

# Chapter 1

## Quantum formalism

### 1.1 Summary of quantum states and observables

In this section we make a summary of fundamental assumptions and postulates of the quantum theory. We stress the correspondance with classical theory, but at the same time focus on the radically different way the quantum theory is interpreted. We summerize how an isolated quantum system is described in terms of abstract vectors and operators in a Hilbert space.

#### 1.1.1 Classical and quantum states

The classical description of a system that is most closely related the standard quantum description is the *phase space description* of the system. The variables are the generalized coordinates  $q = \{q_i; i = 1, 2, \dots, N\}$  and the canonical momenta  $p = \{p_i; i = 1, 2, \dots, N\}$ . (Note, when no ambiguity can arise we denote the whole sets of coordinates simply by  $q$  and  $p$ .) Each degree of freedom is represented by one coordinate  $q_i$  with the corresponding momentum  $p_i$ . A complete specification of the state of the system is given by the full set of coordinates and momenta  $(q, p)$ , which identifies a point in phase space.

There is a unique time evolution of the phase space coordinates  $(q(t), p(t))$ , with a given initial condition  $(q_0, p_0) = (q(t_0), p(t_0))$  at time  $t_0$ . This is so, since the equation of motion, expressed in terms of the phase space coordinates is *linear* in time derivatives. For a Hamiltonian system the dynamics can be expressed in terms of the classical Hamiltonian, which is a function of the phase space variables  $H(q, p)$  and normally is identical to the energy function. The time evolution is

expressed by Hamilton's equations as

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad (1.1)$$

By solving for the canonical momenta the dynamical equations can be expressed in terms of the coordinates  $\{q_i\}$  alone. These define the *configuration space* of the system. The Lagrangian of the system, which is related to the Hamiltonian by

$$L(q, \dot{q}) = \sum_i \dot{q}_i p_i - H(q, p), \quad \dot{q}_i = \frac{\partial H}{\partial p_i} \quad (1.2)$$

determines the dynamics in configuration space through the Euler-Lagrange equations,

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) = 0, \quad i = 1, 2, \dots, N \quad (1.3)$$

This is second order in time derivatives and corresponds to Newton's second law expressed in general coordinates.

If a complete specification of the system cannot be given, a statistical description is often used. The state of the system is then described in terms of a probability function  $\rho(q, p)$  defined on the phase space, and this is the basis of a statistical mechanics description of the system. The time evolution is described through the time derivative of  $\rho$ ,

$$\begin{aligned} \frac{d}{dt} \rho &= \sum_i \left( \frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right) + \frac{\partial}{\partial t} \rho \\ &= \{\rho, H\}_{PB} + \frac{\partial}{\partial t} \rho \end{aligned} \quad (1.4)$$

where the *Poisson bracket*, defined by

$$\{A, B\}_{PB} = \sum_i \left( \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \right) \quad (1.5)$$

has been introduced. One should note that in Eq.(1.4)  $\frac{\partial}{\partial t}$  is the time derivative with fixed phase space coordinates, whereas  $\frac{d}{dt}$  includes the time variation due to the motion in phase space. The time evolution of  $\rho$  (and any other phase space variable), when written in this way, shows a remarkable similarity with the *Heisenberg*

*equation of motion* of the quantum system. The commutator between the variables then takes the place of the Poisson bracket.

The quantum description of the system discussed above also involves the (phase space) variables  $(q, p)$ . But these dynamical variables are now re-interpreted as operators that act on complex-valued functions, the wave-functions  $\psi(q)$ , which usually are defined as a functions over the configuration space. To specify the variables as operators they are often written  $\hat{q}_i$  and  $\hat{p}_i$ . In the standard way we refer to these as *observables*, and the fundamental relation between these observables is the (Heisenberg) commutation relation

$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij} \quad (1.6)$$

with  $\hbar$  as Planck's constant. A more general observable  $\hat{A}$  may be viewed as a function of  $q_i$  and  $p_i$ , and in general two observables  $\hat{A}$  and  $\hat{B}$  will in general not commute. We usually restrict observables to be Hermitean operators, which corresponds to real-valued variables in the classical description.

There is a close relation between the classical description of a mechanical system and the corresponding quantum description, and this relation is most explicit when the dynamics is expressed in terms of phase space variables. The transition from the classical to the quantum description is referred to as *canonical quantization* and is in its simplest form described as a transition between classical variables and quantum observables

$$q_i \rightarrow \hat{q}_i, p_i \rightarrow \hat{p}_i \quad (1.7)$$

where the quantum variables satisfy the fundamental commutation relation (1.6). This transition between the classical and quantum description is often expressed in terms of a substitution between Poisson brackets (for the classical variables) and commutators (for the quantum variables)

$$\{A, B\}_{PB} \rightarrow \frac{1}{i\hbar} [\hat{A}, \hat{B}] \quad (1.8)$$

Clearly this simple substitution rule gives the right commutator between  $\hat{q}_i$  and  $\hat{p}_j$  when used on the Poisson brackets between  $q_i$  and  $p_j$ .<sup>1</sup>

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<sup>1</sup>In general there will, however be an ambiguity in this substitution in the form of the so called *operator ordering problem*. Since classical observables commute, a composite variable  $C = AB = BA$  can be written in several ways. The corresponding quantum observables may be different due to non-commutativity,  $\hat{C} = \hat{A}\hat{B} \neq \hat{B}\hat{A} = \hat{C}'$ . The *Weyl ordering* is a way to solve the ambiguity by replacing a product by its symmetrized version,  $\hat{C} = \frac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A})$ .

Viewed the other way, the classical description can be seen as a special “classical limit” of the quantum description, where Planck’s constant disappears from the equations. This transition to the classical description, as a limit of the quantum theory, is referred to as the *correspondance principle*, and was by Bohr (and others) used as a guiding principle in the development of the early form of quantum mechanics. For radiative transitions between atomic levels the correspondance principle implies that the radiation formula of the quantum theory reproduces the classical one for highly excited atoms, in the limit where the excitation energy approaches the ionization value.

The close relation between the classical and quantum dynamics is clearly seen in the similarity between the classical equations of motion and the *Heisenberg equation of motion* for the quantum system. The latter is usually obtained from the former simply by the substitution (1.7). This correspondance relates directly to *Ehrenfest’s theorem*, which states that the classical dynamical equations keep their validity also in the quantum theory, if the classical variables are replaced by their corresponding quantum expectation values. Thus, the quantum expectation value  $\langle q \rangle$  in many respects behaves like a classical variable  $q$ , and the time evolution of the expectation value follows a classical equation of motion. As long as the wave function is well localized (in the  $q$ -variable), the system is “almost classical”. However if the wave functions more spread or divides into separated parts, then highly “non-classical effects” may arise.

The close correspondance between the classical and quantum theory is in many respects rather surprising, since the physical interpretation of the two theories are radically different. The difference is linked to the statistical interpretation of the quantum theory, which is the subject of one of the later sections. Both classical and quantum descriptions of a system will often be of statistical nature, since the full information (especially for systems with a large number of degree of freedom) may not be achievable. Often interactions with other systems (the surroundings) disturb the system in such a way that only a statistical description is meaningful. If such disturbances are negligible the system is referred to as an *isolated* or *closed system* and for a classical system all the dynamical variables can in principle be ascribed sharp values.

For a quantum system this is not the case. The quantum state of an isolated system is described by the wave function  $\psi(q)$  defined over the (classical) configuration space and this is interpreted as an *probability amplitude*. This means that the absolute value  $|\psi(q)|^2$  defines a probability distribution in configuration space. For a general observable  $\hat{a}$  this leads to a statistical variation or uncertainty

in the measured value, expressed in terms of the variable

$$\Delta A^2 = \langle (\hat{A} - \langle \hat{a} \rangle)^2 \rangle \quad (1.9)$$

Even if this probability distribution in principle can be sharp in the set of variables  $q$ , it cannot at the same time be sharp in the conjugate variables  $p$  due to the fundamental commutation relation (1.6). This is quantified in *Heisenberg's uncertainty relation*

$$\Delta q_i \Delta p_i \geq \frac{\hbar}{2} \quad (1.10)$$

The inherent probabilistic interpretation of the quantum theory in many respects is more closely related to a statistical description of the classical system than to detailed non-statistical description. However, the standard description in terms of a wave function  $\psi(q)$  defined on the configuration space seems rather different from a classical statistical description in terms of a phase space probability distribution  $\rho(q, p)$ . Quantum descriptions in terms of functions similar to  $\rho(q, p)$  are possible (the so-called *Wigner function* is of this type) and in some cases they are useful description. But one important property of the wave functions is hidden in such a reformulation. The *superposition principle* is a fundamental principle of quantum mechanics which makes the dynamical equations expressed in terms of the wave functions linear equations. The (quasi-) probability distributions derived from the standard quantum description are quadratic in  $\psi(q)$ , and therefore the linearity is lost. In the classical statistical theory there is no counterpart to the superposition principle.

The description of the quantum system in terms of wave functions defined as functions over the classical configuration space is only of many equivalent “representations” of the quantum theory. A more abstract formulation exists, based on superposition principle, where the states are (abstract) vectors in a complex vector space. Different representations of the theory correspond to different choices of basis in this vector space. In the following a summary of this abstract (and formal) description is given, in terms of what may be called the fundamental postulates of quantum theory.

### 1.1.2 The fundamental postulates

1. A quantum state of an isolated physical system is described by a vector with

unit norm in a complex vector space (a Hilbert space)<sup>2</sup> equipped with a scalar product.

In the Dirac notation a vector is represented by “ket”  $|\psi\rangle$ , which can be expanded in any complete set of basis vectors  $|a_i\rangle$ ,

$$|\psi\rangle = \sum_i c_i |a_i\rangle \quad (1.11)$$

where the coefficients  $c_i$  are complex numbers. For an infinite dimensional Hilbert space the basis may be a discrete or continuous set of vectors. We refer to the vectors (kets) as *state vectors* and the vector space as the *state space*.

A “bra”  $\langle\psi|$  is regarded as vector in the “dual vector space”, and is related to  $|\psi\rangle$  by an “anti-linear” mapping (linear mapping + complex conjugation)

$$|\psi\rangle \rightarrow \langle\psi| = \sum_i c_i^* \langle a_i| \quad (1.12)$$

The scalar product is a complex-valued composition of a bra and a ket,  $\langle\phi|\psi\rangle$  which is a linear function of  $|\psi\rangle$  and an antilinear function of  $\langle\phi|$ .

2. *The time evolution of the state vector,  $|\psi\rangle = |\psi(t)\rangle$ , is (in the Schrödinger picture) defined by the Schrödinger equation, of the form*

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (1.13)$$

The equation is linear in the time derivative, which means that the time evolution  $|\psi\rangle = |\psi(t)\rangle$  is uniquely determined by the initial condition  $|\psi\rangle_0 = |\psi(t_0)\rangle$ .  $\hat{H}$  is the Hamiltonian of the system which is a *linear, hermitean* operator. It gives rise to a time evolution which is a *unitary*, time dependent, mapping of the quantum states.

3. *Each physical observable of a system is associated with a hermitian operator acting on the Hilbert space. The eigenstates of each such operator form a complete orthonormal set.*

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<sup>2</sup>A Hilbert space is an (infinite-dimensional) vector space with a scalar product (an inner product space) which is *complete* in the norm. This means that any (Cauchy) sequence of vectors  $|n\rangle$ ,  $n = 1, 2, \dots$ , where the norm of the relative vectors  $|n, m\rangle = |n\rangle - |m\rangle$  goes to zero as  $n, m \rightarrow \infty$  will have a limit (vector) belonging to the space.

With  $\hat{A}$  as an observable, hermiticity means

$$\langle \phi | \hat{A} \psi \rangle = \langle \hat{A} \phi | \psi \rangle \equiv \langle \phi | \hat{A} | \psi \rangle \quad (1.14)$$

If the observable has a discrete spectrum, the eigenstates are orthogonal and may be normalized as

$$\langle a_i | a_j \rangle = \delta_{ij} \quad (1.15)$$

Completeness means

$$\sum_i |a_i\rangle \langle a_i| = \hat{\mathbf{1}} \quad (1.16)$$

where  $\hat{\mathbf{1}}$  is the unit operator. In general a hermitean operator will have partly a discrete and partly a continuous spectrum. For the continuous vectors orthogonality is expressed in terms of Dirac's delta function.<sup>3</sup>

4. *If the system is in state  $|\psi\rangle$ , then the result of a measurement of a physical observable  $\hat{A}$  is one of the eigenvalues  $a_n$  of the associated hermitian operator. The probability for measuring a specific eigenvalue  $a_n$  is given by the square modulus of the scalar product of the state  $|\psi\rangle$  with the (normalized) eigen vector  $|a_n\rangle$ ,*

$$p_n = |\langle a_n | \psi \rangle|^2 \quad (1.17)$$

If the observable has a degeneracy, so that several (orthogonal) eigenvectors have the same eigenvalue, the probability is given as a sum over all eigenvectors with the same eigenvalue  $a_n$ . The expectation value of an observable  $A$  obtained by a measurement on the system is

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle . \quad (1.18)$$

and is equal to the mean value obtained by an (infinite) sequence of identical measurements performed on the system, which before each measurement is prepared in the same state  $|\psi\rangle$ .

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<sup>3</sup>For an observable with a discrete spectrum the eigenstates are normalizable and belong to the Hilbert space. For a continuous spectrum the eigenstates are non-normalizable and fall outside the Hilbert space. They can be included in an extension of the Hilbert space. Completeness holds within this extended space, but orthonormality of the vectors has to be expressed in terms of Dirac's delta function rather than the Kronecker delta.

5. An *ideal* measurement of observable  $A$  resulting in a value  $a_n$  projects the state vector from initial value  $|\psi\rangle$  to final state

$$|\psi\rangle \rightarrow |\psi'\rangle = P_n |\psi\rangle. \quad (1.19)$$

where  $P_n$  is the projection on the eigenstate  $|a_n\rangle$ , or more generally on the subspace spanned by the vectors with eigenvalue  $a_n$ .<sup>4</sup>

Note that since the projected state in general will not be normalized to unity, the state should also be multiplied by a normalization factor in order to satisfy the standard normalization condition for physical states.

The projection to the eigenstate which corresponds to the measured eigenvalue in a sense is a minimal disturbance of the system caused by the measurement. It is often referred to as the “collapse of the wave function”, and corresponds to the “collapse” of a probability function of a classical system when additional information is introduced in the description. But one should be aware of the farreaching difference of this “collapse by adding new information” in the classical and quantum description.

### 1.1.3 Coordinate representation and wave functions

A coordinate basis is a continuous set of eigenvectors of the coordinate observables  $\hat{q}_i$

$$\hat{q}_i |q\rangle = q_i |q\rangle \quad (1.20)$$

where  $q$  denotes the set of coordinates  $\{q_i\}$ . For a Cartesian set of coordinates the standard normalization is

$$\langle q'|q\rangle = \delta(q' - q) \quad (1.21)$$

where  $\delta(q' - q)$  is the  $N$ -dimensional Dirac delta-function, with  $N$  as the dimension of the configuration space. The wave functions defined over the configuration space of the system are the components of the abstract state vector  $|\psi\rangle$  on this basis,

$$\psi(q) = \langle q|\psi\rangle \quad (1.22)$$

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<sup>4</sup>Such idealized measurements are often referred to as *projective* measurements.



A general observable is in the coordinate representation specified by its matrix elements

$$A(q', q) \equiv \langle q' | \hat{A} | q \rangle \quad (1.23)$$

It acts on the wave function as an integral operator

$$\langle q | \hat{A} | \psi \rangle = \int d^N q' A(q, q') \psi(q') \quad (1.24)$$

A potential function is an example of a local observable,

$$V(q', q) = V(q) \delta(q' - q) \quad (1.25)$$

The momentum operator is quasi-local in the sense that it can be expressed as a derivative rather than an integral

$$\langle q | \hat{p}_i | \psi \rangle = -i\hbar \frac{\partial}{\partial q_i} \langle q | \psi \rangle \quad (1.26)$$

Formally we can write the matrix elements of the momentum operator as the derivative of a delta function

$$\langle q | \hat{p}_i | q' \rangle = -i\hbar \frac{\partial}{\partial q_i} \delta(q - q') \quad (1.27)$$

(Check this by use of the integration formula for observables in the coordinate representation.)

From the abstract formulation it is clear that the coordinate representation is only one of many equivalent representations of quantum states and observables. The *momentum representation* is defined quite analogous to the coordinate representation, but now with the momentum states  $|p\rangle$  as basis vectors,

$$\psi(p) = \langle p | \psi \rangle \quad (1.28)$$

The transition matrix elements between the two representations is (for Cartesian coordinates),

$$\langle q | p \rangle = (2\pi\hbar)^{-N/2} \exp\left(\frac{i}{\hbar} q \cdot p\right) \quad (1.29)$$

with  $q \cdot p = \sum_i q_i p_i$ , which means that these two (conjugate) representations are related by a Fourier transformation.

Note that often a set of continuous (generalized) coordinates is not sufficient to describe the wave function. For example, the spin variable of a particle with spin has discrete eigenvalues and does not have a direct counterpart in terms of a continuous classical coordinate. With discrete variables present the wave function can be described as a multicomponent function

$$\psi_m(q) = \langle q, m | \psi \rangle \quad (1.30)$$

where  $m$  represents the discrete variable, *e.g.* the spin component in the  $z$ -direction.

The coordinate representation and the momentum representation are only two specific examples of *equivalent representations* of the quantum system. In general the transition matrix element between two representations, defined by two orthonormal sets of basis vectors,  $\{|a_n\rangle\}$  and  $\{|b_m\rangle\}$  is,

$$U_{mn} = \langle a_n | b_m \rangle \quad (1.31)$$

and satisfies the condition

$$\sum_m U_{nm} U_{mn'}^* = \sum_m \langle a_n | b_m \rangle \langle b_m | a'_n \rangle = \delta_{nn'} \quad (1.32)$$

This means that it is a *unitary* matrix, and the corresponding representations are unitarily equivalent.

### 1.1.4 Spin-half system and the Stern Gerlach experiment

The postulates of quantum mechanics have far reaching implications. We have earlier stressed the close correspondance between the classical (phase space) theory and the quantum theory. Now we will study a special representation of the simplest quantum system, the *two-level system*, where some of the basic differences between the classical and quantum theory are apparent.

The electron spin gives an example of a *spin-half system*, and when the (orbital) motion of the electron is not taken into account the Hilbert space is reduced to a two-dimensional (complex) vector space. This two-dimensionality is directly related to the discovery of Stern and Gerlach of the two spin states of silver atoms. Their discovery is clearly incompatible with a classical model of electron spin as due to the rotation of a small body.

We focus on the Stern-Gerlach experiment as shown schematically in Figure 1. A beam of Ag atoms is produced by an oven with a small hole. Atoms with velocity sharply peaked around a given value are selected and sent through a strong

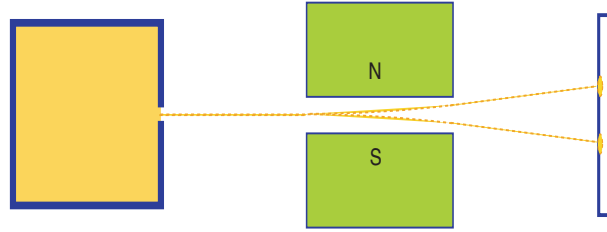


Figure 1.1: The Stern-Gerlach experiment. Atoms with spin  $1/2$  are sent in a beam from an oven. When passing between two magnets, the atoms are deflected vertically, with an angle depending on the vertical spin component. Classically a smooth distribution is expected, since there is no preferred directions for the spin. In reality only two directions are observed, consistent with the quantum prediction of quantization of the spin.

magnetic field. Due to a weak gradient in the field the particles in the beam are deflected, with a deflection angle depending on the component of the magnetic moment in the direction of the gradient. The degree of deflection is measured by registering the particles on a screen.

Let us first analyze the deflection from a classical point of view. We assume the atoms to have a magnetic moment  $\boldsymbol{\mu} = -e/(m_e c)\mathbf{S}$ , where  $\mathbf{S}$  is the intrinsic spin,  $e$  is the electron charge and  $m_e$  is the electron mass. (The main contribution to the magnetic moment comes from the outermost electron.) Between the magnets there is an approximately constant magnetic field  $\mathbf{B} = B\mathbf{e}_1$ , where  $\mathbf{e}_1$  is a unit vector in the direction of the magnetic field. The spin will here rapidly precess around the magnetic field and the average value will be in the direction of the magnetic field,  $\bar{\boldsymbol{\mu}} = m_1\mathbf{e}_1$ . There is a gradient in the magnetic field which produces a force on the atom and changes its momentum

$$\dot{\mathbf{p}} = \nabla(\boldsymbol{\mu} \cdot \mathbf{B}) \approx \mu_1 \partial_1 B \mathbf{e}_1 \quad (1.33)$$

This shows that the deflection angle is proportional to the component of the magnetic moment along the magnetic field. Since we expect the spin direction of the emitted Ag atoms to be randomly distributed in space we expect from this classical reasoning to see a continuous distribution of the atoms on the screen.

The surprising discovery of Stern and Gerlach was that there was no such continuous distribution. Instead the position of the atoms were rather strongly restricted to two spots, which according to the deflection formula would correspond

to the two values

$$\mu_1 = \pm\mu. \quad (1.34)$$

This result cannot be understood within classical theory.

To see this, let us consider two *hypothetical* situations, that instead of measuring the component  $\mu_1$  (by measuring the deflection angle in the  $\mathbf{e}_1$  direction), we had measured  $\mu_2$  along the direction  $\mathbf{e}_2$  rotated by an angle  $+120^\circ$  or  $\mu_3$  along the direction  $\mathbf{e}_3$  rotated by an angle  $-120^\circ$  relative to  $\mathbf{e}_1$ . By elementary vector addition it is clear that the sum of these (hypothetical) results would be

$$\mu_1 + \mu_2 + \mu_3 = \boldsymbol{\mu} \cdot (\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3) = 0 \quad (1.35)$$

But this is incompatible with the result of the Stern-Gerlach experiment, since the possible values  $\pm m$  cannot be restricted to the component  $\mu_1$ , but must, due to rotational symmetry, be the only values possible also for  $\mu_2$  and  $\mu_3$ .

However, the result of the Stern-Gerlach experiment is consistent with the postulates of quantum mechanics, if we assume that the spin component in a given direction is an observable with only two eigenvalues

$$\hat{S}_x |\pm\rangle_x = \pm \frac{\hbar}{2} |\pm\rangle_x \quad (1.36)$$

When the components satisfy the spin algebra

$$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z \quad (+ \text{cycl. perm.}) \quad (1.37)$$

then the component of the spin vector in *any* direction will have the two eigenvalues  $\pm\hbar/2$ .

A typical feature of the spin operator is that its components in different directions do not commute, they are *incompatible* observables. This means that they in general cannot be ascribed sharp values at the same time, since they do not have common eigenvectors. This incompatibility is directly related to the paradox met above when we ascribed a (hypothetical) sharp value to the magnetic moment in all the three directions  $\mu_1$ ,  $\mu_2$  and  $\mu_3$ . The situation that we have met here, that the components of a vector that can be *continuously* rotated has *discrete* eigenvalues, cannot be explained within the framework of classical theory.

## 1.2 Quantum Dynamics

In this section we formulate the dynamical equation of a quantum system and compare the two unitarily equivalent descriptions, the Schrödinger and Heisenberg pictures. We also examine the rather different Feynman's path integral formulation of quantum dynamics. The two-level system and the one-dimensional harmonic oscillator models are studied and we introduce coherent states description.

### 1.2.1 The Schrödinger and Heisenberg pictures

*The Schrödinger picture.*

The time evolution of an isolated quantum system is defined by the *Schrödinger equation*. Originally this was formulated as a wave equation, but it can be reformulated as a differential equation in the (abstract) Hilbert space of ket-vectors as

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (1.38)$$

With the state vector given for an initial time  $t_0$  it will determine the state vector at later times  $t$  (and also for earlier times) as long as the system stays isolated. The information about the dynamics is contained in the Hamiltonian  $\hat{H}$ , which usually can be identified with the energy observable of the system. The original Schrödinger equation, described as a wave equation can be viewed as the coordinate representation of Eq.(1.13).

For a system described by phase space variables  $(q, p)$ , the classical motion in phase space is described by the Hamiltonian function  $H((q, p))$ , which (normally) is the classical energy written as a function of  $q$  and  $p$ . Canonical quantization implies that the quantum Hamiltonian is defined by the same function of the (quantum) phase space variables,  $\hat{H} = H(\hat{q}, \hat{p})$ . However, one should note that in some cases there is an “operator order” ambiguity. This means that two classical expressions for  $H$  that are equivalent due to the commutativity of the classical phase space variables, may be mapped into two non-equivalent quantum observables, due to the non-commutativity of the quantum phase space variables. One way to resolve this ambiguity is the *Weyl ordering* which symmetrizes products in  $q$  and  $p$ .

The time evolution of the state vector can be expressed in terms of a time evolution operator  $\hat{U}(t, t_0)$ , which is a unitary operator that relates the state vector

of the system at time  $t$  with that of time  $t_0$ ,

$$\hat{\mathcal{U}}(t, t_0)|\psi(t_0)\rangle = |\psi(t)\rangle \quad (1.39)$$

The time evolution operator is determined by the Hamiltonian through the equation

$$i\hbar \frac{\partial}{\partial t} \hat{\mathcal{U}}(t, t_0) = \hat{H} \hat{\mathcal{U}}(t, t_0) \quad (1.40)$$

which follows from the Schrödinger equation(1.13).

When  $\hat{H}$  is a time-independent operator, a closed form for the time evolution can be given

$$\hat{\mathcal{U}}(t - t_0) = e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} \quad (1.41)$$

(Note that a function of an observable  $\hat{H}$ , like  $\exp(-\frac{i}{\hbar} \hat{H}(t - t_0))$  can be defined by its action on the eigenvectors  $|E\rangle$  of  $\hat{H}$ ,

$$e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} |E\rangle = e^{-\frac{i}{\hbar} E(t-t_0)} |E\rangle .) \quad (1.42)$$

If however  $\hat{H}$  is time dependent so that the operator at different times do not commute, we may use a more general integral expression

$$\hat{\mathcal{U}}(t - t_0) = \sum_{n=0}^{\infty} \left( \frac{-i}{\hbar} \right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_n) \quad (1.43)$$

where the term corresponding to  $n = 0$  is simply the unit operator  $\hat{\mathbf{1}}$ . Note that the product of the the time dependent operators  $\hat{H}(t_k)$  is a *time-ordered product*.

### *The Heisenberg picture.*

The description of the quantum dynamics given above is usually referred to as the Schrödinger picture. From the discussion of different *representations* of the quantum system we know that unitary transformations of states and observables leads to a different, but equivalent representation of the system. Thus, if we denote the states of a system by  $|\psi\rangle$  and the observables by  $A$  and make a unitary transformation  $\hat{U}$  on *all* states and *all* observables,

$$|\psi\rangle \rightarrow |\psi'\rangle = \hat{U}|\psi\rangle, \quad \hat{A} \rightarrow \hat{A}' = \hat{U} \hat{A} \hat{U}^\dagger, \quad \hat{U} \hat{U}^\dagger = \hat{\mathbf{1}}, \quad (1.44)$$

then all matrix elements are left unchanged,

$$\langle \phi' | \hat{A}' | \psi' \rangle = \langle \phi | \hat{U}^\dagger \hat{U} \hat{A} \hat{U}^\dagger \hat{U} | \psi \rangle = \langle \phi | \hat{A} | \psi \rangle \quad (1.45)$$

and since all measurable quantities can be expressed in terms of such matrix elements, the two descriptions related by a unitary transformation can be viewed as equivalent. This is true also when  $\hat{U} = \hat{U}(t)$  is a time dependent transformation.

The transition to the *Heisenberg picture* is defined by a special unitary transformation

$$\hat{U}(t) = \hat{\mathcal{U}}^\dagger(t, t_0) \quad (1.46)$$

This is the inverse of the time-evolution operator, and when applied to the time-dependent state vector of the Schrödinger picture it will simply cancel the time dependence of the state vector

$$|\psi\rangle_H = \hat{\mathcal{U}}^\dagger(t, t_0) |\psi(t)\rangle_S = |\psi(t_0)\rangle_S \quad (1.47)$$

Here we have introduced a subscript  $S$  for the vector in the Schrödinger picture and  $H$  for the Heisenberg picture. (The initial time  $t_0$  is arbitrary and is often chosen as  $t_0 = 0$ .) The time evolution is now carried by the observables, rather than the state vectors,

$$\hat{A}_H(t) = \hat{\mathcal{U}}^\dagger(t, t_0) \hat{A}_S \hat{\mathcal{U}}(t, t_0) \quad (1.48)$$

and the Schrödinger equation is replaced by the Heisenberg equation of motion

$$\frac{d}{dt} \hat{A}_H = \frac{i}{\hbar} [\hat{H}, \hat{A}_H] + \frac{\partial}{\partial t} \hat{A}_H \quad (1.49)$$

One should note the difference between the (dynamical) time dependence of the observable  $\hat{A}_H(t)$  in the Heisenberg picture and the time dependence allowed for in the expression (1.43) for the time evolution operator. The latter is due to a possible (explicit) time dependence of the Hamiltonian caused by time varying external influence on the system. This gives rise to time variation of the observables in the Schrödinger picture. In the Heisenberg equation of motion observables such a variation will give a contribution through the partial derivative in (1.49). Without such an explicit time dependence, the time evolution is caused only by the non-commutativity of the observable with the Hamiltonian.

### *The interaction picture*

A third representation of the unitary time evolution of a quantum system is the

*interaction picture* which is particularly useful in the context of time-dependent perturbation theory. The Hamiltonian is of the form

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad (1.50)$$

where  $\hat{H}_0$  is the unperturbed Hamiltonian and  $\hat{H}_1$  is the (possibly time dependent) perturbation. The eigenvalue problem of  $\hat{H}_0$  we assume can be solved and the corresponding time evolution operator is

$$\hat{\mathcal{U}}_0(t - t_0) = e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)} \quad (1.51)$$

The transition from the Schrödinger picture to the interaction picture is defined by acting with the inverse of this on the state vectors

$$|\psi(t)\rangle_I = \hat{\mathcal{U}}_0^\dagger(t, t_0) |\psi(t)\rangle_S \quad (1.52)$$

Note that the time variation of the state vector is only partly cancelled by this transformation, since the effect of the perturbation  $\hat{H}_1$  is not included. The time evolution of the observables is given by

$$\hat{A}_I(t) = \hat{\mathcal{U}}_0^\dagger(t, t_0) \hat{A}_S \hat{\mathcal{U}}_0(t, t_0) \quad (1.53)$$

This means that they satisfy the same Heisenberg equation of motion as for a system where the hamiltonian is simply  $\hat{H} = \hat{H}_0$ . The remaining part of the dynamics is described by the interaction Hamiltonian

$$\hat{H}_I(t) = \hat{\mathcal{U}}_0^\dagger(t, t_0) \hat{H}_1 \hat{\mathcal{U}}_0(t, t_0) \quad (1.54)$$

which acts on the state vectors through the (modified) Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = \hat{H}_I(t) |\psi(t)\rangle_I \quad (1.55)$$

The corresponding time evolution operator has the same form as (1.43),

$$\hat{\mathcal{U}}_I(t - t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \hat{H}_I(t_1) \hat{H}_I(t_2) \cdots \hat{H}_I(t_n) \quad (1.56)$$

and this form of the operator gives a convenient starting point for a perturbative treatment of the effect of  $\hat{H}_I$ . We shall apply this method when studying the interaction between photons and atoms in a later section.

We summarize the difference between the three pictures by the following table



	States	Operators
Schrödinger	time dependent	time independent
Heisenberg	time independent	time dependent
Interaction	time dependent	time dependent

## 1.2.2 Path integrals

Feynman's path integral method to study the dynamics of quantum systems is rather different from the methods outlined above. Instead of applying the standard description of states as vectors in a Hilbert space, it focusses directly on transition matrix elements and describe these as integrals over classical trajectories of the system. The method is well suited to describe quantum systems which can be expressed in terms of continuous variables, but for discrete variables like the intrinsic spin of the electron, it is not so well suited. (However, path integral methods which use "Grassman variables" can deal also with discrete variables.

The path integral method is used extensively in quantum field theory, and it has become a standard method which is applied in many parts of physics. For this reason it is natural to include it also here. Although the path integral method can be viewed as a fundamental approach to quantum theory, *i.e.*, a method that completely circumvent the standard description with state vectors and observables, it is often instead derived from the Hamiltonian formulation, and that is the approach we also will take.

Let us consider the time evolution of a quantum system as a wave  $\psi(q, t)$  in configuration space, where  $q = \{q_1, q_2, \dots, q_N\}$  is a set of continuous (generalized) coordinates. In the "bra-ket" notation we write it as

$$\begin{aligned}
 \psi(q, t) &= \langle q | \psi(t) \rangle \\
 &= \langle q | \hat{\mathcal{U}}(t, t_0) | \psi(t_0) \rangle \\
 &= \int d^N q' \langle q | \hat{\mathcal{U}}(t, t_0) | q' \rangle \langle q' | \psi(t_0) \rangle \\
 &\equiv \int d^N q' \langle q | t | q' t_0 \rangle \psi(t_0)
 \end{aligned} \tag{1.57}$$

The information about the dynamics of the system is encoded in the transition matrix element

$$\langle q | t | q' t_0 \rangle = \langle q | \hat{\mathcal{U}}(t, t_0) | q' \rangle \tag{1.58}$$

which gives the probability amplitude for the system which starts in the configuration  $q'$  at time  $t_0$  to end up (in a position measurement) in the configuration  $q$  at a

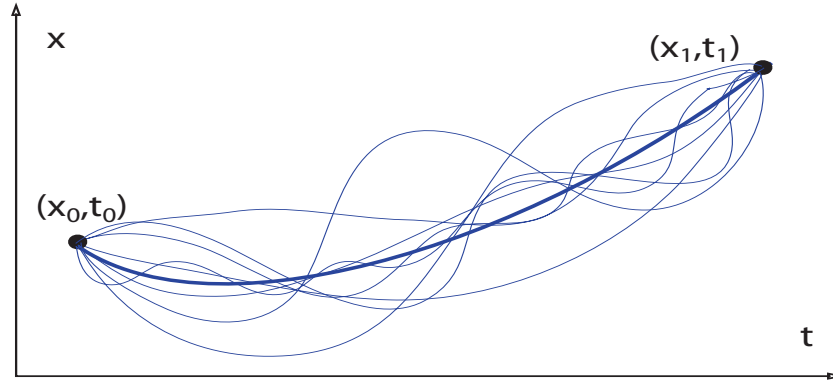


Figure 1.2: The path integral as a “sum over histories”. All possible paths between the initial point  $(x_0, t_0)$  and the final point  $(x_1, t_1)$  contribute to the quantum transition amplitude between the points. The paths close to the classical path, here shown in dark blue, tend to be most important since their contributions interfere constructively.

later time  $t$ . This amplitude is often referred to as a propagator,  $\mathcal{G}(q t, q' t_0)$  and is usually defined as being a “causal” propagator, in the sense that it only propagates forward in time.

$$\mathcal{G}(q t, q' t_0) = \begin{cases} \langle q t | q t_0 \rangle & t > t_0 \\ 0 & t < t_0 \end{cases} \quad (1.59)$$

We will see how a path integral representation of this propagator can be found. For simplicity we shall consider the case of a one-dimensional configuration space. We may visualize this as a particle moving on a line.

First we note that the propagation between  $t_0$  and  $t$  can be viewed as composed of the propagation between a series of intermediate times  $t_k, k = 0, 1, \dots, n$  with  $t_n = t$  and where  $n$  may be arbitrary large

$$\mathcal{G}(x t, x' t_0) = \int dx_{n-1} \dots \int dx_2 \int dx_1 \mathcal{G}(x t, x_{n-1} t_{n-1}) \dots \mathcal{G}(x_2 t_2, x_1 t_1) \mathcal{G}(x_1 t_1, x' t_0) \quad (1.60)$$

This follows from a repeated use of the composition rule satisfied by the time evolution operator

$$\hat{U}(t_f, t_i) = \hat{U}(t_f, t_m) \hat{U}(t_m, t_i) \quad (1.61)$$

where  $t_i, t_m$  and  $t_f$  are arbitrary chosen times. In the expression (1.60) for  $\mathcal{G}(x, t, x', t_0)$  the intermediate times  $t_1, t_2, \dots$  may also be arbitrarily distributed between  $t_0$  and  $t$ , but for simplicity we think of them as having a fixed distance

$$t_{k+1} - t_k = \Delta t \equiv (t - t_0)/n \quad (1.62)$$

To proceed we assume a specific form for the Hamiltonian,

$$\hat{H} = \frac{1}{2m} \hat{p}^2 + V(\hat{x}) \quad (1.63)$$

which is that of a particle of mass  $m$  moving in a one-dimensional potential  $V(x)$ . The propagator for a small time interval  $\Delta t$  is

$$\begin{aligned} \mathcal{G}(x, t + \Delta t, x', t) &= \langle x | e^{-\frac{i}{\hbar} \hat{H} \Delta t} | x' \rangle \\ &\approx \langle x | e^{-\frac{i}{\hbar} \frac{1}{2m} \hat{p}^2 \Delta t} e^{-\frac{i}{\hbar} V(\hat{x}) \Delta t} | x' \rangle \\ &= \langle x | e^{-\frac{i}{\hbar} \frac{1}{2m} \hat{p}^2 \Delta t} | x' \rangle e^{-\frac{i}{\hbar} V(x') \Delta t} \end{aligned} \quad (1.64)$$

We have here made use of

$$e^{i(\hat{A} + \hat{B})\Delta t} = e^{i\hat{A}\Delta t} e^{i\hat{B}\Delta t} + \mathcal{O}(\Delta t^2) \quad (1.65)$$

where  $\hat{A}$  and  $\hat{B}$  are two (non-commuting) operators and the  $\mathcal{O}(\Delta t^2)$  term comes from the commutator between  $\hat{A}$  and  $\hat{B}$ . In the present case  $\hat{A} = \hat{p}^2/(2m\hbar)$ ,  $\hat{B} = \hat{V}/\hbar$ , and these clearly do not commute. However, we will take the limit  $\Delta t \rightarrow 0$  ( $n \rightarrow \infty$ ) and this allows us to neglect the correction term coming from the commutator. The  $x$ -space matrix element of the kinetic term can be evaluated

$$\begin{aligned} \langle x | e^{-\frac{i}{\hbar} \Delta t \frac{\hat{p}^2}{2m}} | x' \rangle &= \int dp \langle x | p \rangle e^{-\frac{i}{\hbar} \frac{p^2}{2m} \Delta t} \langle p | x' \rangle \\ &= \int \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar} p(x-x')} e^{-\frac{i}{\hbar} \frac{p^2}{2m} \Delta t} \\ &= \int \frac{dp}{2\pi\hbar} e^{-\frac{i}{\hbar} \frac{\Delta t}{2m} (p - m \frac{x-x'}{\Delta t})^2} e^{\frac{i}{\hbar} \Delta t \frac{m}{2} \left(\frac{x-x'}{\Delta t}\right)^2} \\ &= N_{\Delta t} e^{i \frac{m(x-x')^2}{2\hbar\Delta t}}. \end{aligned} \quad (1.66)$$

where  $N_{\Delta t}$  is an  $x$ -independent normalization constant,

$$\begin{aligned} N_{\Delta t} &= \int \frac{dp}{2\pi\hbar} e^{-i \frac{\Delta t}{2m\hbar} (p - m \frac{x-x'}{\Delta t})^2} \\ &= \int \frac{dp}{2\pi\hbar} e^{-i \frac{\Delta t}{2m\hbar} p^2} \end{aligned} \quad (1.67)$$

This last expression may look somewhat mysterious, since the integral does not seem to converge for large  $p$ . However, let us focus on a related integral, the Gaussian integral with a *real* coefficient in the exponent. This is convergent,

$$\int_{-\infty}^{+\infty} dp e^{-\lambda p^2} = \sqrt{\frac{\pi}{\lambda}} \quad (1.68)$$

Now we shall simply assume that the correct expression for  $N_{\Delta t}$  is found by making an analytic continuation of this result to imaginary  $\lambda$ . This gives

$$N_{\Delta t} = \sqrt{\frac{m}{2\pi i \hbar \Delta t}} \quad (1.69)$$

For the matrix element of the time evolution operator we now get,

$$\langle x | e^{-\frac{i}{\hbar} \Delta t H} | x' \rangle = N_{\Delta t} e^{i \frac{m(x-x')^2}{2\hbar \Delta t}} e^{-\frac{i}{\hbar} V(x') \Delta t} \quad (1.70)$$

and with  $x' \rightarrow x_k$  and  $x \rightarrow x_{k+1}$  this can be used for each term in the factorized expression (1.60) for the propagator. The result is

$$\mathcal{G}(x t, x' t_0) = (N_{\Delta t})^n \int dx_{n-1} \dots \int dx_2 \int dx_1 e^{i \frac{\Delta t}{\hbar} \sum_{k=0}^n \left[ \frac{m}{2} \left( \frac{x_{k+1} - x_k}{\Delta t} \right)^2 - V(x_k) \right]} \quad (1.71)$$

The exponent can be further simplified in the limit  $n \rightarrow \infty$ ,

$$\frac{i}{\hbar} \Delta t \sum_{k=0}^n \left[ \frac{m}{2} \left( \frac{x_{k+1} - x_k}{\Delta t} \right)^2 - V(x_k) \right] \rightarrow \frac{i}{\hbar} \int_{t_0}^t dt \left[ \frac{1}{2} m \left( \frac{dx}{dt} \right)^2 - V(x) \right] \quad (1.72)$$

where we have now assumed that the sequence of intermediate positions  $x_k$  (which we integrate over) in the limit  $n \rightarrow \infty$  defines a differentiable curve. The expression we arrive at can be identified as the (classical) action associated with the curve defined by the positions  $x_k$  as functions of time,

$$\mathcal{S}[x(t)] = \int_{t_0}^t L(x, \dot{x}) = \int_{t_0}^t \left( \frac{1}{2} m \dot{x}^2 - V(x) \right) \quad (1.73)$$

In the continuum limit ( $n \rightarrow \infty$ ) we therefore write the propagator as

$$\mathcal{G}(x t, x' t_0) = \int \mathcal{D}[x(t)] e^{\frac{i}{\hbar} \mathcal{S}[x(t)]} \quad (1.74)$$

The meaning of this expression is that we integrate over all possible paths  $x(t)$  which interconnect the initial point  $x' = x(t_0)$  with the final point  $x = x(t)$ , with a complex weight factor determined by the classical action of the path. Note that the discretized expression (1.71), with the correct normalization factors included can now be thought of as *defining* the integration measure  $\mathcal{D}[x(t)]$  of the path integral. However, we have noticed some complications in the path integral expression. Thus, it is difficult to control the oscillations in the factor  $e^{\frac{i}{\hbar}S[x(t)]}$  unless we impose some method (analytic continuation) to damp the exponential factor.

In the above derivation we have used the Hilbert space description of quantum mechanics as starting point and discretized the time variable in order to approach a situation where the intermediate positions define a continuous curve. However, the path integral formulation, as originally discussed by Feynman, is usually considered to be a fundamental formulation of quantum mechanics, not limited to the discrete formulation used here. This path integral description has several appealing features. The quantum evolution can be thought of as a sum over “all possible histories” of the system, not only the one that is dynamically possible in a classical theory. In this sense it is quite general, not limited to a system with one dimension or with a given form of the Hamiltonian. But in general we should expect that to give a precise definition to the integration measure may be highly non-trivial. Even in the one-dimensional case we meet normalization factors that diverge in the continuum limit.

### 1.2.3 Path integral for a free particle

The discretization of time is convenient to discuss the connection between the Hamiltonian formulation and the path integral formulation of quantum mechanics. However, the discretization is not faithful to the idea of the path integral as a sum over contributions from (continuous) paths, since the points for different times are integrated over independently. We will here try out another formulation which respects more the idea of paths, and apply it to the example of a free particle.

We then consider a path as a (continuous) curve  $x(t)$  which connects an initial point  $x_0 = x(t_0)$  with a final point  $x_1 = x(t_1)$ , and denote the time difference as  $T = t_1 - t_0$ . With the endpoints of the curve fixed, an arbitrary curve between these points can be written as

$$x(t) = x_{cl}(t) + \sum_{n=1}^{\infty} c_n \sin(n\pi \frac{t - t_0}{T}) \quad (1.75)$$

where  $x_{cl}(t)$  is a solution of the classical equation of motion with the given end

points. The deviation from the classical curve is expanded in a Fourier series. We shall now interpret the path integral as an independent integration over each Fourier components  $c_n$ . Note that for arbitrarily chosen coefficient we now have a continuous curve.

The action for a free particle is given by

$$\begin{aligned}
S[x(t)] &= \int_{t_0}^{t_1} dt \frac{1}{2} m \dot{x}^2 \\
&= S[x_{cl}(t)] + \frac{1}{2} m \int_{t_0}^{t_1} dt \sum_{nn'} c_n c_{n'} \frac{nm\pi^2}{T^2} \cos(n\pi \frac{t-t_0}{T}) \cos(m\pi \frac{t-t_0}{T}) \\
&= S[x_{cl}(t)] + \frac{1}{2} m \int_{t_0}^{t_1} dt \sum_{nn'} c_n c_{n'} \frac{nn'\pi^2}{T^2} \cos(n\pi \frac{t-t_0}{T}) \cos(n'\pi \frac{t-t_0}{T}) \\
&= S[x_{cl}(t)] + \frac{1}{2} m \int_0^\pi d\phi \sum_{nn'} c_n c_{n'} \frac{nn'\pi^2}{T} \cos(n\phi) \cos(n'\phi) \\
&= S[x_{cl}(t)] + \frac{m\pi^2}{4T} \sum_n n^2 c_n^2 \tag{1.76}
\end{aligned}$$

For the propagator this gives

$$\begin{aligned}
\mathcal{G}_0(x_1 t_1, x_0 t_0) &= \int \mathcal{D}[x(t)] e^{\frac{i}{\hbar} S[x(t)]} \\
&= \mathcal{N} e^{\frac{i}{\hbar} S[x_{cl}(t)]} \prod_n \int dc_n e^{i \frac{m\pi^2}{4T\hbar} n^2 c_n^2} \tag{1.77}
\end{aligned}$$

In the last expression we have interpreted the path integral as an integral over the Fourier coefficients  $c_n$ , but we have also introduced a normalization factor, which at this stage is unspecified. Also note that the integrals have to be made well-defined by the same trick as before, by changing the imaginary coefficient to a real one. This gives

$$\begin{aligned}
\mathcal{G}_0(x_1 t_1, x_0 t_0) &= \mathcal{N} e^{\frac{i}{\hbar} S[x_{cl}(t)]} \prod_n \left( \frac{2}{n} \sqrt{\frac{iT\hbar}{m\pi}} \right) \\
&= \mathcal{N}' e^{\frac{i}{\hbar} S[x_{cl}(t)]} \\
&= \mathcal{N}' e^{\frac{i}{\hbar} \frac{1}{2} m \left( \frac{x_1 - x_0}{T} \right)^2} \tag{1.78}
\end{aligned}$$

Note that the product is not well-defined separately from  $\mathcal{N}$  and is absorbed in the total normalization factor  $\mathcal{N}'$ , which we have not been able to determine. This factor depends on the precise definition of the path integral.

We could alternatively have used the discrete time definition to derive the propagator, and this would also have determined the normalization factor  $\mathcal{N}'$ . However, in this simple case the propagator can be evaluated directly, and we use the expression to check our result from the path integral formulation,

$$\begin{aligned}
 \mathcal{G}_0(x_1, t_1, x_0, t_0) &= \langle x_1 | e^{\frac{i}{\hbar} \frac{p^2}{2m} T} | x_0 \rangle \\
 &= \int dp e^{\frac{i}{\hbar} \frac{p^2}{2m} T} \langle x_1 | p \rangle \langle p | x_0 \rangle \\
 &= \int \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar} [\frac{p^2}{2m} T + p(x_0 - x_1)]} \\
 &= \sqrt{\frac{m}{2\pi i \hbar T}} e^{i \frac{m(x_0 - x_1)^2}{2\hbar T}} \quad (1.79)
 \end{aligned}$$

This agrees with the expression (1.78) and determines  $\mathcal{N}'$ . We note that the exponential factor is determined by the action of the classical path between the initial and final points. A similar expression for the propagator, involving the action of the classical path, can be found for any action that is quadratic in both  $q$  and  $\dot{q}$ .

### 1.2.4 The classical theory as a limit of the path integral

One of the advantages of the Feynman path integral is its close relation to the classical theory. This is clear already from the formulation in terms of the classical Lagrangian of the system. Let us formulate the path integral in the general form

$$\begin{aligned}
 \mathcal{G}(q_f, t_f, q_i, t_i) &= \int \mathcal{D}[q(t)] e^{\frac{i}{\hbar} \mathcal{S}[q(t)]} \\
 &= \int \mathcal{D}[q(t)] \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} L(q, \dot{q}) dt\right) \quad (1.80)
 \end{aligned}$$

where the Lagrangian  $L(q, \dot{q})$  depends on a set of generalized coordinates  $q = \{q_i\}$  and their derivatives  $\dot{q} = \{\dot{q}_i\}$ . We note from this formulation that variations in the path  $q(t)$  that give rise to rapid variations in the action  $\mathcal{S}[q(t)]$  tend to give contributions to the path integral that add destructively. This is so because of the rapid change in the complex phase of the integrand.

The classical limit of a quantum theory is often thought of as a formal limit  $\hbar \rightarrow 0$ . From the expression for the path integral we note that smaller  $\hbar$  means

more rapid variation in the complex phase. This indicates that in the classical limit most of the paths will not contribute to the path integral, since variations in the action from the neighbouring paths will tend to “wash out” the contribution. The only paths which retain their importance are those where the action is stationary, *i.e.*, it does not change under small variations in the path.

The stationary paths are characterized by  $\delta\mathcal{S} = 0$ , with

$$\begin{aligned}\delta\mathcal{S} &= \int_{t_i}^{t_f} \left( \frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right) dt \\ &= \int_{t_i}^{t_f} \left[ \frac{\partial L}{\partial q_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) \right] \delta q_i dt\end{aligned}\quad (1.81)$$

In this expression  $\delta q_i$  denotes an (infinitesimal) variation in the path, and  $\delta \dot{q}_i$  the corresponding variation in the time derivative. The last expression in (1.81) is found by a partial integration and applying the constraint on the variation that it vanishes in the end points,  $\delta q_i(t_i) = \delta q_i(t_f) = 0$ . This constraint follows from the fact that the end points of the paths are fixed by the coordinates of the propagator (1.80).

Thus, the important paths are those with stationary action, and these satisfy the Euler-Lagrange equations,

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) = 0 \quad , i = 1, 2, \dots, N \quad (1.82)$$

since  $\delta\mathcal{S}$  should be 0 for *all* (infinitesimal) variations. In a Lagrangian formulation of the classical theory of a system with dynamics determined by  $L(q, \dot{q})$ , these are exactly the classical equations of motion. A simple example is provided by a particle moving in a three-dimensional potential, where

$$L(\vec{r}, \dot{\vec{r}}) = \frac{1}{2} \dot{\vec{r}}^2 - V(\vec{r}) \quad (1.83)$$

In this case it is straight forward to check that the Euler-Lagrange equations give the Newton's 2. law, in the form

$$m\ddot{\vec{r}} = -\vec{\nabla}V(\vec{r}) \quad (1.84)$$



## 1.3 Two-level system and harmonic oscillator

The (one-dimensional) harmonic oscillator is an important system to study, both in the context of classical and quantum physics. One reason is that in many respects it is the simplest system with non-trivial dynamics to study, and physicists always like to reduce more complicated problems to harmonic oscillators if possible. There are also many physical systems that are well described as harmonic oscillators. All periodic motions close to (stable) equilibrium can be viewed as approximate harmonic oscillator motions, and the modes of free (non-interacting) fields can be viewed, both classically and quantum mechanically, as harmonic oscillators.

Even if the harmonic oscillator, in many respects, can be regarded as the simplest (most fundamental) system to study, there is a quantum mechanical system that in a sense is even more fundamental, the two-level system. A special realization of this is the spin-half system already discussed. There are also other physical systems which, to a good approximation, can be regarded as a two level system. One example is an atomic system with two (almost) degenerate ground states, where the dynamics can be described as a transition (tunneling) between these two states. Atomic clocks are quantum systems of this type. Also for transitions between atoms with many energy levels often only two of the levels will be active in the transition and a two-level model is adequate.

As opposed to the harmonic oscillator there is no classical analogue to the quantum two-level system. Classical spin does of course exist, but that correspond to many-level “high-spin” quantum systems rather than to the simplest spin-half system. In recent years the interest for two-level systems have increased with the interest for “quantum information” since the fundamental “qubit” is described by a two-level system.

Inn this section we will study these two fundamental systems, first the two-level system.

### 1.3.1 The two-level system

The Hilbert space of this system is two-dimensional. Let us denote by  $\{|k\rangle, k = 0, 1\}$  the basis vectors of an arbitrarily chosen orthonormal basis. Any state vector can be represented as a two-component, complex matrix  $\Psi$ ,

$$|\psi\rangle = \sum_{k=0}^1 \psi_k |k\rangle \Rightarrow \Psi = \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \quad (1.85)$$

An operator  $\hat{A}$  acting in this space has four independent components and can be represented as a  $2 \times 2$  matrix  $\mathbf{A}$ ,

$$\hat{A}|k\rangle = \sum_l A_{lk} |l\rangle \Rightarrow \mathbf{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad (1.86)$$

It can be expressed in terms of the unit matrix and the Pauli spin matrices as,

$$\mathbf{A} = a_0 \mathbf{1} + \sum_m a_m \sigma_m \quad (1.87)$$

with

$$\begin{aligned} a_0 &= \frac{1}{2}(A_{11} + A_{22}), & a_1 &= \frac{1}{2}(A_{12} + A_{21}), \\ a_2 &= \frac{i}{2}(A_{12} - A_{21}), & a_3 &= \frac{1}{2}(A_{11} - A_{22}) \end{aligned} \quad (1.88)$$

When  $\hat{A}$  is hermitean, all the coefficients  $a_k$  are real. The Pauli matrices are represented as

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

They define the fundamental commutator relations of the observables of the two level system,

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \quad (1.89)$$

where  $\epsilon_{ijk}$  is the Levi-Civita symbol, which is totally antisymmetric in the indices  $ijk$  and satisfy  $\epsilon_{123} = 1$ . The Pauli matrices also satisfy the *anti-commutation* relations

$$\{\sigma_i, \sigma_j\} = 0 \quad (1.90)$$

Let us consider a general (“rotated”) Pauli matrix

$$\sigma_n = \mathbf{n} \cdot \boldsymbol{\sigma} = \begin{pmatrix} \cos \theta & e^{-i\phi} \sin \theta \\ e^{i\phi} \sin \theta & -\cos \theta \end{pmatrix} \quad (1.91)$$

with  $\mathbf{n}$  as a (three-component) unit vector. The two eigenstates of this operator are

$$|\mathbf{n}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}, \quad |-\mathbf{n}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-i\phi} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} \quad (1.92)$$

with  $|\mathbf{n}\rangle$  as the “spin up” state in the  $\mathbf{n}$  direction and  $|-\mathbf{n}\rangle$  as the “spin down” vector. We note that *any* vector in the two-dimensional state space can, up to a normalization factor, be written in the form of  $|\mathbf{n}\rangle$  for some vector  $\mathbf{n}$ . This implies that the *physically distinct* state vectors of the two-level system has the topology of a two-dimensional sphere. They can be identified uniquely by the three-dimensional unit vector  $\mathbf{n}$ . Note however, the difference with a classical configuration space with the topology of a sphere. In the latter case all the points on the sphere correspond to independent configurations. In the quantum two-level model, there are only two *independent states*,  $|0\rangle$  (the “south pole”) and  $|1\rangle$  (the “north pole”). All other points on the sphere correspond to linear superpositions of these.

### 1.3.2 Spin dynamics and magnetic resonance

The spin realization of the two-level system has already been briefly discussed in the context of the Stern-Gerlach experiment. We here consider the spin dynamics in a constant magnetic field in more detail and proceed to show how to solve a time-dependent problem, where the spin is subject to a periodic field.<sup>5</sup>

The basic observables of the spin half-system are the three components of the spin vector

$$\hat{\mathbf{S}} = (\hbar/2)\boldsymbol{\sigma} \quad (1.93)$$

where  $\boldsymbol{\sigma}$  is a vector matrix with the three Pauli matrices as components. They correspond to the three space components of the spin vector.

The observable  $\hat{\mathbf{S}}$  we will identify as the spin of an electron. The corresponding magnetic moment is given by

$$\boldsymbol{\mu} = \frac{e}{m_e c} \hat{\mathbf{S}} \quad (1.94)$$

where  $e$  is the electron charge and  $m_e$  is the electron mass. The spin Hamiltonian is

$$\hat{H} = -\frac{e}{m_e c} \mathbf{B} \cdot \hat{\mathbf{S}}. \quad (1.95)$$

The Heisenberg equation of motion for the spin, which follows from (1.49) is

$$\frac{d}{dt} \hat{\mathbf{S}}_H = \omega_c \mathbf{n} \times \hat{\mathbf{S}}_H, \quad (1.96)$$

---

<sup>5</sup>The effect of a magnetic field on the electron spin, with its corresponding changes in the atomic levels, is usually referred to as the *Zeeman effect*.

where

$$\omega_c = -\frac{eB}{m_e c}. \quad (1.97)$$

and  $\hat{\mathbf{n}}$  is a unit vector  $\mathbf{B} = B\hat{\mathbf{n}}$ .<sup>6</sup> Eq.(1.96) has exactly the same form as the classical spin precession equation with  $\omega_c$  as the precession frequency. A natural interpretation is then that the quantum spin precesses in the magnetic field in the same way as the classical spin. However, as our discussion of the Stern-Gerlach experiment has shown the non-commutativity of the different components of  $\hat{\mathbf{S}}$  makes the quantum spin variable qualitatively different from the classical spin.

The expression for the Hamiltonian (1.95) can be simplified by the choice of coordinate axes. If we choose the (1,2,3) components of the Pauli spin matrices to correspond to the  $(x, y, z)$  directions in space, and  $e\mathbf{B}$  to point in the positive  $z$ -direction, the Hamiltonian gets the form

$$\begin{aligned} \hat{H} &= -\frac{e}{m_e c} B \hat{S}_z \\ &= \frac{1}{2} \hbar \omega_c \sigma_z. \end{aligned} \quad (1.98)$$

The corresponding time evolution operator is

$$\hat{U}(t) = e^{-\frac{i}{\hbar} \hat{H} t} = e^{-\frac{i}{2} \omega_c \sigma_z t} \quad (1.99)$$

and shows explicitly the rotation around the  $z$ -axis.

We now proceed to examine a two-state problem with a *time-dependent* Hamiltonian, which is directly relevant for the so-called *spin magnetic resonance*. The system is the spin variable of a (bound) electron in a magnetic field  $\mathbf{B}$  which now, in addition to a constant part has an oscillating part,

$$\mathbf{B} = B_0 \mathbf{k} + B_1 (\cos \omega t \mathbf{i} + \sin \omega t \mathbf{j}). \quad (1.100)$$

Both  $B_0$  and  $B_1$  are constants. The oscillating field is due to a circularly polarized electromagnetic field interacting with the electron.

The time variation of  $\mathbf{B}$  gives rise to a time-dependent Hamiltonian. Usually a time-dependent problem like this is highly non-trivial, and can only be solved

---

<sup>6</sup> $\omega_c$  may be chosen to be positive by choosing  $eB$  negative. For the electron, with  $e < 0$  this means choosing  $\hat{\mathbf{n}}$  in the direction of  $B$ , so that  $B$  is positive. For a particle with positive charge  $e$   $\hat{\mathbf{n}}$  is chosen in the *opposite* direction of  $\mathbf{B}$ , so that  $B$  is negative.

within some approximation scheme. But the present problem can be solved exactly. We show this by rewriting the Hamiltonian in the following form

$$\begin{aligned}
\hat{H} &= -\frac{e}{m_e c} [B_0 \mathbf{k} + B_1 (\cos \omega t \mathbf{i} + \sin \omega t \mathbf{j})] \cdot \hat{\mathbf{S}} \\
&= -\frac{e}{m_e c} [B_0 \hat{S}_z + B_1 (\cos \omega t \hat{S}_x + \sin \omega t \hat{S}_y)] \\
&= -\frac{e}{m_e c} e^{-\frac{i}{\hbar} \omega t \hat{S}_z} [B_0 \hat{S}_z + B_1 \hat{S}_x] e^{\frac{i}{\hbar} \omega t \hat{S}_z}
\end{aligned} \tag{1.101}$$

where the last expression follows from the commutation relations between the components of  $\hat{\mathbf{S}}$ . This form for the Hamiltonian shows that it can be transformed to a time-independent form by a unitary transformation. In fact, the Hamiltonian can be transformed into the spin Hamiltonian (1.95) that we have already discussed.

In order to show this we perform the *time-dependent* transformation

$$|\psi(t)\rangle \rightarrow |\psi(t)\rangle_1 = e^{\frac{i}{\hbar} \omega t \hat{S}_z} |\psi(t)\rangle \tag{1.102}$$

The transformed state vector satisfies the modified Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle_1 = [e^{\frac{i}{\hbar} \omega t \hat{S}_z} \hat{H} e^{-\frac{i}{\hbar} \omega t \hat{S}_z} - \omega \hat{S}_z] |\psi(t)\rangle_1 \tag{1.103}$$

This is the Schrödinger equation for a time-independent Hamiltonian of the form

$$\begin{aligned}
\hat{H}_1 &= e^{\frac{i}{\hbar} \omega t \hat{S}_z} \hat{H} e^{-\frac{i}{\hbar} \omega t \hat{S}_z} - \omega \hat{S}_z \\
&= -\frac{e}{m_e c} [B_0 \hat{S}_z + B_1 \hat{S}_x] - \omega \hat{S}_z \\
&= \frac{1}{2} \hbar [(\omega_0 - \omega) \sigma_z + \omega_1 \sigma_x]
\end{aligned} \tag{1.104}$$

where we have introduced  $\omega_0 = -eB_0/(m_e c)$  and  $\omega_1 = -eB_1/(m_e c)$ . The transformation above can be interpreted as changing to a rotating reference frame, where the magnetic field looks time-independent.

If we now introduce the parameters

$$\Omega = \sqrt{(\omega_0 - \omega)^2 + \omega_1^2} \tag{1.105}$$

and

$$\cos \theta = \frac{\omega_0 - \omega}{\sqrt{(\omega_0 - \omega)^2 + \omega_1^2}}, \quad \sin \theta = \frac{\omega_1}{\sqrt{(\omega_0 - \omega)^2 + \omega_1^2}} \tag{1.106}$$

the transformed Hamilton gets the form

$$\hat{H}_1 = \frac{1}{2}\hbar\Omega (\cos\theta\sigma_z + \sin\theta\sigma_x) \quad (1.107)$$

It has the same form as (1.98) except the magnetic field is rotated by an angle  $\theta$  relative to the  $z$ -axis. Thus, the time evolution in the transformed frame is simply

$$\hat{U}_1(t) = e^{-\frac{i}{2}\Omega t (\cos\theta\sigma_z + \sin\theta\sigma_x)} \quad (1.108)$$

Now the time evolution operator, in the original frame, can be found by applying the time dependent transformation in reverse,

$$\begin{aligned} \hat{U}(t) &= e^{-\frac{i}{2}\omega t\sigma_z}\hat{U}_1(t) \\ &= e^{-\frac{i}{2}\omega t\sigma_z}e^{-\frac{i}{2}\Omega t(\cos\theta\sigma_z + \sin\theta\sigma_x)} \end{aligned} \quad (1.109)$$

which in matrix form is

$$\begin{aligned} \hat{U}(t) &= \begin{pmatrix} e^{-\frac{i}{2}\omega t} & 0 \\ 0 & e^{\frac{i}{2}\omega t} \end{pmatrix} \begin{pmatrix} \cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2} & -i\sin\theta\sin\frac{\Omega t}{2} \\ -i\sin\theta\sin\frac{\Omega t}{2} & \cos\frac{\Omega t}{2} + i\cos\theta\sin\frac{\Omega t}{2} \end{pmatrix} \\ &= \begin{pmatrix} (\cos\frac{\omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2})e^{-\frac{i}{2}\omega t} & -i\sin\theta\sin\frac{\Omega t}{2}e^{-\frac{i}{2}\omega t} \\ -i\sin\theta\sin\frac{\Omega t}{2}e^{\frac{i}{2}\omega t} & (\cos\frac{\Omega t}{2} + i\cos\theta\sin\frac{\Omega t}{2})e^{\frac{i}{2}\omega t} \end{pmatrix} \end{aligned} \quad (1.110)$$

The above result shows that the time-varying magnetic field  $\mathbf{B}_1$  will induce oscillations in the spin between the two eigenstates  $|0\rangle$  and  $|1\rangle$  of the time-independent spin Hamiltonian  $\hat{H}_0 = -\hbar eB_0/(m_e c)\sigma_z$ ,

$$|\psi(t)\rangle = c_0(t)|0\rangle + c_1(t)|1\rangle \quad (1.111)$$

Let us choose as initial conditions,  $c_0(0) = 1, c_1(0) = 0$ , which means that the spin starts in the ground state of  $\hat{H}_0$ . This gives,

$$\begin{aligned} c_0(t) &= (\cos\frac{\omega t}{2} + i\cos\theta\sin\frac{\Omega t}{2})e^{\frac{i}{2}\omega t} \\ c_1(t) &= -i\sin\theta\sin\frac{\Omega t}{2}e^{\frac{i}{2}\omega t} \end{aligned} \quad (1.112)$$

The time-dependent occupation probability of the upper level is

$$|c_1(t)|^2 = \sin^2\theta\sin^2\frac{\Omega t}{2} \quad (1.113)$$

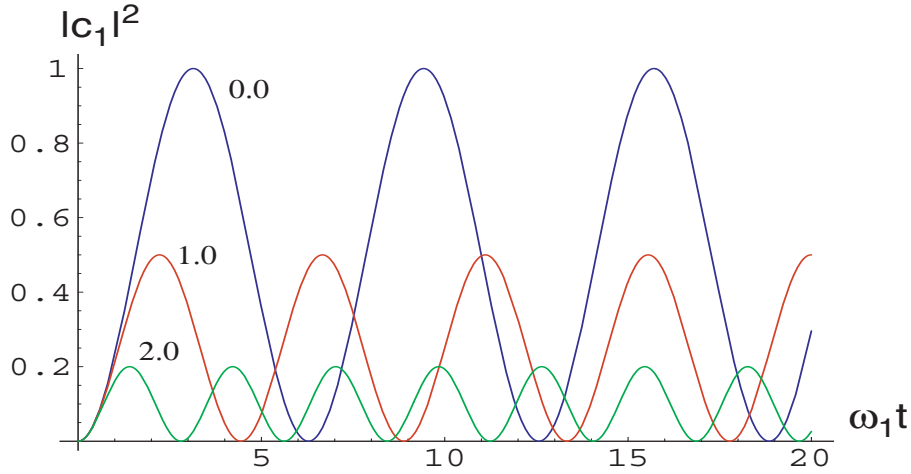


Figure 1.3: Rabi oscillations in a two-level system, caused by an oscillating field. The oscillations in the occupation of the upper level are shown as function of time. The oscillations are shown for three different values of the detuning parameter  $(\omega_0 - \omega)/\omega_1$ .

The amplitude of the oscillations is

$$\sin^2 \theta = \frac{\omega_1^2}{(\omega_0 + \omega)^2 - \omega_1^2} \quad (1.114)$$

The expression shows a *resonance effect*, when the frequency of the oscillating field matches the energy difference between the two levels,  $\omega = \omega_0$ . For this frequency the maximum value of  $|c_1(t)|^2$  is 1, which means that there is a complete transitions between the two levels  $|0\rangle$  and  $|1\rangle$  during the oscillations. The frequency of the oscillations is

$$\Omega = \sqrt{(\omega_0 - \omega)^2 + \omega_1^2} \quad (1.115)$$

with a resonance value

$$\Omega_{res} = |\omega_1| = \left| \frac{eB_1}{m_e c} \right| \quad (1.116)$$

Thus, the frequency depends on the amplitude of the oscillating field. In Fig.1.3.2 the oscillations are shown as a function of time

The model studied here has important applications in the context of *nuclear magnetic resonance* and in atomic beam physics. It is often referred to as the *Rabi effect*, and the oscillation frequency is called the *Rabi frequency*.

### 1.3.3 Harmonic oscillator and coherent states

The Hamiltonian of a one-dimensional (quantum) harmonic oscillator we write in the standard way as

$$\hat{H} = \frac{1}{2m}(\hat{p}^2 + m^2\omega^2\hat{x}^2) \quad (1.117)$$

which means that it is realized as the energy observable of a particle with mass  $m$  in the oscillator potential  $\hat{V} = (\omega^2/2m)\hat{x}^2$ .

The most elegant approach to solve the energy eigenvalue problem is the algebraic method shown in all introductory text books on quantum mechanics. It is based on the closed commutator algebra formed by the operators  $\hat{x}$ ,  $\hat{p}$  and  $\hat{H}$ ,<sup>7</sup>

$$[\hat{x}, \hat{p}] = i\hbar, \quad [\hat{x}, \hat{H}] = i\frac{\hbar}{m}\hat{p}, \quad [\hat{p}, \hat{H}] = -i\hbar m\omega^2\hat{x} \quad (1.118)$$

This is conveniently reformulated in terms of the *raising* and *lowering* operators

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p}), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} - i\hat{p}) \quad (1.119)$$

which gives

$$\hat{H} = \frac{1}{2}\hbar\omega(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) \quad (1.120)$$

The commutator algebra is now reformulated as

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad [\hat{H}, \hat{a}] = -\hbar\omega, \quad [\hat{H}, \hat{a}^\dagger] = \hbar\omega \quad (1.121)$$

We briefly summarize the construction of energy eigen states. Since  $\hat{H}$  is a positive definite operator, there is a lowest energy state, which is annihilated by  $\hat{a}$ ,

$$\hat{a}|0\rangle = 0 \quad (1.122)$$

---

<sup>7</sup>The commutator algebra of the observables defines a *Lie algebra*. When the Hamiltonian belongs to such a finite-dimensional Lie algebra, the general methods for finding *representations* of the Lie algebra can be used to construct the eigenstates and find the eigenvalues of the Hamiltonian.)



The repeated application of  $\hat{a}^\dagger$  on this state generate a series of states  $|n\rangle$ ,  $n = 0, 1, 2, \dots$ , which according to the commutator with  $\hat{H}$  all are energy eigenstates. These states form a complete set of states in the Hilbert space. The explicit action of the operators on these states follows from the algebraic relations and are here summarized as

$$\begin{aligned}\hat{a}|n\rangle &= \sqrt{n}|n-1\rangle \\ \hat{a}^\dagger|n-1\rangle &= \sqrt{n}|n\rangle, \\ \hat{H}|n\rangle &= \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle\end{aligned}\quad (1.123)$$

Expansion of state vectors  $|\psi\rangle$  in the orthonormal basis  $\{|n\rangle\}$  defines a representation which we shall refer to as the  $n$ -representation. The transition between this representation and the standard coordinate (or  $x$ -) representation is defined by the matrix elements

$$\langle x|n\rangle \equiv \psi_n(x) \quad (1.124)$$

For given  $n$  this corresponds to the energy eigenfunction in the coordinate representation. We refer to standard treatments of the harmonic oscillator, where these eigenstates are expressed in terms of Hermite polynomials.

After this brief reminder on standard treatments of the harmonic oscillator, we turn to the main theme of this section, which is discussion of the so-called *coherent states*. These are defined as the eigenstates of the annihilation operator  $\hat{a}$ ,

$$\hat{a}|z\rangle = z|z\rangle \quad (1.125)$$

What is unusual about this definition of states is that  $\hat{a}$  is not a hermitian operator (and therefore not an observable in the usual sense). However, the states  $|z\rangle$  defined in this way do form a complete set, in fact an overcomplete set, and they define a new representation, the *coherent state representation* with many useful properties.

Note that, since  $\hat{a}$  is non-hermitian, the eigenvalues  $z$  will in general be complex rather than real. Based on the relation between  $\hat{a}$  with  $\hat{x}$  and  $\hat{p}$  it is useful to write  $z$  as,

$$z = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x_c + ip_c) \quad (1.126)$$

This indicates that  $z$  can be interpreted as a complex *phase space* variable, with  $\text{Re}z$  proportional to  $x$  and  $\text{Im}z$  proportional to  $p$ . However, since  $x$  has already

been used for the eigenvalues of  $\hat{x}$  and  $p$  for  $\hat{p}$ , we have introduced  $x_c$  and  $p_c$  for the phase-space components of  $z$ . Such a distinction is necessary, since  $|z\rangle$  is not an eigenstate for  $\hat{x}$  and  $\hat{p}$ , although both  $x$  and  $p$  will be strongly peaked around  $x_c$  and  $p_c$ , respectively. Expressed in terms of the expectation values we have have

$$\langle z|\hat{a}|z\rangle = z, \quad \langle z|\hat{a}^\dagger|z\rangle = z^* \quad (1.127)$$

which for the expectation values of position and momentum gives

$$\langle x\rangle_z = x_c, \quad \langle p\rangle_z = p_c \quad (1.128)$$

To study the coherent states further we first focus on the ground state of the harmonic oscillator which is a coherent state with  $z = 0$ , as follows from (1.122). For the ground state we have the following expectation values for  $x$  and  $p$ , in the ground state,

$$\begin{aligned} \langle x\rangle_0 &= \langle p\rangle_0 = 0 \\ \langle x\rangle_0^2 &= \frac{\hbar}{2m\omega} \langle 0|(\hat{a} + \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger)|0\rangle = \frac{\hbar}{2m\omega} \\ \langle p\rangle_0^2 &= \frac{m\omega\hbar}{2} \langle 0|(\hat{a} - \hat{a}^\dagger)(\hat{a} - \hat{a}^\dagger)|0\rangle = \frac{m\omega\hbar}{2} \end{aligned} \quad (1.129)$$

From this follows that the uncertainties in  $x$  and  $p$  for the ground state satisfy

$$\Delta x_0^2 \Delta p_0^2 = \frac{\hbar}{2m\omega} \frac{m\omega\hbar}{2} = \frac{\hbar^2}{4} \quad (1.130)$$

This is the minimum value for the product allowed by Heisenberg's uncertainty principle. Thus, the ground state is a *minimum uncertainty* state. A similar calculation for the excited states show that they are not,

$$\Delta x_n^2 \Delta p_n^2 = \frac{\hbar^2}{4} (2n + 1)^2 \quad (1.131)$$

We shall proceed to show that all *coherent states are minimum uncertainty states*. Since they are optimally focussed in  $x$  and  $p$  the coherent states are the quantum states that are closest to the classical states, which are defined as points in phase space.

To show this we introduce the unitary operator

$$\begin{aligned} \hat{\mathcal{D}}(z) &= e^{(z\hat{a}^\dagger - z^*\hat{a})} \\ &= e^{\frac{i}{\hbar}(p_c\hat{x} - x_c\hat{p})} \end{aligned} \quad (1.132)$$

where  $z$  is a complex number, related to  $x_c$  and  $p_c$  (1.126). It is the quantum version of a *displacement operator in phase space*. It transform  $\hat{a}$  and  $\hat{a}^\dagger$  as

$$\hat{D}(z)^\dagger \hat{a} \hat{D}(z) = \hat{a} + z, \quad \hat{D}(z)^\dagger \hat{a}^\dagger \hat{D}(z) = \hat{a}^\dagger + \zeta^* \quad (1.133)$$

which is shown by use of the *Campbell-Baker Hasdorff* formula

$$e^{\hat{B}} \hat{A} e^{-\hat{B}} = \hat{A} + [\hat{B}, \hat{A}] + \frac{1}{2} [\hat{B}, [\hat{B}, \hat{A}]] + \dots \quad (1.134)$$

It acts on  $x$  and  $p$  in the following way

$$\hat{D}(z)^\dagger \hat{x} \hat{D}(z) = \hat{x} + x_c, \quad \hat{D}(z)^\dagger \hat{p} \hat{D}(z) = \hat{p} + p_c \quad (1.135)$$

which explains the interpretation of  $\hat{D}$  as a displacement operator in phase space.

With the displacement operator  $\hat{D}$  acting on the ground state a continuum of new states can be generated,

$$|z\rangle = \hat{D}(z)|0\rangle \quad (1.136)$$

and it is straight forward to demonstrate from the above relations that these are coherent states as defined by (1.125). The eigenvalues  $z$  take all values in the complex plane, which means that there is one coherent state for each point in the (two-dimensional) phase space. Furthermore, since  $\hat{D}(z)$  simply adds a constant to observables  $\hat{x}$  and  $\hat{p}$ , which means that  $\hat{x} - \langle x \rangle$  and  $\hat{p} - \langle p \rangle$  are unchanged by the displacements, the shifted state  $|z\rangle$  has the same uncertainty in  $x$  and  $p$  as the ground state. Thus, all coherent states  $|z\rangle$  are minimum uncertainty states.

### *Coherent states in the coordinate representation*

The coordinate representation of the coherent states are defined by

$$\psi_z(x) = \langle x|z\rangle \quad (1.137)$$

where the *bra* corresponds to a position eigenstate and the *ket* to a coherent state. The  $z = 0$  state is the ground state of the harmonic oscillator and is known to have the gaussian form

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} \quad (1.138)$$

This expression can readily be generalized to arbitrary coherent states, since they satisfy a linear differential equation

$$\frac{1}{\sqrt{2m\hbar\omega}} \left( m\omega x + \hbar \frac{d}{dx} \right) \psi_z(x) = z \psi_z(x) \quad (1.139)$$

or,

$$\frac{d}{dx}\psi_z(x) = \left(-\frac{m\omega}{\hbar}x + \sqrt{\frac{2m\omega}{\hbar}}z\right)\psi_z(x) \quad (1.140)$$

The equation has the solution

$$\psi_z(x) = N_z e^{-\left(\frac{m\omega}{2\hbar}x^2 - \sqrt{\frac{2m\omega}{\hbar}}zx\right)} \quad (1.141)$$

where  $N_z$  is a  $z$ -dependent normalization factor. We rewrite it in the form

$$\psi_z(x) = N'_z e^{-\left(\frac{m\omega}{2\hbar}(x-x_c)^2 - \frac{i}{\hbar}x p_c\right)} \quad (1.142)$$

with a new normalization factor  $N'_z$ . The phase space coordinates  $x_c$  and  $p_c$  correspond to the real and imaginary parts of  $z$  as given by (1.126). The normalization integral determines  $N'_z$  to be, up to a phase factor, the same as the prefactor of the ground state wave function (1.138). At this stage the phase factor is arbitrary. However, implicitly this phase has already been fixed by the definition (1.136). To show this we shall find the expression for  $\psi_z(x)$  in alternative, more direct way.

$$\begin{aligned} \psi_z(x) &= \langle x | \hat{\mathcal{D}}(z) | 0 \rangle \\ &= \langle x | e^{\frac{i}{\hbar}(p_c \hat{x} - x_c \hat{p})} | 0 \rangle \\ &= e^{\frac{i}{2\hbar}x_c p_c} \langle x | e^{\frac{i}{\hbar}p_c \hat{x}} e^{-\frac{i}{\hbar}x_c \hat{p}} | 0 \rangle \\ &= e^{\frac{i}{2\hbar}x_c p_c} e^{\frac{i}{\hbar}p_c x} e^{-x_c \frac{d}{dx}} \langle x | 0 \rangle \\ &= e^{\frac{i}{2\hbar}x_c p_c} e^{\frac{i}{\hbar}p_c x} \psi_0(x - x_c) \end{aligned} \quad (1.143)$$

In this calculation we have used that  $\exp(-\frac{i}{\hbar}x_c \hat{p})$  is a translation operator in  $x$ -space. With the ground state wave function given by (1.138), the full expression for the coherent state in the  $x$ -representation is

$$\psi_z(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\left(\frac{m\omega}{2\hbar}(x-x_c)^2 - \frac{i}{\hbar}x p_c - \frac{i}{2\hbar}x_c p_c\right)} \quad (1.144)$$

This expression agrees with (1.142) and also gives the expression for the  $x$ -independent phase factor of the normalization factor.

*Time evolution of coherent states*

In the Heisenberg picture the time evolution of the creation and annihilation operators are

$$\begin{aligned}\hat{a}^\dagger(t) &= \hat{U}(t,0)^\dagger \hat{a}^\dagger \hat{U}(t,0) \\ &= e^{i\omega\hat{a}^\dagger\hat{a}}\hat{a}^\dagger e^{-i\omega\hat{a}^\dagger\hat{a}} \\ &= e^{i\omega t}\hat{a}^\dagger\end{aligned}\tag{1.145}$$

and

$$\begin{aligned}\hat{a}(t) &= \hat{U}(t,0)^\dagger \hat{a} \hat{U}(t,0) \\ &= e^{i\omega\hat{a}^\dagger\hat{a}}\hat{a} e^{-i\omega\hat{a}^\dagger\hat{a}} \\ &= e^{-i\omega t}\hat{a}\end{aligned}\tag{1.146}$$

From the last one follows,

$$\hat{a} \hat{U}(t,0)|z\rangle = e^{-i\omega t}\hat{U}(t,0)\hat{a}|z\rangle = e^{-i\omega t}z \hat{U}(t,0)|z\rangle\tag{1.147}$$

which gives the time evolution

$$\hat{U}(t,0)|z\rangle = e^{i\alpha(t)}|e^{-i\omega t}z\rangle\tag{1.148}$$

where  $\alpha(t)$  is an undetermined complex phase. The equation shows that a coherent state continues to be a coherent state during the time evolution. This means that it keeps its property of maximal localization in the phase space variables. The motion is given by

$$z(t) = e^{-i\omega t} z(0)\tag{1.149}$$

which means for the real and imaginary parts

$$\begin{aligned}m\omega x_c(t) &= \cos\omega t m\omega x_c(0) + \sin\omega t p_c(0) \\ p_c(t) &= \cos\omega t p_c(0) - \sin\omega t m\omega x_c(0)\end{aligned}\tag{1.150}$$

This shows that the coherent state moves in such a way that the phase space variables  $x_c$  and  $p_c$  change in exactly the same way as the variables of a classical harmonic oscillator. This is consistent with *Ehrenfest's theorem*, since  $x_c$  and  $p_c$  coincide with the expectation values  $\langle x \rangle$  and  $\langle p \rangle$ . Since the coherent states keep their (maximal) localization, they are as close as we can get to classical states

within the quantum description.

### *The coherent state representation*

The coherent states are expressed in the  $n$ -representation in the following way

$$\begin{aligned}
 \langle n|z\rangle &= \langle n|\hat{\mathcal{D}}(z)|0\rangle \\
 &= \langle n|e^{(z\hat{a}^\dagger - z^*\hat{a})}|0\rangle \\
 &= \langle n|e^{-\frac{1}{2}|z|^2} e^{z\hat{a}^\dagger} e^{-z^*\hat{a}}|0\rangle \\
 &= e^{-\frac{1}{2}|z|^2} \langle n|e^{z\hat{a}^\dagger}|0\rangle \\
 &= e^{-\frac{1}{2}|z|^2} \langle n|\sum_{m=0}^{\infty} \frac{z^m}{m!} (\hat{a}^\dagger)^m|0\rangle \\
 &= e^{-\frac{1}{2}|z|^2} \frac{z^n}{\sqrt{n!}}
 \end{aligned} \tag{1.151}$$

From this follows that the overlap between two coherent states is

$$\begin{aligned}
 \langle z|z'\rangle &= \sum_n \langle z|n\rangle \langle n|z'\rangle \\
 &= e^{-\frac{1}{2}(|z|^2 + |z'|^2)} \sum_n \frac{(z'z^*)^n}{n!} \\
 &= e^{-\frac{1}{2}(|z|^2 + |z'|^2) + z'z^*}
 \end{aligned} \tag{1.152}$$

and the absolute value is

$$|\langle z|z'\rangle| = e^{-\frac{1}{2}|z-z'|^2} \tag{1.153}$$

The coherent states corresponding to two different values of  $z$  are not orthogonal states, but the overlap falls off exponentially fast with the distance between the two points. This overlap gives a measure of the intrinsic uncertainty of the coherent state as a probability amplitude in phase space.

An interesting property of the coherent states is that, even if they are not orthogonal, they satisfy a completeness relation. To see this we calculate the integral

$$\int d^2z |z\rangle \langle z| = \int d^2z e^{-|z|^2} \sum_{n,m} \frac{z^n z^{*m}}{\sqrt{n!m!}} |n\rangle \langle m|$$

$$\begin{aligned}
&= \int_0^{2\pi} d\theta \int_0^\infty dr r e^{-r^2} \sum_{n,m} \frac{r^{(n+m)}}{\sqrt{n!m!}} e^{i\theta(n-m)} |n\rangle \langle m| \\
&= 2\pi \int_0^\infty dr e^{-r^2} \sum_n \frac{r^{2n+1}}{n!} |n\rangle \langle n| \\
&= \pi \sum_n |n\rangle \langle n| \\
&= \pi \hat{\mathbf{1}}
\end{aligned} \tag{1.154}$$

We rewrite this as the completeness relation

$$\int \frac{d^2z}{\pi} |z\rangle \langle z| = \hat{\mathbf{1}} \tag{1.155}$$

With the help of the completeness relation the *coherent state representation* can be defined as an alternative to the coordinate representation and the momentum representation. The wave function, which is a function of the complex phase space variable  $z$ , is defined by the state vector  $|\psi\rangle$  as

$$\psi(z) = \langle z|\psi\rangle \tag{1.156}$$

and the inverse relation is

$$|\psi\rangle = \int \frac{d^2z}{\pi} |z\rangle \langle z|\psi\rangle = \int \frac{d^2z}{\pi} |z\rangle \psi(z) \tag{1.157}$$

One of the implications of the above relation is that the coherent states do not form a linearly independent set of states, they form instead an overcomplete set. Thus,

$$|z\rangle = \int \frac{d^2z'}{\pi} |z'\rangle \langle z'|z\rangle = \int \frac{d^2z'}{\pi} |z'\rangle e^{-\frac{1}{2}(|z|^2+|z'|^2)+z'^*z} \tag{1.158}$$

which demonstrates the lack of linear independence. A consequence of this is that the expansion of a state vector  $|\psi\rangle$  in terms of the coherent states cannot be uniquely defined. Nevertheless, the expansion given by (1.157) is *unique* because of constraints that implicitly are posed on the wave functions  $\psi(z)$ . To see this we rewrite it in terms of the  $n$ -representation

$$\begin{aligned}
\psi(z) &= \sum_n \langle z|n\rangle \langle n|\psi\rangle \\
&= \sum_n \langle n|\psi\rangle e^{-\frac{1}{2}|z|^2} \frac{z^{*n}}{\sqrt{n!}} \\
&\equiv e^{-\frac{1}{2}|z|^2} f(z^*)
\end{aligned} \tag{1.159}$$

The function

$$f(z^*) = \sum_n \langle n | \psi \rangle \frac{z^{*n}}{\sqrt{n!}} \quad (1.160)$$

is an *analytic function* of  $z^*$  since it depends only on  $z^*$  and not on  $z$ . This is the constraint on the wave functions  $\psi(z)$  that makes the coherent state representation well-defined, *the wave functions are up to a common factor  $e^{-\frac{1}{2}|z|^2}$  restricted to be analytic functions.*

Thus, wave functions and observables of the originally one-dimensional problem can be rewritten in terms of analytic functions defined on the two-dimensional phase space. One should, however, be aware of the fact that several relations in this representation are unfamiliar, because of the non-orthogonality between the basis states  $|z\rangle$ .

The coherent states are important in many respects because of their close relation with classical states. They were introduced in the context of the quantum description of light, where they describe states of *classical light* within the quantum theory.

### 1.3.4 Fermionic and bosonic oscillators: an example of supersymmetry

There is a formal similarity between the two-level system which we shall examine in this section. To make the similarity explicit, we write the Hamiltonian of the two-level system as

$$\hat{H}_F = \frac{1}{2} \hbar \omega \sigma_z \quad (1.161)$$

and introduce the raising and lowering operators

$$\hat{b}^\dagger = \sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y), \quad \hat{b} = \sigma_- = \frac{1}{2}(\sigma_x - i\sigma_y) \quad (1.162)$$

In matrix form the operators are

$$\hat{H}_F = \frac{1}{2} \hbar \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{b}^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{b} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

We now have the algebraic relations

$$\{\hat{b}, \hat{b}^\dagger\} = 1, \quad \hat{H}_F = \frac{1}{2} \hbar \omega [\hat{b}^\dagger, \hat{b}] \quad (1.163)$$



where  $\{\hat{b}, \hat{b}^\dagger\}$  is the *anticommutator*  $\hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b}$ . The corresponding relations for a harmonic oscillator are

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad \hat{H}_B = \frac{1}{2}\hbar\omega \{\hat{a}^\dagger, \hat{a}\} \quad (1.164)$$

We note that the (formal) transition between the two systems corresponds to interchanging commutators with anticommutators.

There are many physical realizations of these two systems. We will now focus on a simple *many-particle realization*. Let us assume that a single state is available for many identical particles. The state may be considered to be one of the field modes of a free field. The identical particles may be either fermions or bosons.

In the fermion case the the state space will contain only two states.  $|0\rangle$  is the *vacuum state* with no particle present and  $|1\rangle$  is the excited state with one particle present. Due to the Pauli exclusion principle the single-particle state cannot be occupied by more than one particle. The occupation energy of this state is  $\hbar\omega$ . With this interpretation of the two-level system the operator  $\hat{b}^\dagger$  is a *creation operator* for a fermion and  $\hat{b}$  is an annihilation operator. The Hamiltonian is defined so that the vacuum energy is  $-\frac{1}{2}\hbar\omega$ .

In the boson case there is an infinite number of states, since the single-particle state can be occupied by an arbitrary number of particles. The states  $|n\rangle$  now are interpreted as states with  $n$  bosons present. The operator  $\hat{a}^\dagger$  is a creation operator for bosons and  $\hat{a}$  an annihilation operator. The boson vacuum state has a vacuum energy  $+\frac{1}{2}\hbar\omega$  which is the ground state energy of the harmonic oscillator.

With the interpretation above in mind we may refer to the two-level system as a *fermionic oscillator* and the standard harmonic oscillator as a *bosonic oscillator*.

In recent years the idea has been extensively developed that nature has a (hidden) symmetry between fermions and bosons called *supersymmetry*. There is at this stage no physical evidence for the presence of this symmetry as a fundamental symmetry of nature. Nevertheless the idea has been pursued, since supersymmetry is an important input in string theories and supergravity theories.

We discuss here a simple realization of supersymmetry (or Fermi-Bose symmetry) as a symmetry for the two-level model and the quantum harmonic oscillator.

The symmetrized model has a Hamiltonian that can be written as a sum of the two Hamiltonians

$$\hat{H} = \hat{H}_F + \hat{H}_B = \frac{1}{2}\hbar\omega[\{\hat{a}^\dagger, \hat{a}\} + [\hat{b}^\dagger, \hat{b}]] \quad (1.165)$$

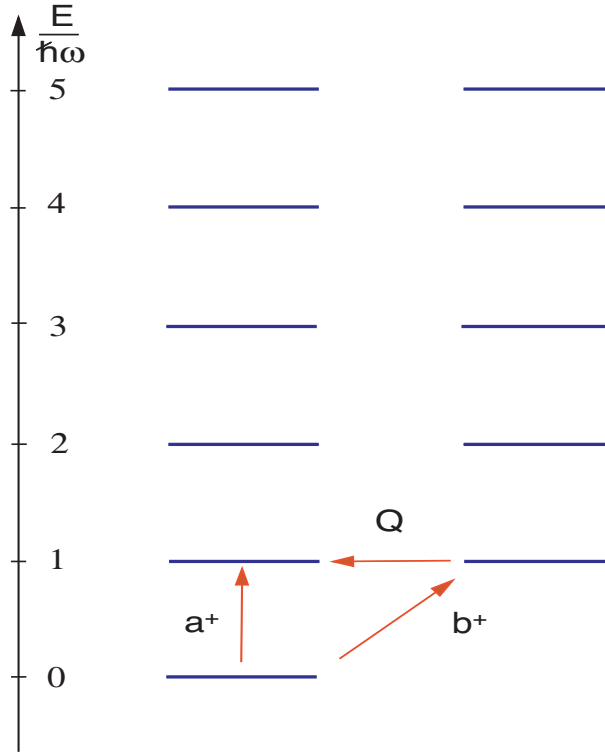


Figure 1.4: The energy spectrum of a supersymmetric oscillator. The bosonic creation operator  $\hat{a}^\dagger$  acts vertically, while the fermionic creation operator  $\hat{b}^\dagger$  acts in the diagonal direction. The supercharge  $\hat{Q}$  is a symmetry operator that maps between pairs of degenerate excited states. The ground state which is non-degenerate is annihilated by  $\hat{Q}$  and  $\hat{Q}^\dagger$ .

Since the level spacing of the two Hamiltonians have been chosen to be equal there is a double degeneracy of all the excited levels, while the ground state is non-degenerate, as shown in Fig.1.3.4.

The supersymmetry is made explicit in terms of a *supercharge*, defined as

$$\hat{Q} = \sqrt{\hbar\omega} \hat{a}^\dagger \hat{b}, \quad \hat{Q}^\dagger = \sqrt{\hbar\omega} \hat{a} \hat{b}^\dagger \quad (1.166)$$

Together with the Hamiltonian it defines a *supersymmetry algebra*

$$\begin{aligned} \{\hat{Q}, \hat{Q}^\dagger\} &= \hat{H} \\ [\hat{Q}, \hat{H}] &= [\hat{Q}^\dagger, \hat{H}] = 0 \end{aligned}$$

$$\begin{aligned}\{\hat{Q}, \hat{Q}\} &= 2\hat{Q}^2 = 0 \\ \{\hat{Q}^\dagger, \hat{Q}^\dagger\} &= 2\hat{Q}^{\dagger 2} = 0\end{aligned}\quad (1.167)$$

This is not a standard Lie algebra, since it involves both commutators and anti-commutators. It is referred to as a *graded Lie algebra*.  $\hat{Q}$  and  $\hat{Q}^\dagger$  are the fermionic (or odd) elements and  $\hat{H}$  is the bosonic (or even) element of this graded algebra.

The supersymmetry gives, as a general feature, a vacuum energy which is 0, due to cancellation of the contributions from the bosonic and fermionic variables. This type of cancellation is important in *supersymmetric quantum field theories*, where the divergent contributions to the vacuum energy are avoided.

## 1.4 Problems

### 1.4.1 Time evolution operator

Let us assume that the dynamics of a quantum system is determined by a time-dependent Hamiltonian  $\hat{H}(t)$ . Show that the corresponding Schrödinger equation can formally be integrated from an initial time  $t_0$  to a final time  $t$  and that this expression can be used to give the time evolution operator of the form (1.43). To find this expression, use the integrated Schrödinger equation iteratively, with the term containing  $\hat{H}(t)$  (right-hand side) as the input term. As first input use  $|\psi(t)\rangle = |\psi(t_0)\rangle$ . Use then the output expression (left-hand side) for  $|\psi(t)\rangle$  as the new input etc. This gives an expression for  $|\psi(t)\rangle$  which can be written as a sum of terms with an increasing number of Hamiltonians acting on  $|\psi(t_0)\rangle$ . From this expression the time evolution operator can be extracted.

### 1.4.2 Operator identities

Assume  $\hat{A}$  and  $\hat{B}$  to be two operators, generally not commuting.

a) Show the following relation (Campbell-Baker-Hausdorff)

$$e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}} = \hat{B} + \lambda[\hat{A}, \hat{B}] + \frac{\lambda^2}{2}[\hat{A}, [\hat{A}, \hat{B}]] \dots \quad (1.168)$$

by expanding in powers of  $\lambda$ .

b) Show in a similar way the relation

$$e^{\lambda\hat{A}}e^{\lambda\hat{B}} = e^{\lambda\hat{A} + \lambda\hat{B} + \frac{\lambda^2}{2}[\hat{A}, \hat{B}] + \dots} \quad (1.169)$$

If  $[\hat{A}, \hat{B}]$  commutes with both  $\hat{A}$  and  $\hat{B}$  show that (1.169) is exact without higher order terms indicated by ... .

### 1.4.3 Ehrenfest's theorem

A (quantum) particle with mass  $m$  moves in a potential  $V(x)$ . Show that the expectation values  $\langle x \rangle$  and  $\langle p \rangle$  satisfy similar equations of motion as those of a classical particle in the potential  $V(x)$ . Is there any difference? Discuss under what conditions the classical and quantum expectation value equations are essentially identical.

### 1.4.4 Gaussian wave function

A wave function for a free particle with mass  $m$  in one dimension is in the momentum representation described by the Gaussian

$$\psi(p) = N e^{-\frac{\lambda}{2}(p-p_0)^2} \quad (1.170)$$

$\lambda$  is a parameter that determines the width of the Gaussian and  $N$  is a normalization factor. Find the corresponding time dependent wave function  $\psi(x, t)$  in the coordinate representation. Show that  $|\psi(x, t)|^2$  is a Gaussian and examine how the maximum of the wave packet moves with time and how the width changes.

### 1.4.5 Potential step

A particle of mass  $m$  moves in a one-dimensional potential. The potential is piecewise constant with  $V = 0$  for  $x < 0$  and  $V = -u$  for  $x > 0$ . Initially the particle is moving towards the potential step with position  $x < 0$  and momentum  $p > 0$ . The problem is to compare the motion of a classical particle with that of a quantum particle. Somewhat surprisingly there is an important qualitative difference.

First, discuss what happens to a particle according to the classical description. Next, solve the quantum problem for a stationary situation where the incoming particle is described by a plane wave moving towards the potential step. Is there a difference between the behaviour of the particle in the classical and quantum description? Consider the limit of an infinitely deep step,  $u \rightarrow \infty$ .

Can the above result be reconciled with Ehrenfest's theorem? To examine this, introduce a wave packet for the incoming particle by modulating the stationary state with a Gaussian function of the incoming momentum, as discussed in

problem (1.4.4). Examine first the motion of the incoming and outgoing particle in terms of maxima of the wave packets. Also consider the *form* of the transmitted wave. Is the Gaussian form preserved when passing the potential jump?

In order to do the momentum integrations some simplifications have to be made:

- In the momentum-dependent *amplitudes* of the reflected and transmitted waves replace the momentum variable  $p$  with its peak value  $p_0$ .
- Also consider  $p$  to be small at the scale set by the potential step,  $p \ll \sqrt{2mu}$ .

### 1.4.6 Stationary phase

A simpler way to determine the motion of the *maximum* of a wave packet is to use a "stationary phase argument". Instead of introducing an explicit (Gaussian) wave function profile, we consider the  $k$ -dependence of the plane waves of the incoming and outgoing particle. The plane waves will in general have the form

$$\psi(x, t) = Ne^{i(kx - \frac{\hbar k^2 t}{m} + \alpha(k))} \quad (1.171)$$

where  $N$  is a real normalization factor and  $\alpha$  is a ( $k$ -dependent) phase factor. Let us assume that the real wave function does not have a single momentum component like in (1.171), but it is strongly peaked around the value  $\hbar k$  in momentum space. The stationary phase argument states that the corresponding  $x$ -space wave function is peaked around a point (in  $x$ -space) determined by the condition that the phase factor of (1.171) is stationary with respect to variations in  $k$ . This gives the free particle motion

$$x = x_0 + vt \quad (1.172)$$

with

$$x_0 = \frac{\partial \alpha}{\partial k}, \quad v = \frac{\hbar k}{m} \quad (1.173)$$

Use the stationary phase argument to study the motion of the particle in (1.4.5) and check that the result is the same as found for the motion of the peak of the wave packets.

### 1.4.7 Faster than light?

Consider the tunneling of a particle through a piecewise constant potential

$$V(x) = \begin{cases} 0 & x < -a \\ V_0 & -a < x < a \\ 0 & a < x \end{cases} \quad (1.174)$$

Let us assume that a particle of mass  $m$  approaches the potential barrier from the left with an energy smaller than  $V_0$ . There is a certain probability of the particle to be scattered back from the barrier and a probability for the particle to tunnel through.

An interesting question concerns the tunneling time of the particle through the potential barrier. There are arguments that the particle penetrates the potential with a speed which is larger than that of the incoming free particle. Indeed there exist claims that in a corresponding optical system the effect can be used to send signals faster than light.

Examine, by use of the stationary phase argument, both the delay time of the reflected wave and the tunneling time of the transmitted wave. What happens when  $a$  increases? Does the result give support for the claim that the barrier speeds up the particle (even to superluminal speed)? Check that also in this case Ehrenfest's theorem is satisfied.

### 1.4.8 Forced harmonic oscillator

A one-dimensional oscillator is subject to a periodic perturbation. The Hamiltonian of the oscillator has the form

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t) \quad (1.175)$$

with

$$\hat{H}_0 = \frac{1}{2m}(\hat{p}^2 + m^2\omega_0^2\hat{x}^2), \quad \hat{H}_1(t) = F\hat{x}\cos(\omega t) \quad (1.176)$$

$F$  gives the strength of the perturbation, and  $\omega$  the frequency of the perturbation, which we consider as variable, while the oscillator frequency  $\omega_0$  is fixed.

Use the expression for the time-evolution operator in the interaction picture to find the time development of a state that starts in the ground state of  $\hat{H}_0$  at time  $t = 0$ . Determine the state as a function of time only to first order in  $\hat{H}_1$ . Find the time evolution of the expectation value  $\langle x \rangle$ . What happens when the frequency  $\omega$  gets close to  $\omega_0$ ?

### 1.4.9 Schwinger representation for angular momenta

Let  $\hat{a}_1, \hat{a}_1^\dagger$  and  $\hat{a}_2, \hat{a}_2^\dagger$  be the annihilation and creation operators of two independent harmonic oscillators. A set of quadratic operators are defined by

$$\begin{aligned}\hat{J}_1 &= \frac{\hbar}{2}(\hat{a}_2^\dagger \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_2) \\ \hat{J}_2 &= \frac{i\hbar}{2}(\hat{a}_2^\dagger \hat{a}_1 - \hat{a}_1^\dagger \hat{a}_2) \\ \hat{J}_3 &= \frac{\hbar}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2) \\ \hat{j} &= \frac{\hbar}{2}(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2)\end{aligned}\tag{1.177}$$

Show that the operators satisfy the angular momentum commutation relations

$$\begin{aligned}[\hat{J}_1, \hat{J}_2] &= i\hbar \hat{J}_3 \text{ (+ cyclic permutations)} \\ \hat{\mathbf{J}}^2 &= \hat{j}(\hat{j} + 1)\hbar^2.\end{aligned}\tag{1.178}$$

### 1.4.10 Displacement operator in phase space

Show that the operator

$$\hat{\mathcal{D}}(\zeta) = e^{(\zeta \hat{a}^\dagger - \zeta^* \hat{a})}\tag{1.179}$$

acts as a displacement operator in phase space, in the sense

$$\hat{\mathcal{D}}(\zeta) \hat{x} \hat{\mathcal{D}}(\zeta)^\dagger = \hat{x} - \xi, \quad \hat{\mathcal{D}}(\zeta) \hat{p} \hat{\mathcal{D}}(\zeta)^\dagger = \hat{p} - \nu\tag{1.180}$$

where

$$\zeta = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega \xi + i\nu)\tag{1.181}$$

Does the displacement operator in the  $x$ -direction,  $\hat{\mathcal{D}}(\sqrt{\frac{m\omega}{2\hbar}}\xi)$  commute with that in the  $p$ -direction,  $\hat{\mathcal{D}}(\frac{1}{\sqrt{2m\hbar\omega}}i\nu)$ ? Find a relation between the two products  $\hat{\mathcal{D}}(\sqrt{\frac{m\omega}{2\hbar}}\xi)\hat{\mathcal{D}}(\frac{1}{\sqrt{2m\hbar\omega}}i\nu)$  and  $\hat{\mathcal{D}}(\frac{1}{\sqrt{2m\hbar\omega}}i\nu)\hat{\mathcal{D}}(\sqrt{\frac{m\omega}{2\hbar}}\xi)$ .

### 1.4.11 Coherent states

Check, by use of operator identities, the expression for a coherent state  $|z\rangle$  in the  $n$ -representation, as given by Eq.(1.151). (Fill in missing details.)

