration variables

$$\tilde{y}_j \;=\; \sum_k^n (S^{-1})_{jk} y_k \;; \quad y_k \;=\; \sum_k^n S_{kj}\tilde{y}_j \;. \tag{2.250}$$

The bilinear form in (2.246) reads then in terms of $\tilde{y}_j$

$$\begin{aligned} \textstyle\sum_{j,k}^n y_j a_{jk} y_k \quad &= \sum_{j,k}^n \sum_{\ell m}^n \tilde{y}_\ell S_{j\ell} a_{jk} S_{km} \tilde{y}_m \\ &= \sum_{j,k}^n \sum_{\ell m}^n \tilde{y}_\ell (S^T)_{\ell j} a_{jk} S_{km} \tilde{y}_m \\ &= \sum_{j,k}^n \tilde{y}_j \tilde{a}_{jk} \tilde{y}_k \end{aligned} \tag{2.251}$$

where, according to (2.248, 2.249)

$$\tilde{a}_{jk} \;=\; \sum_{l,m}^n (S^T)_{jl} a_{lm} S_{mk} \;. \tag{2.252}$$

For the determinant of $\tilde{\mathbf{a}}$ holds

$$det(\tilde{\mathbf{a}}) = \prod_{j=1}^n \tilde{a}_{jj} \tag{2.253}$$

as well as

$$\begin{aligned} det(\tilde{\mathbf{a}}) \;&=\; det(\mathbf{S}^{-1}\mathbf{a}\mathbf{S}) \;=\; det(\mathbf{S}^{-1})\, det(\mathbf{a}) \;, det(\mathbf{S}) \\ &=\; (det(\mathbf{S}))^{-1}\; det(\mathbf{a})\; det(\mathbf{S}) \;=\; det(\mathbf{a}) \;. \end{aligned} \tag{2.254}$$

One can conclude

$$det(\mathbf{a}) \;=\; \prod_{j=1}^{n} \tilde{a}_{jj} \; . \tag{2.255}$$

We have assumed $det(\mathbf{a}) \neq 0$. Accordingly, holds

$$\prod_{j=1}^{n} \tilde{a}_{jj} \neq 0 \tag{2.256}$$

such that none of the eigenvalues of **a** vanishes, i.e.,

$$\tilde{a}_{jj} \neq 0 \; , \quad \text{for } j \;=\; 1,\, 2,\, \ldots,\, n \tag{2.257}$$

Substitution of the integration variables (2.250) allows one to express (2.250)

$$I \;=\; \int_{-\infty}^{+\infty} d\tilde{y}_1 \;\ldots\; \int_{-\infty}^{+\infty} d\tilde{y}_n \, \left| det\left(\frac{\partial(y_1, \ldots, y_n)}{\partial(\tilde{y}_1, \ldots, \tilde{y}_n)} \right) \right| \quad e^{i \sum_k^n \tilde{a}_{kk} \tilde{y}_k^2} \; . \tag{2.258}$$

where we introduced the Jacobian matrix

$$\mathbf{J} \;=\; \frac{\partial(y_1, \ldots, y_n)}{\partial(\tilde{y}_1, \ldots, \tilde{y}_n)} \tag{2.259}$$

with elements

$$J_{js} \;=\; \frac{\partial y_j}{\partial \tilde{y}_s} \; . \tag{2.260}$$

According to (2.250) holds

$$\mathbf{J} \;=\; \mathbf{S} \tag{2.261}$$

and, hence,

$$det(\frac{\partial(y_1, \ldots, y_n)}{\partial(\tilde{y}_1, \ldots, \tilde{y}_n)}) \;=\; det(\mathbf{S}) \; . \tag{2.262}$$

From (2.249) follows

$$1 \;=\; \det\left(\mathbf{S}^T \mathbf{S}\right) \;=\; (\,\det \mathbf{S}\,)^2 \tag{2.263}$$

such that one can conclude

$$\det \mathbf{S} \;=\; \pm 1 \tag{2.264}$$

One can right then (2.258)

$$
\begin{aligned}
I &= \int_{-\infty}^{+\infty} d\tilde{y}_1 \ \ldots \int_{-\infty}^{+\infty} d\tilde{y}_n \ \ e^{i \sum_k^n \tilde{a}_{kk} \tilde{y}_k^2} \\
&= \int_{-\infty}^{+\infty} d\tilde{y}_1 \ e^{i\tilde{a}_{11}\tilde{y}_1^2} \ \ldots \ \int_{-\infty}^{+\infty} d\tilde{y}_n \ e^{i\tilde{a}_{nn}\tilde{y}_n^2} \ = \ \prod_{k=1}^{n} \int_{-\infty}^{+\infty} d\tilde{y}_k \ e^{i\tilde{a}_{kk}\tilde{y}_k^2}
\end{aligned} \tag{2.265}
$$

which leaves us to determine integrals of the type

$$
\int_{-\infty}^{+\infty} dx \ e^{icx^2} \tag{2.266}
$$

where, according to (2.257) holds $c \neq 0$.

We consider first the case $c > 0$ and discuss the case $c < 0$ further below. One can relate integral (2.266) to the well-known Gaussian integral

$$
\int_{-\infty}^{+\infty} dx \ e^{-cx^2} \ = \ \sqrt{\frac{\pi}{c}} \, , c > 0 \ . \tag{2.267}
$$

by considering the contour integral

$$
J \ = \ \oint_{\gamma} dz \ e^{icz^2} = 0 \tag{2.268}
$$

along the path $\gamma = \gamma_1 + \gamma_2 + \gamma_3 + \gamma_4$ displayed in Figure **??**. The contour integral (2.268) vanishes, since e^{icz^2} is a holomorphic function, i.e., the integrand does not exhibit any singularities anywhere in $\mathbb{C}$. The contour intergral (2.268) can be written as the sum of the following path integrals

$$
J \ = \ J_1 \ + \ J_2 \ + \ J_3 \ + \ J_4 \, ; \quad J_k \ = \ \oint_{\gamma_k} dz \ e^{icz^2} \tag{2.269}
$$

The contributions J_k can be expressed through integrals along a real coordinate axis by realizing that the paths γ_k can be parametrized by real coordinates x

$$
\begin{aligned}
\gamma_1 : z = x \qquad & J_1 = \int_{-p}^{p} dx\ e^{icx^2} \\
\gamma_2 : z = ix + p \qquad & J_2 = \int_{0}^{p} i\ dx\ e^{ic(ix+p)^2} \\
\gamma_3 : z = \sqrt{i}\ x \qquad & J_3 = \int_{\sqrt{2}p}^{-\sqrt{2}p} \sqrt{i}\ dx\ e^{ic(\sqrt{i}x)^2} \\
& \quad = -\sqrt{i} \int_{-\sqrt{2}p}^{\sqrt{2}p} dx\ e^{-cx^2} \\
\gamma_4 : z = ix - p \qquad & J_4 = \int_{-p}^{0} i\ dx\ e^{ic(ix-p)^2}\ , \\
& \text{for } x, p \in \mathbb{R}.
\end{aligned}
\tag{2.270}
$$

Substituting $-x$ for x into integral J_4 one obtains

$$
\begin{aligned}
J_4 &= \int_{p}^{0} (-i)\ dx\ e^{ic(-ix+p)^2} \\
&= \int_{0}^{p} i\ dx\ e^{ic(ix-p)^2} \quad = \quad J_2\ .
\end{aligned}
\tag{2.271}
$$

We will now show that the two integrals J_2 and J_4 vanish for $p \to +\infty$. This follows from the following calculation

$$
\begin{aligned}
\lim_{p\to+\infty} |J_{2 \text{ or } 4}| &= \lim_{p\to+\infty} \left|\int_{0}^{p} i\ dx\ e^{ic(ix+p)^2}\right| \\
&\leq \lim_{p\to+\infty} \int_{0}^{p} |i|\ dx\ |e^{ic(p^2-x^2)}|\ |e^{-2cxp}|\ .
\end{aligned}
\tag{2.272}
$$

It holds $|e^{ic(p^2-x^2)}| = 1$ since the exponent of e is purely imaginary. Hence,

$$
\begin{aligned}
\lim_{p\to+\infty} |J_{2 \text{ or } 4}| &\leq \lim_{p\to+\infty} \int_{0}^{p} dx\ |e^{-2cxp}| \\
&= \lim_{p\to+\infty} \frac{1 - e^{-2cp}}{2\ c\ p} \quad = \quad 0\ .
\end{aligned}
\tag{2.273}
$$

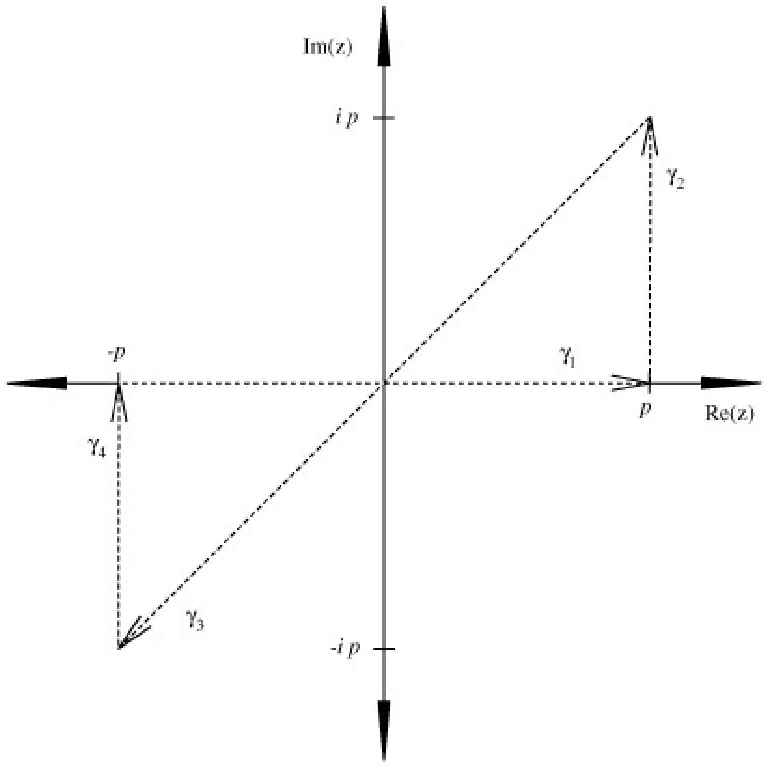

Figure 2.3: Contour path γ in the complex plain.

J_2 and J_4 do not contribute then to integral (2.268) for $p = +\infty$. One can state accordingly

$$J \;=\; \int_{-\infty}^{\infty} dx\; e^{icx^2} \;-\; \sqrt{i}\;\int_{-\infty}^{\infty} dx\; e^{-cx^2} \;=\; 0\;. \tag{2.274}$$

Using 2.267) one has shown then

$$\int_{-\infty}^{\infty} dx\; e^{icx^2} \;=\; \sqrt{\frac{i\pi}{c}}\;. \tag{2.275}$$

One can derive the same result for $c < 0$, if one chooses the same contour integral as (2.268), but with a path γ that is reflected at the real axis. This leads to

$$J \;=\; \int_{-\infty}^{\infty} dx\; e^{icx^2} \;+\; \sqrt{-i}\;\int_{\infty}^{-\infty} dx\; e^{cx^2} \;=\; 0 \tag{2.276}$$

and ($c < 0$)

$$\int_{-\infty}^{\infty} dx\; e^{icx^2} \;=\; \sqrt{\frac{-i\pi}{-|c|}} \;=\; \sqrt{\frac{i\pi}{c}}\;. \tag{2.277}$$

We apply the above results (2.275, 2.277) to (2.265). It holds

$$I \;=\; \prod_{k=1}^{n} \sqrt{\frac{i\pi}{\tilde{a}_{kk}}} = \sqrt{\frac{(i\pi)^n}{\prod_{j=1}^{n} \tilde{a}_{jj}}}\;. \tag{2.278}$$

Noting (2.255) this result can be expressed in terms of the matrix **a**

$$I \;=\; \sqrt{\frac{(i\pi)^n}{det(\mathbf{a})}} \tag{2.279}$$

which concludes our proof.