# Open Systems in QM. The Density Matrix. Coherence. Entanglement

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# Contents

# 1 Mixed and Entangled States.

Let us consider a closed system consisting of two *interacting* parts which are described respectively by sets of generalised coordinates $x = x_1, ... x_N$ and $q = q_1, ..., q_M$. Suppose that we are interested in the properties (i.e. to measure physical observables) and in the behaviour (i.e. to follow the time dependence) of only one part of the system, say, $x$ and are not interested in the part $q$. Such a situation typically arises when a physical system under considerations is not isolated and interacts with its surroundings, e.g. a particle in an accelerator, an atom in a non ideal gas, propagating radiation in a medium, etc. Such systems are called *open systems* and the $q$-part is often referred to as *environment*.

Classically, open systems are described exactly as the closed systems, i.e. by prescribing the time dependence of the coordinates $x(t)$ and momenta $p(t)$ for given initial conditions $x(t_0)$ and $p(t_0)$. Any physical observable $f(x, p_x)$ which "belongs" to the x–part and is independent of $q$ can be calculated at any time $t$ by simply inserting the values of $x(t)$ and $p(t)$. Of course the dynamics of $x$ and $p$ is not independent – their equations of motion depend on the coordinates and momenta $q$ and $p_q$ of the rest of the system and one must deal with the entire system by solving all the equation simultaneously. The point to note however is that nothing conceptually new is required in classical mechanics as far as the *kinematical* description of an open system is concerned. Moreover when it ceases to interact with the other parts of the composite system also its dynamical description becomes identical to a closed system.

Let us now address the same situation in quantum mechanics. The entire system is of course described by a general, in principle time–dependent, wave function $\Psi(x, q, t)$ but we can not write a wave function for the x–part only. One sometimes says that an open system *does not have a wave function* or that it is in a *mixed state*. The peculiarity of the quantum mechanical description however goes even beyond this – *the system can be in a mixed state even when it is closed, i.e. not interacting with the environment.* Indeed let the $x$- and the $q$- parts of system be described by the Hamiltonian $H = H_x + H_q$ – a sum of independent (commuting) parts. A possible wave function of the system is a product $X_n(x)Q_m(q)$ or more generally $(\sum_n a_n X_n(x))(\sum_m b_m Q_m(q))$ where $X_n(x)$ and $Q_m(q)$ are the corresponding eigenfunctions of $H_x$ and $H_q$ respectively. The probabilities of $x$ and $q$ for such wave functions are independent of each other as expected for independent parts.

However the above product form of the wave function is not the most general. In fact because of the linearity of the Schrödinger equation one can have a more general *superposition*

$$\Psi(x, q) = \sum_{mn} c_{mn} X_n(x) Q_m(q) \tag{1}$$

with non separable $c_{mn}$. Such wave functions are called *entangled* and have no classical analogue. The celebrated Einstein-Podolsky-Rosen gedanken experiment deals with one of the simplest examples of an entangled state - two noninteracting spins in a singlet state of a total spin

$$\Psi(\sigma_1, \sigma_2) = \frac{1}{\sqrt{2}} \left[ \chi_\uparrow(\sigma_1)\chi_\downarrow(\sigma_2) - \chi_\downarrow(\sigma_1)\chi_\uparrow(\sigma_2) \right]$$

The content of this Chapter is how to describe mixed systems both kinematically and dynamically.

## 2   The Density Matrix.

The wave function $\Psi(x, q, t)$ contains of course all the information about the $x$-part. On this basis it is possible to find a kinematic description of this open system only in terms of its own coordinates.

### 2.1   The definition

Let us consider an arbitrary physical observable $f(x, p_x)$ belonging only to the $x$–part. To find all the information about this observable which is contained in $\Psi(x, q, t)$ one must proceed in a standard way, i.e. consider the corresponding operator $f_{op}$, find its eigenfunctions $\phi_n(x)$ and eigenvalues $f_n$ and form overlaps

$$a_n(q) = \int dx \; \phi_n^*(x)\Psi(x, q, t)$$

These overlaps depend not only on $n$ but also on $q$ - the coordinates of the environment, i.e. of the unobserved part. This of course means that the absolute value squares of these overlaps $|a_n(q)|^2$ give probabilities to measure $f_n$ together with *a particular* $q$ of the environment. To obtain the probability $w_n$ of $f_n$ one must integrate over $q$ to obtain

$$w_n(t) \;\; = \;\; \int dq |a_n(q)|^2 = \int dq| \int dx \; \phi_n^*(x)\Psi(x, q, t)|^2 = \tag{2}$$
$$= \;\; \int dx dx' \phi_n^*(x)\phi_n(x')\rho(x, x', t)$$

where we have defined a bilocal function depending on two sets of $x$'s

$$\rho(x, x', t) = \int dq \Psi(x, q, t)\Psi^*(x', q, t) \tag{3}$$

Since $f_{op}$ above is arbitrary the function $\rho(x, x', t)$ carries all the information about the $x$–part of the system and must be considered as the object which replaces the wave function when one deals with open systems. It is called *the density matrix* and was introduced in quantum mechanics by F. Bloch and L. Landau. The origin of the word matrix in its name is intuitively clear and will be further explained in the next section.

   To appreciate the need for a bilocal $\rho(x, x')$ let us consider an expectation value of the operator $f_{op}$ which acts on the $x$-part of the system

$$< f_{op} >= \int \Psi^*(x, q, t) f_{op}\Psi(x, q, t) dx dq$$

We wish to express it in terms of $\rho(x, x', t)$. If $f_{op}$ is just a function $f(x)$ of x then $< f(x) >= \int f(x)\rho(x, x)dx$. But in general $f_{op}$ depends also on the derivatives like $p_{op} = -i\hbar\partial/\partial x$. One should therefore first act with $f_{op}$ on the first argument of $\rho(x, x', t)$ and set $x = x'$ afterwards,

$$< f_{op} >= \int [f_{op}\rho(x, x', t)]_{x=x'} \, dx \tag{4}$$

## 2.2  Closed system in a mixed state

Let us consider the limiting situation which we have already mentioned in the previous Section, i.e. when the two parts $x$ and $q$ of the system cease to interact. Each part is now a closed system and the simplest possibility is that the wave function $\Psi(x, q, t)$ is just a product

$$\Psi(x, q, t) = \phi(x, t) \, Q(q, t) \tag{5}$$

In this case the result of any measurement on the $x$–part is independent of what happens to the $q$–part and the density matrix has a separable product form

$$\rho(x, x', t) = \phi(x, t)\phi^*(x', t) \tag{6}$$

Such density matrices describe *pure states*.

If $\rho(x, x', t)$ is not a product of $x$– and $x'$–dependent functions the system is said to be in a *mixed state* which is the most general state of a quantum mechanical system. The density matrix description is therefore more general than the description using wave functions. As we have already indicated *even a closed system is not always found in a pure state.* Although the x–part does not interact with the rest of the system, i.e. with the $q$–part, their combined wave function may not have the factorized form (5). This in fact will happen only in particular circumstances when a special care is taken in order to "prepare" the system with such wave function. In general the $x$- and $q$-parts will be entangled and described by a wave function which is a superposition of products, cf., Eq. (1).

Perhaps the simplest way to illustrate this it to consider a general Hamiltonian

$$H = H_x + H_q + V_{xq}(t) \tag{7}$$

consisting of a sum of $x$- and $q$- dependent parts $H_x$, $H_q$ and the time dependent interaction $V_{xq}(t)$ which is "switched off" after some time $t_0$

$$V_{xq}(t) \to 0 \ \text{ at } \ t > t_0$$

In practice this can happen when the x- and q-parts get separated in the course of their dynamics at distances larger than the "range" of $V_{xq}$.

We can represent the wave function of such a system as an expansion

$$\Psi(x, q, t) = \sum_{mn} A_{mn}(t)\phi_m(x)Q_n(q) \tag{8}$$

in terms of the complete set of the eigenstates $\phi_m(x)$ and $Q_n(q)$ of $H_x$ and $H_q$ respectively. The time dependence of the coefficients $A_{mn}(t)$ is determined by the Schrödinger equation $(i\hbar\partial_t - H)\Psi(x, q, t) = 0$ which in the basis $\phi_m(x)Q_n(q)$ becomes coupled equations

$$i\hbar\frac{\partial B_{mn}(t)}{\partial t} = \sum_{m'n'}\langle mn|V_{xq}(t)|m'n'\rangle B_{m'n'}(t) \tag{9}$$

for conveniently defined coefficients $B_{nm}(t)$

$$A_{mn}(t) = B_{mn}(t)\exp[-i(E_m + \epsilon_n)(t - t_0)/\hbar] \tag{10}$$

where $E_m$ and $\epsilon_n$ are the energies of $\phi_m(x)$ and $Q_n(q)$ respectively.

The solution of the above coupled equations depends on the interaction $V_{xq}$ in a complicated way. The density matrix of the x-part is

$$\rho(x, x', t) = \int dq\, \Psi(x, q, t)\Psi^*(x', q, t) = \sum_{mm'} C_{mm'}(t)\phi_m(x)\phi_{m'}^*(x') \tag{11}$$

where

$$C_{mm'}(t) = \sum_n A_{mn}(t)A_{m'n}^*(t)$$

This $\rho(x, x', t)$ describes a general mixed state of the subsystem $x$ interacting with $q$ and accordingly is not in the form of the product (6).

When after the "switching off" time $t_0$ the parts $x$ and $q$ cease to interact, $V_{xq}(t) \to 0$, the coefficients $B_{mn}$ become time independent so that

$$A_{mn}(t) = A_{mn}(t_0)\exp[-i(E_m + \epsilon_n)(t - t_0)/\hbar]$$

and correspondingly

$$C_{mm'}(t) = C_{mm'}(t_0)\exp[-i(E_m - E_{m'})(t - t_0)/\hbar]\,, \quad (t \geq t_0) \tag{12}$$

This form of $C_{mm'}(t)$ and the expression (11) with such $C_{mm'}(t)$ show that despite the vanishing of the interaction between the two parts the density matrix (11) still does not describe a pure state unless it so happened that $A_{mn}(t_0)$ had at $t_0$ a *factorized form* $A_{mn}(t_0) = a_m b_n$ with some arbitrary $a_m$ and $b_n$. In general the fact that the x–part becomes isolated after $t = t_0$ does not lead to the factorized form of its density matrix. The simpler dynamics of system after $t_0$ is reflected "only" in the simple time dependence of the coefficients $C_{mm'}(t)$. As we will see below this means that the time evolution equation for the density matrix in this case can be written in a general closed form.

## 2.3 Properties of the density matrix.

It is useful to consider $\rho(x, x')$ as a matrix with $x$ and $x'$ playing the role of the (continuous) raw and column indices[1]. This matrix is hermitian,

$$\rho(x, x') = \rho^*(x', x) \tag{13}$$

and its diagonal elements

$$\rho(x, x) = \int dq |\Psi(x, q)|^2 \tag{14}$$

determine the probability distribution of the coordinates $x$. Integrated over $x$ it gives

$$\int dx \rho(x, x) = 1 \tag{15}$$

for a normalized $\Psi(x, q)$.

What is the meaning of the "off diagonal" elements $\rho(x, x')$ with $x \neq x'$? We have already touched upon this issue in relation to Eq. (4). The off diagonal $\rho(x, x')$ contain information about observables the operators of which depend on the derivatives, i.e. are non diagonal in $x$. The simplest example is the probability distribution of momenta $p$ in a one dimensional system

$$w_p = \frac{1}{2\pi\hbar} \int e^{ip(x-x')/\hbar} \rho(x, x') dx dx' \tag{16}$$

where we used Eq.(2) with $\phi_n$ taken as momentum eigenstates $(1/\sqrt{2\pi\hbar}) \exp(ipx/\hbar)$.

It is useful to write the relation (2) as

$$w_n = \int dx \, dx' \rho_n(x', x) \rho(x, x') = Tr\rho_n\rho \tag{17}$$

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[1] We omit the explicit dependence of $\rho$ on t in the rest of this section

where we have introduced the density matrix $\rho_n(x, x') = \phi_n(x)\phi_n^*(x')$ of the pure state $\phi_n(x)$, interpreted the integrations over $x$ and $x'$ as summations over the continuous matrix indices and used the symbolic matrix multiplication of $\rho$ and $\rho_n$ together with the trace operation. We can see that taking trace of a product of two density matrices is a generalization to the mixed states of the projection operation for pure states.

## 2.4 Spectral representation of $\rho$

A given general density matrix $\rho(x, x')$ can be diagonalized

$$\int \rho(x, x')\xi_m(x') \, dx' = w_m \xi_m(x) \tag{18}$$

Since it is hermitian the eigenvalues $w_m$ are real and the eigenfunctions $\xi_m(x)$ are orthogonal. Since they are determined up to a multiplicative constant one can normalize them so have

$$\int dx \, \xi_m^*(x)\xi_n(x) = \delta_{mn} \tag{19}$$

Using these functions one can represent $\rho(x, x')$ in the spectral decomposition form

$$\rho(x, x') = \sum_m w_m \xi_m(x)\xi_m^*(x') \tag{20}$$

Because of the normalization condition (15) one has

$$\sum_m w_m = 1 \tag{21}$$

We also have that

$$w_m \geq 0 \tag{22}$$

Indeed using the spectral decomposition (20) and then the definition (3) of $\rho(x, x')$ we find[2]

$$w_m = \int dx dx' \xi_m^*(x)\rho(x, x')\xi_m(x') = \int dq |M_m(q)|^2 \ \text{ with } \ M_m(q) = \int dx \xi_n^*(x)\Psi(x, q)$$

which is obviously $\geq 0$.

Combining (21) and (22) we conclude that

$$0 \leq w_m \leq 1 \tag{23}$$

The eigenvalues $w_m$ have thus the properties of probabilities and one sometimes interprets (20) as an *incoherent superposition* of pure states $\xi_m(x)$ each realized with the probability $w_m$.

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[2]Thanks to Yoav Palti for this proof

## 2.5 From pure to maximally mixed. Entropy of a mixed state

Obviously for a pure state one must have one $w_n = 1$ while the rest are equal to zero. The opposite case of a "maximally" mixed state is obtained when all $w_n$'s are equal, $w_n = 1/N$ where N is the total number of states. Of course in general N is infinite and such a case is not realistically achieved but frequently as we will discuss below one deals with a finite number of *relevant* states for which the distribution $w_n = 1/N$ has in fact a fairly common occurrence. Such a degenerate distribution means that (like with other degeneracies familiar from, say degenerate energy or angular momentum levels) *there is no unique set of eigenstates of $\rho$* and one can choose any orthogonal set in the N dimensional subspace. This situation must be contrasted with the pure state situation in which one unique state is selected.

There exist a function of $\rho$ which provides a simple characterization of the intermediate situations between the two extremes – the pure and the maximally mixed states. This is the familiar statistical entropy

$$S = -Tr\ \rho \ln \rho = -\sum_m w_m \ln w_m \qquad (24)$$

This expression is equal to zero – its minimum value – in a pure state and reaches the maximum $S_{max} = \ln N$ in the other extreme. The reader is referred to Ref. [1] for further discussion of these and other properties of this expression and its uses in statistical and information theory.

## 2.6 Density operator

It is useful to view the expression (20) as a matrix element of the density operator

$$\rho_{op} = \sum_m w_m |\xi_m><\xi_m| \qquad (25)$$

in the coordinate representation $x$,

$$\rho(x, x') = <x|\rho_{op}|x'>$$

In order to find this operator in any other representation defined by a complete orthonormal set $\{\phi_n(x)\}$ one must simply expand

$$
\begin{aligned}
\rho(x, x') &= \sum_{mn} \rho_{mn} \phi_m(x) \phi_n^*(x')\ , \\
\rho_{mn} &= \int dx\, dx'\, \phi_m^*(x) \phi_n(x') \rho(x, x')
\end{aligned}
\qquad (26)
$$

The properties of $\rho$ which we found in the x–representation hold in general,

$$\rho_{mn} = \rho_{nm}^* \quad , \quad Tr\,\rho = \sum_n \rho_{nn} = \int \rho(x,x)dx = 1 \tag{27}$$

According to Eq.(2) the diagonal elements of $\rho_{mn}$ represent the probabilities to find the system in the pure states $\phi_n(x)$. The off diagonal elements carry information about physical observables for which the corresponding operators are *not diagonal* in the set $\{\phi_n(x)\}$. For the reasons which will become clear below in certain situations such off diagonal elements are termed "coherences".

If the basis $\phi_n(x)$ coincides with the eigenstates $\xi_n(x)$ of $\rho$ then

$$\rho_{mn} = w_n \delta_{mn} \tag{28}$$

We also note that expression (4) for the expectation value of an operator can be written in a compact way using the matrix notation

$$
\begin{aligned}
< f_{op} > &= \int dx \sum_{mn} \rho_{mn}[f_{op}\phi_m(x)\phi_n^*(x')]_{x=x'} \\
&= \sum_{mn} \rho_{mn} f_{nm} = Tr(\rho f_{op})
\end{aligned}
\tag{29}
$$

It is instructive to compare this expression with Eq. (17).

## 2.7  Pure vs mixed state - how to know?

The density matrix in a pure state remains a product in any representation

$$\rho(x,x') = \phi(x)\phi^*(x') = \sum_{mn} a_m a_n^* \phi_n(x)\phi_m^*(x') \quad \rightarrow \quad \rho_{mn} = a_m a_n^* \tag{30}$$

where $a_n$'s are just the coefficients of the expansion of $\phi(x)$ in the basis $\phi_n(x)$. A very general property of the density operator representing a pure state is that its square is equal to itself

$$(\rho^2)_{mk} = \sum_n \rho_{mn}\rho_{nk} = \sum_n a_m a_n^* a_n a_k^* = a_m a_k^* = \rho_{mk} \quad \rightarrow \quad \rho^2 = \rho \tag{31}$$

Such an operator is called *projection operator* or in mathematical terms, *idempotent operator*. All its higher powers are obviously also equal, $\rho^n = \rho$. As we already

know the eigenvalues $w_n$ of such an operator are all zero except one which is equal to unity, $w_n = \delta_{n,1}$ and corresponds to the eigenstate $\xi_1(x) = \phi(x)$. When acting on an arbitrary function $\psi(x)$ the density operator of a pure state $\phi(x)$ simply projects on this state,

$$\int dx' \, \rho(x, x')\psi(x') = <\phi|\psi> \phi(x) \tag{32}$$

The property (31) of a pure state implies

$$Tr \, \rho^2 = Tr \, \rho = 1 \tag{33}$$

which suggests an easy check of whether a given $\rho$ represents a pure or a mixed state. In the general case the following inequality holds

$$
\begin{aligned}
Tr \, \rho^2 &= \sum_n w_n^2 \le (\sum_n w_n)^2 = (Tr \, \rho)^2 = 1 \quad \rightarrow \\
&\rightarrow \quad Tr\rho^2 \le 1 \quad \rightarrow \quad \sum_{mn} |\rho_{mn}|^2 \le 1
\end{aligned}
\tag{34}
$$

which impose severe limitations on possible values of $\rho_{mn}$. Let us also notice that the maximally mixed states discussed in Sec. 2.5 which have $w_n$'s all equal, $w_n = 1/N$ when working in a finite, N-dimensional subspace have

$$Tr \, \rho^2 = \sum_n w_n^2 = 1/N \tag{35}$$

# 3  Dynamical Equations for the Density Matrix.

## 3.1  Liouville–von Neumann equation

We will now discuss the equations which determine the density matrix in various physical situations . Our starting point will be the Schrödinger equation for the wave function $\Psi(x, q, t)$ of the entire composite system. It is convenient to rewrite it for

$$R(x, q; x', q'; t) = \Psi(x, q, t)\Psi^*(x', q', t)$$

which is the density matrix of the composite system,

$$
\begin{aligned}
i\hbar \frac{\partial R(x, q; x', q'; t)}{\partial t} &= i\hbar \frac{\partial \Psi(x, q, t)}{\partial t}\Psi^*(x', q', t) + \Psi(x, q, t)i\hbar \frac{\partial \Psi^*(x', q', t)}{\partial t} \\
&= (H\Psi(x, q, t))\Psi^*(x', q', t) - \Psi(x, q, t)(H'^*\Psi^*(x', q', t)) \\
&= (H - H'^*)R(x, q; x', q'; t)
\end{aligned}
\tag{36}
$$

where $H$ and $H'$ is the same Hamiltonian of the system but acting on the non primed and primed variables respectively. $R(x, q; x', q'; t)$ can be considered as a matrix element of the operator $R_{op} = |\Psi ><\Psi|$ and the Schrödinger equation (36) can be written as

$$i\hbar < x, q|\frac{\partial R_{op}}{\partial t}|x', q' >=$$ (37)
$$=< x, q|H_{op}|\Psi ><\Psi|x', q' > - < x, q|\Psi ><\Psi|H_{op}|x', q' >=$$
$$=< x, q|H_{op}R_{op}|x', q' > - < x, q|R_{op}H_{op}|x', q' > .$$

or in the operator form

$$i\hbar\frac{\partial R_{op}}{\partial t} = [H_{op}, R_{op}]$$ (38)

This equation is the quantum mechanical analogue of the classical Liouville equation and is called the Liouville–von Neumann equation. We note that it has the form of the Heisenberg equation for operators but with the opposite sign. This sign change reflects the mutual consistency of the Heisenberg and the Schrödinger pictures of the time evolution in quantum mechanics. Indeed one can easily check using the cyclic properties of trace that precisely because of the difference in the sign the time derivative of the expectation value of an operator

$$< \Psi|F_{op}|\Psi >= Tr(F_{op}|\Psi ><\Psi|) = TrF_{op}R_{op}$$

will be the same irrespective of whether one considers $F$ evolving in time according to the Heisenberg equation

$$i\hbar\frac{\partial F_{op}}{\partial t} = [F_{op}, H_{op}]$$

or allows $R_{op}$ to be time dependent according to Eq. (38).

## 3.2   Closed but mixed

### 3.2.1   The equation

Let us now consider a particular case of $H_{op} = \hat{H}_x + \hat{H}_q$, i.e. when the interaction $\hat{V}_{xq} = 0$ so that the x–part is a closed system. Then a closed equation for $\rho(x, x'; t)$ exists and has the Liouville–von Neumann form

$$i\hbar\frac{\partial \rho_{op}(t)}{\partial t} = [\hat{H}_x, \rho_{op}]$$ (39)

which is easily shown by using the definition, Eq. (3) of $\rho(x, x')$, writing it in a formal way as

$$\rho_{op} = Tr_q \, R_{op}$$

and applying the operation $Tr_q$ to Eq. (38),

$$
\begin{aligned}
i\hbar \frac{\partial \rho_{op}(t)}{\partial t} &= \hat{H}_x(Tr_q R_{op}) - (Tr_q R_{op})\hat{H}_x + Tr_q(\hat{H}_q R_{op}) - Tr_q(R_{op}\hat{H}_q) \\
&= \hat{H}_x \rho_{op} - \rho_{op}\hat{H}_x = [\hat{H}_x, \rho_{op}]
\end{aligned}
\tag{40}
$$

The terms involving $\hat{H}_q$ cancel because of the cyclic property of the trace. Indeed writing explicitly

$$
Tr_q\left([\hat{H}_q, \, R_{op}]\right) = \int dq dq' (<q|\hat{H}_q|q'><q'|R_{op}|q> - <q|R_{op}|q'><q'|\hat{H}_q|q>)
\tag{41}
$$

and renaming $q \longleftrightarrow q'$ in the last term we see that this expression vanishes.

We thus see that in this case the equation for the density matrix of a closed part of the composite system has the same Liouville – von Neumann form as for the density matrix $R$ of the entire system. Its formal solution can be written as

$$\rho_{op}(t) = \exp(-i\hat{H}_x t/\hbar) \, \rho_{op}(0) \, \exp(i\hat{H}_x t/\hbar) \tag{42}$$

In terms of the eigenfunctions $\phi_n(x)$ and eigen energies $E_n$ of $\hat{H}_x$ one can use

$$<x|\exp(-i\hat{H}_x t/\hbar))|x'> = \sum_n \phi_n(x)\phi_n^*(x')\exp(-iE_n t/\hbar)$$

and write this solution as a linear combination

$$\rho(x, x'; t) \equiv <x|\rho(t)|x'> = \sum_{mn} \rho_{mn}\phi_m(x)\phi_n^*(x')\exp[-i(E_m - E_n)t/\hbar] \tag{43}$$

with the constants $\rho_{mn}$ determined by initial conditions at $t = 0$. This solution is what we have already discussed before, cf. Eqs. (11,12) and is an obvious generalization of the solution

$$\sum_m c_m \phi_m(x)\exp(-iE_m t/\hbar)$$

of the Schrödinger equation for a pure system wave function. In both cases the key technical point in finding the solutions is to determine the eigenfunctions $\phi_n(x)$ and eigenenergies of the Hamiltonian $H_x$.

We notice that the expression (24) for the entropy of $\rho$ remains constant in time if $\rho$ evolves according to Eq. (40), i.e. for a closed system. This can be verified directly by evaluating $dS/dt$ or by observing that the time evolution (42) is a unitary transformation and that $S$ is invariant under any unitary transformation of the density matrix $\rho$ since it depends only on the eigenvalues $w_m$ of $\rho$.

### 3.2.2 Static limit

It is useful and instructive to discuss the time independent solutions of the Liouville – von Neumann equation (39)

$$[\hat{H}_x, \rho_{op}] = 0 \tag{44}$$

As with any operator which commutes with the Hamiltonian this equation means that $\rho_{op}$ has the same eigenfunctions $\phi_n(x)$ as $\hat{H}_x$. Which means that its spectral decomposition form Eq. (20) is

$$\rho(x, x') = \sum_m w_m \phi_m(x) \phi_m^*(x') \tag{45}$$

The weights $w_n$ are not determined by the equation (44) and can be arbitrary subject to the standard conditions Eqs. (21,22). Their values for a given physical system depend on the preparation of the system. The limiting case $w_n = \delta_{nm}$ corresponds to the system in a pure state $\phi_m(x)$ with a given energy $E_m$. Other familiar cases are the canonical and microcanonical distributions with the inverse temperature $\beta$ and the energy $E$ respectively

$$w_n = \frac{e^{-\beta E_n}}{\sum_m e^{-\beta E_m}} \qquad , \qquad w_n = \frac{\delta(E - E_n)}{\sum_m \delta(E - E_m)} \tag{46}$$

### 3.2.3 Degenerate levels. Finite size density matrices

Degenerate energy levels deserve special attention. The energy eigenfunctions in this case are characterized by an extra index or indices to distinguish the degenerate sub levels. Atomic levels $E_{nl}$ in a hydrogen atom serve as an example with corresponding eigenfunctions $\phi_{nlm_lm_s}$ depending on additional quantum numbers of the angular momentum and spin projections $m_l$ and $m_s$. In such cases one has solutions of Eq. (44) with a given energy which are finite matrices in the degenerate subspace of this eigenenergy.

To write this formally let us denote by $\phi_{n\nu_n}(x)$ the degenerate eigenstates of $\hat{H}_x$ with energy $E_n$. Then

$$\rho(x,x') = \sum_{\nu_n,\nu'_n} \rho_{n\nu_n,n\nu'_n}\phi_{n\nu_n}(x)\phi^*_{n\nu'_n}(x') \tag{47}$$

is a particular case of the solution Eq. (45) with an arbitrary (apart of the general conditions Eq. (27)) matrix of coefficients $\rho_{n\nu_n,n\nu'_n}$ in the degenerate (and usually finite) subspace spanned by $\phi_{n\nu_n}(x)$ with fixed $n$. Such finite size density matrices in degenerate energy level subspaces are found fairly often in realistic physical systems. The reason is that it is much easier to select the energy of the system than to fix the additional physical quantities (like angular momentum projections, etc) which resolve the degeneracy.

## 3.3 Open systems

### 3.3.1 Relaxation time approximation

When the interaction $V_{xq}$ between the parts of the system is not zero there appears an additional term in the equation for $\rho$,

$$i\hbar\frac{\partial \rho_{op}(t)}{\partial t} = [\hat{H}_x, \rho_{op}] + Tr_q\left([\hat{V}_{xq}, R_{op}]\right) \tag{48}$$

Writing this term explicitly

$$Tr_q\left([\hat{V}_{xq}, R_{op}]\right) = \int dqdq'\Big(<q|\hat{V}_{xq}|q'><q'|R_{op}|q> - $$
$$- <q|R_{op}|q'><q'|\hat{V}_{xq}|q>\Big)$$

we notice that unlike what happened with $Tr_q\left([\hat{H}_q, R_{op}]\right)$ term in Eq. (41) this expression does not vanish. While one still could rename $q \longleftrightarrow q'$ in say the last term but the order of $<q|R_{op}|q'>$ and $<q'|V_{xq}|q>$ can obviously not be changed since they are (in general non commuting) matrices in the $x$-subspace.

The remaining dependence of the above expression on the matrix elements of R with respect to the states of the $q$-part of the system means that the equation (48) is not closed. One must in principle consider additional equations for $<q|R|q'>$, solve these equations in terms of $\rho$ and then insert the solution in the equation (48) arriving at a closed equation. In practice however one often deals with the unobserved $q$-part

which to a good approximation behaves as an "environment". This means that it is not disturbed much by the interaction with the $x$-part. The solution for $< q|R|q' >$ and the way it influences the equation (48) for $\rho$ will then have universal features.

There exist formal methods to find the most suitable description of interactions with such environments but these methods are quite involved and actually are still a part of an active field of research, cf. Ref. [5]. Instead we will use a simple ansatz - the relaxation time approximation to illustrate several important features of the dynamics of open systems. This approximation applies when the $q$–part of the composite system is in a thermal equilibrium with temperature T and moreover plays the role of the thermostat (heat bath) with respect to the $x$–part. This means that its interaction with the $x$–part is such that it tends to bring the $x$–part to the equilibrium with the same temperature without changing its own equilibrium state during this process.

As is well known from statistical physics the density matrix in a thermal equilibrium has the form

$$\rho_0 = Z^{-1} \exp(-\hat{H}_x/T)$$

with $Z = Tr \exp(-\hat{H}_x/T)$. Using this expression one writes the following approximation for the equation for $\rho$

$$\frac{\partial \rho}{\partial t} + \frac{i}{\hbar}[H_x \,, \rho] = -\frac{1}{\tau}(\rho - \rho_0) \tag{49}$$

The right hand side replaces $-i/\hbar$ times the last term in (48). To understand its effect let us denote $\Delta\rho(t) = \rho(t) - \rho_0$ and using that $\rho_0 \sim \exp(-H_x/T)$ commutes with $H_x$ rewrite the above equation as

$$\frac{\partial \Delta\rho}{\partial t} + \frac{i}{\hbar}[H_x \,, \Delta\rho] = -\frac{1}{\tau}\Delta\rho \tag{50}$$

It is straightforward to show that the formal solution of this equation is

$$\rho(t) - \rho_0 = \exp(-iH_x t/\hbar)\left[\rho(0) - \rho_0\right] \exp(iH_x t/\hbar)\exp(-t/\tau) \tag{51}$$

One sees that in this approximation one has an exponential relaxation towards the equilibrium with the relaxation time constant $\tau$. The value of $\tau$ must be regarded as a phenomenological parameter which should be chosen to fit a given experimental situation. This approximation is called the relaxation time approximation.

### 3.3.2   T1 and T2 - thermal relaxation and dephasing times

Since $\rho_0$ is $\sim \exp(-H_x/T)$ it commutes with $\exp(iH_x t/\hbar)$ and therefore the above solution can be written as

$$\rho(t) = \rho_0(1 - e^{-t/\tau}) + \exp(-iH_x t/\hbar)\,\rho(0)\,\exp(iH_x t/\hbar)\exp(-t/\tau) \tag{52}$$

In the basis of the eigenstates of $H_x$ the last term in this solution is just the right hand side of Eq. (43) multiplied by $\exp(-t/\tau)$. It exhibits the interplay between the effect of the second term in the equation for $\rho$ which alone would produce the oscillatory (or constant in time for degenerate energy levels) behaviour and the damping effect of the last term in this equation. As the last term in the above solution for $\rho(t)$ decreases and vanishes for $t \gg \tau$ the first term grows to its maximum of $\rho_0$ reaching the thermal equilibrium limit.

It is possible and useful to separate diagonal and off diagonal terms in the solution Eq. (52) written in the basis of $H_x$[3]

$$
\begin{aligned}
w_n(t) \equiv \rho_{nn}(t) &= Z^{-1}e^{-E_n/T}(1-e^{-t/\tau}) + w_n(0)e^{-t/\tau} \\
\rho_{mn,m\neq n}(t) &= \rho_{mn,m\neq n}(0)e^{-i(E_m-E_n)t/\hbar}e^{-t/\tau}
\end{aligned}
\tag{53}
$$

Since $w_n(t)$'s give the probabilities of possible $E_n$'s their time development reflects the energy exchange between the system and the environment, i.e. the heat bath driving the system towards the thermal equilibrium. The off diagonal terms describe oscillations of the relative phases and their decay reflects the "dephasing" effect of the interaction with the random environment.

One often distinguishes the speed of the two processes - the thermal relaxation and the dephasing by using two different relaxation time parameters - $\tau 1$ and $\tau 2$ or more commonly denoted as $T1$ and $T2$. This was apparently first introduced in the context of the Bloch equation describing MRI control of nuclear spins. It will be discussed below in Section 4.

Detailed model calculations, in which the environment is typically represented by a collection of harmonic oscillators, Ref. [6] have shown that the decoherence time scales are typically (but not always) many orders of magnitude shorter than the thermal relaxation, Ref. [7].

We note that unlike in closed systems the entropy of the solution Eq. (52) depends on time. As an example consider the case when the system was initially in a pure state $\rho(0) = |\phi><\phi|$. Expanding in the eigenstates $|\phi_n>$ of $H_x$ it is $\rho(0) = \sum_{mn} c_m c_n^* |\phi_m><\phi_n|$ so that $\rho_{mn} = c_m c_n^*$. The entropy Eq. (24) associated with such $\rho$ is increasing from zero for the initial pure state to the thermal equilibrium value $S_{thermal} = <E>/T + \ln Z = (<E> + F)/T$ in terms of the average energy $<E> = \sum_m E_m \exp(-E_m/T)/Z$ and the free energy $F = -T \ln Z$.

---

[3]Readers are encouraged to write these equations and repeat this discussion for the (very common) case of energy levels with degeneracies, cf., Section 3.2.3

# 4  Two Level Systems. The Bloch Equations

## 4.1  Why only two levels?

Hilbert space of any *realistic* quantum mechanical system is infinitely dimensional. However one frequently isolates and deals with a finite number of levels. This is possible when the dynamics of the amplitudes to populate these levels is to a good approximation decoupled from the rest of the Hilbert space. Spin is a typical example. In the non relativistic approximation in most systems the Hamiltonian is a sum of an orbital and the spin part so that one can treat these parts separately and for the spin part have a reduced problem with a finite (= 2s+1) number of levels .

When it comes to the density matrix there is actually a deeper reason for restricting the considerations to a finite number of levels. As we have seen in Section 1 any system emerging off an interaction with another system will in general be in a mixed state and must be described by a density matrix. Most of quantum systems studied in a laboratory are of this type since they experience some degree of uncontrolled interaction inside a device where they were prepared or measured or on their way towards the experimental area. These could be interactions with, e.g. leftover molecules in a vacuum chamber, stray electromagnetic waves present in space, the walls and other parts of the real world laboratory, etc.

Of course experimentalists are making special efforts to reduce these uncontrollable interactions to a minimum and to resolve pure states of the system characterized by a complete set of quantum numbers. Technically this is more difficult to achieve for states which are *degenerate* or in close energetic proximity to other states. Such states are *much more easily mixed* by uncontrolled disturbances and their resolution requires more elaborate methods and devices. E.g., a momentum state of a free particle is relatively easily selected by measuring its time of flight through a known distance. Its spin however can be selected only by a special, e.g. Stern–Gerlach type of a device.

We have already addressed this situation in Section 3.2.3. Not resolving degenerate or almost degenerate levels means that the system is in a mixed state "with respect" to this, usually finite and small, number of levels. For a free particle that would mean that $\rho(\mathbf{r}, s; \mathbf{r}', s') = \exp[i\mathbf{p}(\mathbf{r} - \mathbf{r}')]\rho(s, s')$, i.e. a factorized density matrix describing a pure state in the orbital variables and non factorized but finite (say $2 \times 2$ for spin 1/2) density matrix for the spin. An atom or a nucleus with a non zero ground state spin J emerges out of an accelerator with a quite accurately resolved velocity but in a $(2J + 1) \times (2J + 1)$ density matrix for spin variables.

## 4.2   Expansion in a complete set of matrices.

Motivated by above observations we will now illustrate some of the concepts discussed in the preceding sections by considering the density matrix description of a simplest case of the finite number of levels – the two level system. The corresponding density matrix is a hermitian $2 \times 2$ matrix with unit trace

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{12}^* & 1 - \rho_{11} \end{pmatrix} \tag{54}$$

In order to describe an arbitrary such matrix and to be able to easily control its most general variations it is convenient to introduce a fixed basis in the space of all $2 \times 2$ matrices. The simplest such basis would be the obvious

$$\rho = \rho_{11} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \rho_{12} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \rho_{12}^* \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + (1 - \rho_{11}) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} ,$$

as every $2 \times 2$ matrix can be written as such linear combination with, in general, complex coefficients. It is however much more convenient to use for $\rho$ another set of four matrices consisting of the unit matrix I and the three Pauli matrices $\sigma_x$, $\sigma_y$, $\sigma_z$. We recall that in the standard representation *in which $\sigma_z$ is diagonal* this set is

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{55}$$

The matrices in this set are hermitian so that the expansion of $\rho$ will involve only real coefficients. Renaming for convenience

$$\sigma_x, \sigma_y, \sigma_z \;\to\; \sigma_1, \sigma_2, \sigma_3$$

we have

$$\rho = \rho_0 I + \sum_{i=1}^{3} \rho_i \sigma_i \quad ; \qquad \rho_0, \; \rho_i - \text{real} \tag{56}$$

But the main advantage of this set is the existence of the relations

$$Tr \, \sigma_i = 0 \quad ; \quad Tr \, \sigma_i \sigma_j = 2\delta_{ij} \tag{57}$$

The first follows, e.g. from the explicit form of the $\sigma$'s whereas the second relation follows from the first and from the basic relation for the Pauli matrices

$$\sigma_i \, \sigma_j = \delta_{ij} + i \, \epsilon_{ijk} \, \sigma_k \tag{58}$$

Eq. (57) can be viewed as the "orthogonality" property between the members of the set $\{I\,,\,\sigma_i\}$ so that for instance the coefficients in (56) can be easily found by multiplying both sides with the corresponding matrix and applying the trace operation,

$$\rho_0 = \frac{1}{2}Tr\,\rho = \frac{1}{2} \qquad , \qquad \rho_i = \frac{1}{2}\,Tr\,\sigma_i\,\rho \equiv \frac{1}{2} <\sigma_i> \tag{59}$$

It is useful to observe that when (59) are inserted in the expansion (56) the analog of the completeness relation for the set $I\,,\,\sigma_i$ is found

$$\sum_i (\sigma_i)_{\alpha\beta}(\sigma_i)_{\gamma\delta} = 2(\delta_{\alpha\delta}\delta_{\beta\gamma} - \frac{1}{2}\delta_{\alpha\beta}\delta_{\gamma\delta}) \tag{60}$$

All the above conclusions hold independently of the particular representation (55) for the Pauli matrices. Indeed transforming to a different representation is equivalent to a unitary transformation

$$\sigma_i \to \sigma_i' = U\sigma_i U^+ \tag{61}$$

The relations (57) retain their form also for the primed $\sigma$'s. One can therefore expand $\rho$ in the primed set $\rho = \rho_0\,I + \sum_i \rho_i'\sigma_i'$ with the coefficients $\rho_i'$ given by the same Eqs. (59) in terms of the primed $\sigma$'s. The unit matrix and the corresponding expansion coefficient $\rho_0$ obviously do nor change.

It is easy and instructive to examine how the primed $\rho$'s are related to the unprimed ones. For this we note that the unitary transformation (61) is equivalent to an orthogonal transformation among the $\sigma$–matrices. Indeed one can expand

$$\sigma_i' \equiv U\sigma_i U^+ = \sum_j A_{ij}\sigma_j$$

since the left hand side is a hermitian $2 \times 2$ matrix with zero trace. For a given $U$ the expansion coefficients form a $3 \times 3$ matrix $A_{ij}$

$$A_{ik} = \frac{1}{2}Tr\sigma_k\sigma_i' = \frac{1}{2}Tr\left(\sigma_k U\sigma_i U^+\right)$$

The matrix elements $A_{ik}$ are real[4] and obey the relations

$$\sum_k A_{ik} A_{jk} = \delta_{ij} \;\; ; \;\; \sum_k A_{ki} A_{kj} = \delta_{ij} \tag{62}$$

which can be verified by explicit calculations using the completeness relations (60) together with $Tr\, \sigma_i' \sigma_j' = Tr\, \sigma_i \sigma_j = 2\delta_{ij}$. These relations written in a compact form

$$AA^T = 1 \;\; ; \;\; A^T A = 1$$

show that $A$ is an orthogonal matrix. Thus the unitary transformation in the spinor Hilbert space causes orthogonal transformation among the 3 spin matrices $\sigma_i$.

Now we can compare the expansion of a given $\rho$ in terms of the primed and unprimed $\sigma$'s. In this way we find that

$$\sum_i \rho_i' \sigma_i' = \sum_j \rho_j \sigma_j \;\; \rightarrow \;\; \rho_i' = \frac{1}{2} \sum_j \rho_j Tr \sigma_i' \sigma_j = \sum_j A_{ij} \rho_j \tag{63}$$

Thus under unitary transformations of the basis of the two dimensional Hilbert space of the spin variables the coefficients $\rho_i$ are transforming as *components of an ordinary 3–vector under rotations* of a reference frame.

In the language of the group theory the matrices U in (61) are matrices of the fundamental representation of the SU(2) group of the spin variables (strictly speaking they belong to the group U(2) but the difference is just a phase which can be ignored in the present case). The matrices $A_{ij}$ form the so called adjoint representation of this group. As is well known this representation is isomorphic to the O(3) group of rotations as we have indeed just "discovered".

## 4.3   Polarisation vector. Bloch sphere

It is customary to denote the averages in Eq. (59) as

$$P_i = <\sigma_i> \tag{64}$$

---

[4]To recheck - $A_{ik}$ can be written as a trace of Hermitian operator

$$2A_{ik} = Tr\sigma_k \sigma_i' = \frac{1}{2} Tr[\sigma_k \sigma_i' + \sigma_i' \sigma_k]$$

and therefore is real. More explicit calculation

$$2A_{ik}^* = Tr\sigma_k^* \sigma_i'^* = Tr\sigma_k^T \sigma_i'^T = Tr\,(\sigma_i' \sigma_k)^T = 2A_{ik}$$

and to refer to these quantities as the components of the polarization vector $\mathbf{P}$ writing

$$\rho = \frac{1}{2}(I + \mathbf{P} \cdot \boldsymbol{\sigma}) \tag{65}$$

where the vector notation is introduced for $P_1$, $P_2$, $P_3$ and $\sigma_1$, $\sigma_2$, $\sigma_3$. The matrix elements of $\rho$, Eq. (54) are related to $P_i$ as

$$\rho_{11} = \frac{1}{2}(1 + P_3) \ , \ \ \rho_{22} = \frac{1}{2}(1 - P_3) \ , \ \ \rho_{12} = \rho_{21}^* = \frac{1}{2}(P_1 - iP_2) \tag{66}$$

The meaning of $\mathbf{P}$ is physically transparent. First let us look at its direction $\mathbf{n} = \mathbf{P}/P$. Since $I$ commutes with $\mathbf{P} \cdot \boldsymbol{\sigma}$ in the expression (65) it is clear that the eigenstates of $\rho$ coincide with the eigenstates of $\mathbf{n} \cdot \boldsymbol{\sigma}$ . Thus $\mathbf{n}$ determines the direction of polarization of the spin of the state described by the density matrix $\rho$ . The degree of the polarization of this state, i.e. the eigenvalues of $\rho$ are determined by the magnitude of $P$. Indeed the eigenvalues of $\mathbf{n} \cdot \boldsymbol{\sigma}$ are equal to $+1$ and $-1$ for any $\mathbf{n}$ since (a) $\mathbf{n} \cdot \boldsymbol{\sigma}$ can be obtained from $\sigma_3$ by rotation, (b) according to the discussion after Eq.(61) this rotation is equivalent to a unitary transformation of $\sigma_3$ and (c) the unitary transformation does not change the eigenvalues. Therefore the eigenvalues of $\rho$ are

$$w_1 = \frac{1}{2}(1 + P) \ \ , \ \ w_2 = \frac{1}{2}(1 - P)$$

where $P = \sqrt{P_1^2 + P_2^2 + P_3^2}$. As a simple example consider for instance the case $P_1 = P$, $P_2 = P_3 = 0$. Then

$$\rho = \frac{1}{2}(I + P\sigma_1)$$

so that the eigenfunctions of $\rho$ are those of $\sigma_1$ and the eigenvalues are as given above.

To understand better the physical meaning of $P$ we note that the particular case when $P = 0$ the state described by $\rho$ is maximally mixed, $Tr \, \rho^2 = 1/2$, cf., Sections 2.5, 2.7. The eigenstates of $\rho$ *are not determined* in this case and in fact can be chosen as any pair of orthogonal spinors. The opposite pure state situation corresponds to the polarization vector with unit length, $P = 1$. Indeed using

$$Tr\rho^2 = Tr\frac{1}{4}(I + \mathbf{P} \cdot \boldsymbol{\sigma})^2 = \frac{1}{4}Tr\left[1 + 2\mathbf{P} \cdot \boldsymbol{\sigma} + (\mathbf{P} \cdot \boldsymbol{\sigma})^2\right] = \frac{1}{2}(1 + P^2)$$

the condition (34) for a general $\rho$ (and $P$ as the vector length by definition non negative) gives $0 \leq P \leq 1$ while the pure state limit $Tr\rho^2 = 1$ is with $P = 1$.

The above discussion can be summarized in a compact way by the concept of a Bloch sphere. This is a sphere which has a unit radius $P = 1$ in the 3 dimensional

space of the "vectors" $\mathbf{P}$. Every point of this sphere defines a different quantum state of a two level system. The points on the surface of the sphere where $P = 1$ denote all possible pure states, while all the points in the interior denote all possible mixed state. The center $P = 0$ is maximally mixed state for which $\rho = (1/2)I$. For any other point the direction $\mathbf{n} = \mathbf{P}/P$ of the vector $\mathbf{P}$ drawn to this point defines the eigenstates of $\rho$. They are the eigenstates of the spin projection $\mathbf{n} \cdot \boldsymbol{\sigma}$. The magnitude of this $P$ or more precisely its deviation from unity defines how much this state is mixed.

## 4.4   Dynamical Bloch equations

We now consider dynamical equations for a two level system. We start with the case when the system is closed. The Liouville – von Neumann equation ( 40) written for a $2 \times 2$ density matrix (65) and projected on $\sigma_i$ is

$$\frac{dP_i}{dt} = \frac{i}{2\hbar} \sum_k P_k \, Tr \, (\sigma_i[\sigma_k \, , \, H]) = -\frac{1}{\hbar} \sum_{kl} \epsilon_{jkl} P_k Tr \, H\sigma_l \tag{67}$$

or in other words

$$\frac{d\mathbf{P}}{dt} = -\frac{1}{\hbar}\mathbf{P} \times Tr \, H\boldsymbol{\sigma} \tag{68}$$

The Hamiltonian must be a $2 \times 2$ matrix and could therefore be written as

$$H = H_0 + \sum_i H_i\sigma_i$$

with real coefficients. In the equation for $\mathbf{P}$ above only the $H_i$ components appear. The term $H_0$ which is proportional to a unit matrix gives a constant shift to the energy eigenvalues and does not effect the eigenfunctions. It therefore does not lead to any physical effects and can be disregarded. As a concrete example let us consider the case of a spin $1/2$ particle (say electron or a proton) in a magnetic field $\mathbf{B}$. In the Chapter Motion in External Electromagnetic Field we discuss the Schrödinger equation for such a particle. In the case when $\mathbf{B}$ is uniform in space the spin part of the Hamiltonian

$$H = -\boldsymbol{\mu} \cdot \mathbf{B} \ , \ \ \boldsymbol{\mu} = \gamma\mathbf{s} = \frac{\hbar\gamma}{2}\boldsymbol{\sigma} \tag{69}$$

can be treated separately from the orbital motion. Here $\gamma$ is the gyromagnetic ratio.

Since

$$TrH\sigma_i = -\hbar\gamma B_i$$

the equation for the polarization vector becomes

$$\frac{d\mathbf{P}}{dt} = \gamma(\mathbf{P} \times \mathbf{B}) \tag{70}$$

This equation has the same form as the classical equation for a magnetic moment $\mathbf{M} \equiv \mathbf{P}$. The vector $\mathbf{P}$ precesses around the (instantaneous) direction of $\mathbf{B}$. For a constant $\mathbf{B}$ the frequency of the precession is equal $\gamma B$, i.e. the difference between the energies of the two eigenstates of the system divided by $\hbar$.

Realistic spin degrees of freedom can never be completely isolated from the surrounding medium. In many cases the influence of the latter can be considered as that of a thermal bath which drives the spin to thermal equilibrium. The dynamics can then be described by the relaxation time approximation Eq. (50). In Section 3.3.2 we have indicated that different relaxation time constants commonly denoted as $T1$ and $T2$ are expected to describe the processes of the thermal equilibration and dephasing.

Let us examine how is this applied in the present two level spin system. Let us start with the simplest case of the time independent $\mathbf{B}$. The expression for the average energy

$$\langle E \rangle = Tr H \rho = \frac{1}{2}\mathbf{P} \cdot Tr H \boldsymbol{\sigma} = -\frac{\hbar\gamma}{2}\mathbf{P} \cdot \mathbf{B}$$

shows that the density matrix dynamics as described by the motion of the polarization vector $\mathbf{P}$ in the Bloch sphere can be viewed as a combination of two - the component parallel to $\mathbf{B}$ in which the energy is changing and another in the planar section of the sphere perpendicular to $\mathbf{B}$, i.e. with the constant projection $\mathbf{P} \cdot \mathbf{B}$ and conserved $\langle E \rangle$. Clearly for a closed system only the second type will be realized while open system with thermal bath environment will have both.

These insights indicate that the $T1$ relaxation time should be associated with the component $\mathbf{P}_{\parallel}$ of $\mathbf{P}$ parallel to $\mathbf{B}$ while the dephasing time constant $T2$ with the perpendicular to $\mathbf{B}$ component $\mathbf{P}_{\perp}$. This understanding is used in the important case of the nuclear magnetic resonance (NMR) in which periodic time dependent magnetic field $\mathbf{B}_1(t)$ is applied in addition to the constant field $\mathbf{B}$ and perpendicular to it.

The environment for this system is assumed to be described by the thermal equilibrium density matrix

$$\rho_{th} \equiv \frac{exp(-H/T)}{Tr \exp(-H/T)}$$

for the Hamiltonian Eq. (69) with a constant $\mathbf{B}$. Using

$$H = -E_0 \mathbf{n} \cdot \boldsymbol{\sigma} \quad \text{with} \quad E_0 \equiv \hbar\gamma B/2 \quad , \quad \mathbf{n} = \mathbf{B}/B$$

and diagonalizing $\exp(-H/T)$ it is straightforward to obtain[5]

$$\rho_{th} = \frac{1}{2}\left[1 + \frac{\mathbf{B}\cdot\boldsymbol{\sigma}}{B}\tanh\left(\frac{\gamma\hbar B}{2T}\right)\right] \tag{71}$$

with the corresponding polarization vector

$$\mathbf{P}_{th} = Tr\rho_{th}\boldsymbol{\sigma} = (\mathbf{B}/B)\tanh(\gamma\hbar B/2T)$$

Using this and the considerations of the two relaxation time constants a very successful *phenomenological* equation to describe NMR was suggested by F. Bloch in 1946,

$$\frac{d\mathbf{P}}{dt} = \gamma\left[\mathbf{P}\times(\mathbf{B} + \mathbf{B}_1(t))\right] - \frac{\mathbf{P}_\perp}{T2} - \frac{\mathbf{P}_\parallel - \mathbf{P}_{th}}{T1} \tag{72}$$

Important and physically interesting details of the applications of the Bloch equation are discussed in the special literature on NMR, cf., Ref. [10].

# 5 Coherence and its Loss (Decoherence) in Quantum Systems

What is coherence? It is difficult to give a short definition. It is essentially a degree of sensitivity of physical phenomena involving waves (optical, quantum, others) to relative phases of the waves. Interference is the obvious and most often discussed such phenomenon. A decrease of the sensitivity to wave phases caused by external conditions is called decoherence or dephasing of waves.

Quantum mechanically the presence of an external potential (i.e. with no own degrees of freedom, or with "frozen" degrees of freedom having energy gaps too large to be excited) can not cause decoherence – e.g. it will not "suppress" interferences. Only interactions with "unobserved" degrees of freedom ("environment") which can change their state can cause decoherence. We will now discuss this in some details.

## 5.1 Interference in the presence of an environment

### 5.1.1 Ideal case - no environment. Pure state

Let us consider interference of two quantum "waves" $\Psi_1(x)$ and $\Psi_2(x)$ where $x$ denotes the generalized coordinates $x = x_1, ..., x_N$. The classical example is the quantum

---

[5]The eigenvalues and eigenfunctions of $H$ are respectively $E_\pm = \pm E_0$ and $|\pm\mathbf{n}\rangle$ with $\mathbf{n}\cdot\boldsymbol{\sigma}|\pm\mathbf{n}\rangle = \pm|\pm\mathbf{n}\rangle$. So $e^{-\beta H} = e^{-\beta E_0}|\mathbf{n}\rangle\langle\mathbf{n}| + e^{\beta E_0}|-\mathbf{n}\rangle\langle-\mathbf{n}|$. Using $\mathbf{n}\cdot\boldsymbol{\sigma} = |\mathbf{n}\rangle\langle\mathbf{n}| - |-\mathbf{n}\rangle\langle-\mathbf{n}|$ and $1 = |\mathbf{n}\rangle\langle\mathbf{n}| + |-\mathbf{n}\rangle\langle-\mathbf{n}|$ obtain $e^{-\beta H} = \sinh\beta E_0 + \cosh\beta E_0\,\mathbf{n}\cdot\boldsymbol{\sigma}$ from which Eq. (71) follows.

version of the Young two slits experiment or incoming and reflected waves described in a simpler example in the next section. The interference of the "waves" $\Psi_1$ and $\Psi_2$ arises, e.g., if one measures

$$
\begin{aligned}
w(x) &= |\Psi_1(x) + \Psi_2(x)|^2 = |\Psi_1(x)|^2 + |\Psi_2(x)|^2 + 2Re[\Psi_1(x)\Psi_2^*(x)] = \\
&= w_1(x) + w_2(x) + 2\sqrt{w_1(x)w_2(x)}\cos[\phi_1(x) - \phi_2(x)]
\end{aligned} \tag{73}
$$

with

$$
w_1(x) = |\Psi_1(x)|^2 \quad , \quad w_2(x) = |\Psi_2(x)|^2
$$

and $\phi_{1,2}(x)$ denoting the phases of $\Psi_{1,2}(x)$. The last term in the expression for $w(x)$ represents the degree of the interference and determines the range of the values of $w(x)$

$$
(\sqrt{w_1(x)} - \sqrt{w_2(x)})^2 \leq w(x) \leq (\sqrt{w_1(x)} + \sqrt{w_2(x)})^2 \tag{74}
$$

which for $w_1 = w_2$ is

$$
0 \leq w(x) \leq 4w_1(x) = 4w_2(x)
$$

This range can typically be examined by scanning the values of the coordinate $x$.

### 5.1.2 Interference in a mixed state

Let us examine what happens with this term in the presence of an "environment", i.e. when the waves interact with uncontrolled and unobserved part of the system. Denoting the degrees of freedom of the unobserved part as $q = q_1, ..., q_M$ we have that the $x$-part of the system is in a mixed state and the two waves must be described by the wave functions $\Psi_1(x, q)$ and $\Psi_2(x, q)$. The expression for $w(x)$ becomes

$$
w(x) = \int dq|\Psi_1(x,q) + \Psi_2(x,q)|^2 = w_1(x) + w_2(x) + 2Re \int dq[\Psi_1(x,q)\Psi_2^*(x,q)] \tag{75}
$$

with

$$
w_1(x) = \int dq|\Psi_1(x,q)|^2 \quad , \quad w_2(x) = \int dq|\Psi_2(x)|^2
$$

All the terms are now "averaged" over the states of the environment. However while the expressions for $w_1(x)$ and $w_2(x)$ are averages over positive functions the averaging in the interference term is over the expression involving the difference of the phases of the two waves

$$
2Re \int dq[\Psi_1(x,q)\Psi_2^*(x,q)] = 2\int dq|\Psi_1(x,q)||\Psi_2(x,q)|\cos[\phi_1(x,q) - \phi_2(x,q)] \tag{76}
$$

One can see that only for particular cases of environment independent phases or environment independent phase difference

$$\delta(x) \equiv \phi_1(x, q) - \phi_2(x, q)$$

one will observe a significant interference effect.

For the waves interacting in a different manner with (passing through different parts of) a sufficiently random environment one will have the phase difference $\delta(x, q)$ changing as a function of environment coordinates $q$. The integration range of $q$ is determined by the amplitudes product $|\Psi_1(x, q)||\Psi_2(x, q)|$. If the change of the phase difference $\Delta\delta(x, q)$ over this range is $\gg 2\pi$ one will in general have a significant decreasing of the integral $\int dq$ over a range of $x$'s in the interference term. Such a situation corresponds to dephasing or decoherence.

### 5.1.3 Comparison with optics

The notions of coherence and dephasing appear naturally in optics. There one deals with waves which vibrate rapidly in time at every point of space through which they propagate. Ignoring for simplicity the polarization properties of light one can represent monochromatic light by a scalar function

$$U(\mathbf{r}, t) = A \cos[\mathbf{k} \cdot \mathbf{r} - \omega t + \phi_0] \tag{77}$$

However, monochromatic light is an idealization and in reality one has random fluctuations in the amplitude and the phase. For thermal light these fluctuations are mainly due to the randomness of spontaneous emission from atoms in the source of light. For the light emitted by laser sources the origin of the fluctuations are temperature variations, mechanical vibrations of the cavity and, always present, spontaneous emissions.

Given such fluctuations light which is most closed to monochromatic (called quasi-monochromatic) may be represented as a generalization of the above expression

$$U(\mathbf{r}, t) = A(\mathbf{r}, t) \cos[\phi(\mathbf{r}, t) - \bar{\omega} t] \tag{78}$$

with time dependent $A(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ having an effective bandwidth $\Delta\omega$ which is much smaller than its mean frequency $\bar{\omega}$

$$\frac{\Delta\omega}{\bar{\omega}} \ll 1 \tag{79}$$

Let us now consider superposition of two such quasi-monochromatic waves

$$
\begin{aligned}
U(\mathbf{r}, t) &= U_1(\mathbf{r}, t) + U_2(\mathbf{r}, t) = \\
&= A_1(\mathbf{r}, t) \cos[\phi_1(\mathbf{r}, t) - \bar{\omega}t] + A_2(\mathbf{r}, t) \cos[\phi_2(\mathbf{r}, t) - \bar{\omega}t]
\end{aligned} \tag{80}
$$

The instantaneous intensity is proportional to the square of $U(\mathbf{r}, t)$

$$
I(\mathbf{r}, t) = U^2(\mathbf{r}, t) = I_1(\mathbf{r}, t) + I_2(\mathbf{r}, t) + I_{12}(\mathbf{r}, t) \tag{81}
$$

where

$$
\begin{aligned}
I_1(\mathbf{r}, t) &= A_1^2(\mathbf{r}, t) \cos^2[\phi_1(\mathbf{r}, t) - \bar{\omega}t] \\
I_2(\mathbf{r}, t) &= A_2^2(\mathbf{r}, t) \cos^2[\phi_2(\mathbf{r}, t) - \bar{\omega}t]
\end{aligned} \tag{82}
$$

and the interference term

$$
\begin{aligned}
I_{12}(\mathbf{r}, t) &= A_1(\mathbf{r}, t) A_2(\mathbf{r}, t) \{\cos[\phi_1(\mathbf{r}, t) + \phi_2(\mathbf{r}, t) - 2\bar{\omega}t] + \\
&\quad + \cos[\phi_1(\mathbf{r}, t) - \phi_2(\mathbf{r}, t)]\}
\end{aligned} \tag{83}
$$

Because of the time variations of optical fields, one can not measure the instantaneous intensity but only its average over some time interval $\Delta t$

$$
\langle I(\mathbf{r}, t) \rangle \equiv \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} I(\mathbf{r}, t') dt' \tag{84}
$$

Optical time scales are

$$
T = \lambda/c \sim 600nm/(300 \cdot 10^6 \, m/\sec) \sim 2 \cdot 10^{-15} \sec
$$

which are much shorter than typical measurement $\Delta t$

$$
\Delta t \gg T \quad \rightarrow \quad \bar{\omega}\Delta t \gg 1 \tag{85}
$$

This means that the first term in $I_{12}(\mathbf{r}, t)$ vanishes upon the averaging while the $\cos^2$'s in the intensities $I_1$ and $I_2$, Eq. (82), can be replaced by their average values of $1/2$. This gives

$$
\begin{aligned}
\langle I(\mathbf{r}, t) \rangle &= \frac{1}{2}\langle A_1^2(\mathbf{r}, t) \rangle + \frac{1}{2}\langle A_2^2(\mathbf{r}, t) \rangle + \\
&\quad . \quad + \langle A_1(\mathbf{r}, t) A_2(\mathbf{r}, t) \cos[\phi_1(\mathbf{r}, t) - \phi_2(\mathbf{r}, t)] \rangle
\end{aligned} \tag{86}
$$

As we see the averaging over the environment coordinates $q$ in the expressions like Eq. (75) is played in optics by the averages over the time interval $\Delta t$ of the measurement of the optical wave.

The relevant time scale of the amplitudes and the phases in the expression (86) is given by the reciprocal bandwidth $1/\Delta\omega$. For ideal monochromatic waves with $\Delta\omega \to 0$ these quantities are independent of time and one would have a full interference pattern. For realistic quasi-monochromatic waves the correlations of the random variations of the phases are most important in determining the results of the time averaging of the interference term, i.e. of the possible dephasing induced by the measurement process. We refer to Ref. [8] for the discussions of how such correlations are seen in the common interference setups. In short one can conclude that the role of the "environment" in optical waves is played by the matter which emits the wave and/or through which the wave propagates.

## 5.2   A simple example - interference of scattering waves

Let us consider interference of incoming and scattered waves in a scattering. For simplicity let us limit ourselves to just one dimension.

### 5.2.1   Elastic scattering - coherence

The incoming wave at $x \to -\infty$ is

$$\psi_i(x)_{x\to-\infty} = Ae^{ikx}$$

Let us assume that this wave gets reflected off a wall placed near $x = 0$. The precise position of the wall and its nature will be immaterial in our discussion.

Let us start with the elastic scattering situation, i.e when the wall does not have (or has frozen) internal degrees of freedom. The reflected wave will then have the form

$$\psi_r(x)_{x\to-\infty} = Are^{-ikx}$$

where $r$ is the reflection coefficient. Again for simplicity let us assume "total reflection" , i.e. $|r| = 1$, $r = e^{2i\delta}$ where $2\delta$ is a "reflection phase" consistent with the possibility that if the wall is not infinitely high the wave penetrates into the region "behind the wall".

The entire wavefunction is

$$\psi(x)_{x\to-\infty} = A(e^{ikx} + re^{-ikx})$$

The probability density to measure $x$ at large $x \to -\infty$

$$\rho(x) = |\psi(x)|^2 = |A|^2(1 + 1 + 2Re\, e^{ikx}r^*e^{ikx}) = 2|A|^2\{1 + \cos[2(kx - \delta)]\} \quad (87)$$

The last term is the result of the interference of the incoming and scattered waves. Its presence causes $\rho(x)$ to oscillate between $\rho_{max} = 4|A|^2$ and $\rho_{min} = 0$ showing maximum interference "contrast" as $x$ changes over the wavelength $\lambda = 2\pi/k$. The waves are fully coherent.

We will now see how the presence of other, unobserved degrees of freedom (environment) influences the interference term.

### 5.2.2    Inelastic scattering - dephasing

Let is assume that the wall and/or the medium behind it has degrees of freedom which we denote by $q$. These can be "vibrations" of the wall or the medium, etc. Their precise nature or dynamics are not important.

The incoming wave is now

$$\Psi_{\text{incoming}}(x, q)_{x \to -\infty} = Ae^{ik_0 x}Q_0(q)$$

where $Q_0(q)$ is the initial wave function of the wall and the medium behind it. In passing we mention that this discussion can be easily generalized to the case of the initial thermal state of the wall.

The reflected wave in this case

$$\Psi_{\text{reflected}}(x, q)_{x \to -\infty} = A\sum_n r_n e^{-ik_n x}Q_n(q)$$

where $Q_n(q)$ are possible states in which the wall/medium can remain after the scattering and $r_n$'s are the corresponding reflection coefficients. The $k_n$ are wave numbers of the reflected waves which in principle can be different if the energies of $Q_n(q)$ are different from the initial $Q_0(q)$.

The entire wave function at asymptotic $x \to -\infty$ is

$$\Psi(x, q)_{x \to -\infty} = A[e^{ik_0 x}Q_0(q) + \sum_n r_n e^{-ik_n x}Q_n(q)]$$

The probability density to measure $x$ at large $x \to -\infty$ is now $\rho(x) = \int |\Psi(x, q)|^2 dq$ which are in fact just diagonal components of the density matrix $\rho(x, x')$ in this case. We obtain

$$\rho(x)_{x \to -\infty} = \int |\Psi(x, q)|^2_{x \to -\infty} dq = |A|^2\{1 + \sum_n |r_n|^2 + 2Re\, e^{ik_0 x}r_0^*e^{ik_0 x}\}$$

where we used the orthonormality of $Q_n$'s, $\int Q_n^*(q)Q_m(q)dq = \delta_{mn}$. Using in addition that $\sum_n |r_n|^2 = 1$ we find

$$\rho(x)_{x\to-\infty} = 2|A|^2\{1 + |r_0|\cos[2(k_0 x - \delta_0)]\} \tag{88}$$

Comparing with the elastic scattering expression (87) we see that the presence of the intrinsic degrees of freedom of the wall/medium is reflected in the presence of $|r_0|$ - the elastic reflection coefficient multiplying the interference term. Since in general $|r_0|$ is smaller than unity the probability $\rho(x)$ now oscillates in a smaller range between $\rho_{max} = 2|A|^2(1 + |r_0|)$ and $\rho_{min} = 2|A|^2(1 - |r_0|)$. This is the effect of the "decoherence" by the "environment". For a typical situation of the environment having many "channels" $Q_n(q)$ the probability of the just the elastic reflection is expected to be very small, $|r_0| \to 0$, leading to the vanishing interference or complete decoherence.

## 5.3 Decoherence and measurements

Decoherence via interactions with unobserved environment plays an important role in the modern attempts to develop the measurement theory beyond a mysterious wave function collapse. A brief review of such attempts can be found in e.g. Ref. [9].

# 6 Quantum Mechanics in Phase Space. Wigner Distribution

## 6.1 Pure states

Phase space description of classical particles is the basis of Hamiltonian formulation and is very useful especially in statistical mechanics and kinetic theory. In quantum mechanics the wave function and the Schrödinger equation describing it are most frequently considered in the coordinate space $\psi(x)$ or using the formal language in the coordinate representation $\langle x|\psi\rangle$. In this form it explicitly gives the probability amplitude of the coordinate[6] but contains full information about the momentum probability amplitude as well. One just needs to evaluate its Fourier transform, i.e. to go to the momentum representation

$$\phi(p) = \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dx\, \psi(x)\, e^{ipx/\hbar}$$

---

[6]For simplicity we limit this discussion here to just one degree of freedom but it is straightforward to generalize this to any number.

Given this it is natural to ask if one can construct on the basis of these two representation of $\psi$ an analogue of the classical combined probability distribution function $f(x, p)$ of both $x$ and $p$ in the phase space. Of course one expects that the uncertainty princ ould prevent such exact analogy. However it turns out that one can introduce functions of both $x$ and $p$ which have many similar properties with the classical phase space distributions.

The most frequently used such function was introduced by Wigner to study quantum corrections to classical statistical mechanics. It is called the Wigner distribution and is defined as

$$W(x, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} da \, \psi^*(x - \frac{a}{2}) \psi(x + \frac{a}{2}) \, e^{ipa/\hbar} \tag{89}$$

The function $W(x, p)$ is real valued and the $x$ and $p$ probability distributions are given naturally by "classical" relations

$$\int dp \, W(x, p) = |\psi(x)|^2 \qquad \text{and} \qquad \int dx \, W(x, p) = |\phi(p)|^2 \tag{90}$$

The first equality is obvious while the last equality is easiest to prove going "backward"

$$
\begin{aligned}
|\phi(p)|^2 &= \frac{1}{2\pi\hbar} \int dy dy' \, \psi^*(y')\psi(y) \, e^{i(p(y-y'))/\hbar} = \\
&= (\text{change to } y' = x - \frac{a}{2} \, , \, y = x + \frac{a}{2}) = \\
&= \frac{1}{2\pi\hbar} \int dx da \, \psi^*(x - \frac{a}{2})\psi(x + \frac{a}{2}) \, e^{i(pa)/\hbar} = \int dx \, W(x, p)
\end{aligned}
$$

We also note that $W(x, p)$ is normalized

$$\int dx dp \, W(x, p) = 1 \tag{91}$$

The above equalities are perhaps the main reason which makes the function $W(x, p)$ the closest quantum analogy with the classical phase space distribution. But as will be detailed below it is not a corresponding distribution of quantum probabilities.

Wigner distribution is straightforwardly generalized to 3 dimensions $(x, p) \to (\mathbf{r}, \mathbf{p})$ and to any number of degrees of freedom. It can also be simply extended to the mixed states defined by density matrices $\rho(x, x')$.

## 6.2 Mixed states. Operators

If one replaces the product of the wavefunctions in the definition Eq. (89) by the density matrix one obtain the generalization of the Wigner distribution to mixed states

$$W(x,p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} da\, \rho(x + \frac{a}{2}, x - \frac{a}{2})\, e^{ipa/\hbar} \equiv \tag{92}$$

$$\equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} da\, \langle x + \frac{a}{2}|\rho_{op}|x - \frac{a}{2}\rangle\, e^{ipa/\hbar}$$

with the inverse relation

$$\rho(x + \frac{y}{2}, x - \frac{y}{2}) = \int dp\, W(x,p)\, e^{ipy/\hbar} \quad \rightarrow \quad \rho(x,x') = \int dp\, W(\frac{x+x'}{2}, p)\, e^{ip(x'-x)/\hbar}$$

The relations (90) become

$$\int dp\, W(x,p) = \rho(x,x) \equiv <x|\rho_{op}|x> \quad , \quad \int dx\, W(x,p) = <p|\rho_{op}|p> \tag{93}$$

The normalization takes the form

$$\int dxdp\, W(x,p) = Tr\rho = 1 \tag{94}$$

and the overlap of two states

$$(2\pi\hbar) \int dxdp\, W_1(x,p)W_2(x,p) = Tr\rho_1\rho_2 \tag{95}$$

In analogy with Eq. (92) one can define the Wigner transformation for any operator $G_{op}$

$$g(x,p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} da\, \langle x + \frac{a}{2}|G_{op}|x - \frac{a}{2}\rangle\, e^{ipa/\hbar}$$

and in this way to map the standard formulation of quantum mechanics in working with functions in the phase space. We refer to Ref. [3] for a review. Let us just add that Wigner transformation is used also outside quantum mechanics. E.g. in signal analysis it allows to combine the time and frequency domain and similarly in mechanical vibrations, or sound waves.

## 6.3 Properties of the Wigner distribution

Inspite of the equalities (90) the function $W(x, p)$ is not the probability distribution in the phase space. The simplest reason is that $W(x, p)$ can take negative values. In fact a theorem exists, Ref. [2], which states that $W(x, p)$ is non negative over the entire phase space only if the corresponding wavefunction $\psi(x)$ is the exponential of a quadratic polynomial. For other wave functions $W(x, p)$ gets negative in some regions of the $x, p$ space.

As a simple illustration of this theorem let us consider the Wigner distributions of the eigenfunctions of harmonic oscillator, Fig. 1. The ground state wave function which is Gaussian has positive Wigner distribution while the excited states have negative valued parts of the distribution.
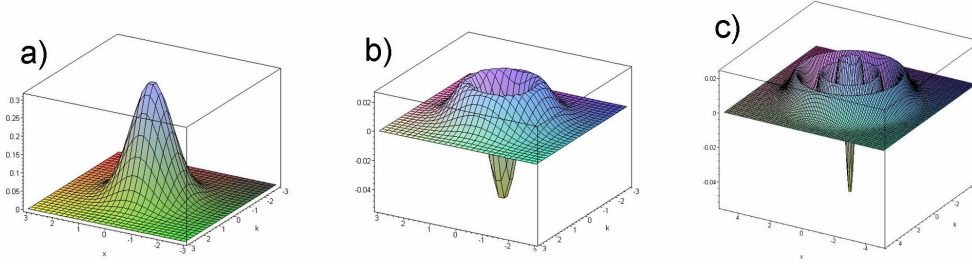


Figure 1: Wigner distributions for the first three eigenstates of harmonic oscillator. By J.S. Lundeen in English Wikipedia

In fact the (easily derivable) expression relating overlaps of two wave functions and the corresponding Wigner distributions

$$|\langle \psi_1 | \psi_2 \rangle|^2 \equiv |\int dx\, \psi_1^*(x)\psi_2(x)|^2 = (2\pi\hbar) \int dx dp W_1(x, p) W_2(x, p) \qquad (96)$$

shows that one must have W's with negative parts to get $\langle \psi_1 | \psi_2 \rangle = 0$ for orthogonal wave functions. The possible negativity of $W(x, p)$ leads to calling it quasi-probability rather than probability distribution.

Another property of the Wigner distribution which makes it different from the conventional probability distribution is that it obeys boundedness inequality

$$-\frac{1}{\pi\hbar} \leq W(x, p) \leq \frac{1}{\pi\hbar} \qquad (97)$$

It can be proved using the Cauchy-Schwartz inequality noticing that the definition Eq. (89) can be viewed as an overlap of two normalized functions[7]. This bound is consistent with the uncertainty principle and means that quantum particle state can not occupy less than $2\pi\hbar$ volume in the phase space. In particular one can not have the classical delta function like $W(x,p)$ at some $x,p$ point. This bound disappears in the classical limit $\hbar \to 0$.

## 6.4  Dynamics of $W(x,p)$. The Moyal equation

Dynamical equation for the time dependence of the Wigner distribution for closed systems can be derived from the Liouville–von Neumann equation (39) for the density matrix and the relation Eq. (92). One "sandwiches" Eq. (39) between $\langle x + a/2|$ and $|x - a/2\rangle$ and Fourier transforms with respect to $a$. The resulting equation is called Moyal or Wigner-Moyal equation. For N degrees of freedom $x = x_1, ..., x_N$ , $p = p_1, ..., p_N$ and a general classical Hamiltonian $H(p,x)$ it has the form[8]

$$\frac{\partial W}{\partial t} = \{\{H, W\}\} \tag{98}$$

with the notation

$$\{\{H, W\}\} = \frac{2}{\hbar} H \sin \frac{\hbar}{2} \sum_{i=1}^{N} \left( \overleftarrow{\partial}_{x_i} \overrightarrow{\partial}_{p_i} - \overleftarrow{\partial}_{p_i} \overrightarrow{\partial}_{x_i} \right) W \tag{99}$$

standing for the Moyal bracket which is an obvious generalization of the classical Poisson bracket for the quantum dynamics in the phase space. One clearly recovers the Poisson bracket in the formal limit $\hbar \to 0$ of the above expression.

---

[7] Here are the details

$$W(x,p) = \frac{1}{\pi\hbar} \langle \xi_1 | \xi_2 \rangle \equiv \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy \xi_1^*(y) \xi_2(y) \text{ with } \xi_{1,2}(y) = \frac{1}{\sqrt{2}} \psi(x \mp \frac{y}{2}) e^{\mp ipy/2\hbar}$$

which are normalized $\langle \xi_1 | \xi_1 \rangle = \langle \xi_2 | \xi_2 \rangle = 1$. Using the Cauchy-Schwartz inequality gives

$$W^2(x,p) = \frac{1}{(\pi\hbar)^2} |\langle \xi_1 | \xi_2 \rangle|^2 \leq \frac{1}{(\pi\hbar)^2} |\langle \xi_1 | \xi_1 \rangle| |\langle \xi_2 | \xi_2 \rangle| = \frac{1}{(\pi\hbar)^2}$$

[8] This Section is intentionally made very brief. Its purpose is to make a reader aware of these developments without going into the details, derivations, etc. Ref. [3] provides a good review of the subject. Cf., also Ref. [7]

It is instructive to consider three dimensional $W(\mathbf{r}, \mathbf{p})$ with the Hamiltonian

$$H(\mathbf{p}, \mathbf{r}) = \mathbf{p}^2/2m + U(\mathbf{r})$$

The Moyal equation (98) then can be written

$$\frac{\partial W}{\partial t} + \frac{1}{m}\mathbf{p} \cdot \nabla_r W - \nabla_r U \cdot \nabla_p W = \sum_{l=1}^{\infty} \frac{(-1)^l (\hbar/2)^{2l}}{(2l+1)!} U \left( \overleftarrow{\nabla}_r \cdot \overrightarrow{\nabla}_p \right)^{2l+1})W \quad (100)$$

where we have separated the $\hbar$ independent terms which have a familiar form of the classical kinetic equation. The right-hand side of the above equation contains a series with coefficients in powers of $\hbar$. Formally this series is essentially the Taylor expansion of

$$\frac{2}{\hbar}U(\mathbf{r}) \sin \frac{\hbar}{2} \left( \overleftarrow{\nabla}_\mathbf{r} \cdot \overrightarrow{\nabla}_\mathbf{p} \right) W(\mathbf{r}, \mathbf{p})$$

without the $l = 0$ term.

# 7 Path Integrals for Open Systems

## 7.1 The Feynman − Vernon Influence Functional

Path integrals offer a different view on the dynamics of an open system. Let us return to considering the density operator $R_{op}$ of the entire composite system. According to Eq. (38) its evolution in time can be written as [9]

$$R_{op}(t_f) = \exp[-iH_{op}(t_f - t_i)/\hbar] \, R_{op}(t_i) \, \exp[iH_{op}(t_f - t_i)/\hbar] \quad (101)$$

or in components

$$R(x_f, q_f; x'_f, q'_f; t_f) \equiv < x_f, q_f| \, R_{op}(t_f) \, |x'_i, q'_i > =$$

$$\int dx_i dq_i dx'_i dq'_i \, K(x_f, q_f; x_i, q_i; t_f - t_i) K^*(x'_f, q'_f; x'_i, q'_i; t_f - t_i) \, R(x_i, q_i; x'_i, q'_i; t_i) \quad (102)$$

where the propagator $K(x_f, q_f; x_i, q_i; t_f - t_i) = < x_f, q_f| \exp[-iH(t_f - t_i)/\hbar]|x_i, q_i >$ is introduced. The density matrix $\rho(x_f, x'_f; t_f)$ of the x–part of the composite system at time $t_f$ is obtained from $R(x_f, q_f; x'_f, q'_f; t_f)$ by setting $q_f = q'_f$ and integrating over these coordinates. Let us assume that the initial density describes a product state,

$$R(x_i, q_i; x'_i, q'_i; t_i) = \rho(x_i, x'_i; t_i)Q(q_i, q'_i; t_i) \quad (103)$$

---

[9] We assume for simplicity that the Hamiltonian of the entire system is time independent

i.e. a state of the system with uncorrelated parts. Let us also use the path integral expression for the propagator

$$K(x_f, q_f; x_i, q_i; t_f - t_i) = \int Dq Dx \exp[(i/\hbar)(S_x + S_q + S_{xq})] \tag{104}$$

with the obvious notation for the parts of the action describing the $x$– and $q$– subsystems and their interaction.

We can use the factorization of the exponent and of the initial state in order to separate the integrations writing first all the integrals involving the $q$–variables and then the integrals over the $x$. In this way we obtain a formal closed expression for the propagation of $\rho$ ,

$$\rho(x_f, x'_f; t_f) = \int dx_i dx'_i J(x_f, x'_f; x_i, x'_i; t_f - t_i) \rho(x_i, x'_i; t_i) \tag{105}$$

with the propagation function given by the double path integral

$$J(x_f, x'_f; x_i, x'_i; t_f - t_i) = \tag{106}$$

$$= \int Dx(t) Dx'(t) \exp\left\{\frac{i}{\hbar}(S_x[x(t)] - S_x[x'(t)])\right\} F[x(t), x'(t)]$$

Here we introduced the Feynman–Vernon influence functional

$$F[x(t), x'(t)] = \tag{107}$$

$$= \int dq_f dq_i dq'_i Q(q_i, q'_i; t_i) K_q(q_f, t_f; q_i, t_i; [x(t)]) K_q^*(q'_f, t_f; q'_i, t_i; [x'(t)])$$

where $K_q$ is the propagator of the $q$–part for a fixed path $x(t)$, i.e.

$$K_q(q_f, t_f; q_i, t_i; [x(t)]) = \int_{q(t_i)=q_i}^{q(t_f)=q_f} Dq(t) \exp\left\{\frac{i}{\hbar}(S_q[q(t)] + S_{xq}[x(t), q(t)])\right\} \tag{108}$$

is the integral over the paths $q(t)$ for a fixed $x(t)$. $K_q$ is clearly a functional of $x(t)$ which is emphasized by our placing of $[x(t)]$ in its argument.

The expression (106) shows that quantum dynamics of an open system interacting with any surrounding medium can be described by a double path integral with the influence and properties of the surroundings incorporated in the functional $F[x(t), x'(t)]$. Two very different surroundings can be indistinguishable in their influence on an open system if they "generate" the same functional $F$. If we have just

an external potential $V(x)$ acting on the system the action will consists of $S_x$ and in addition

$$\int_{t_i}^{t_f} V[x(t)]dt$$

replacing the action $S_q + S_{xq}$ and the integration over $q(t)$. In this case $F$ will have a simple form

$$F = \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} \{V[x(t)] - V[x'(t)]\} \, dt\right)$$

Also in a more general situation one can say that the surrounding medium exert a sort of an external "force" on the system but of course the expression for $F$ is much more complex than the one above reflecting the "back reaction" in the behavior of the surroundings on the dynamics of the $x$ part.

## 7.2   Modeling environment with harmonic oscillators

As an example let us consider the influence functional of a single oscillator coupled linearly to the $x$–part for which for simplicity we will also take a single degree of freedom with mass M and the potential $V(x)$. The corresponding action is

$$S = \int_{t_i}^{t_f} \left\{ \left[\frac{1}{2}M\dot{x}^2 - V(x)\right] - cxq + \frac{m}{2}\left[\dot{q}^2 - \omega^2 q^2\right] \right\} \tag{109}$$

What we denoted earlier as $S_{xq} + S_q$ are the last two terms in this expression. The coefficient $c$ controls the strength of the coupling of the x– and the q– parts. The path integral (108) represents in this case the propagator of the harmonic oscillator driven by the external linear time dependent force $cx(t)$. Explicit expressions for such propagators are well known, cf., Ref. [11]. To keep things simple we also assume that initially the oscillator was in its ground state i.e. had the density matrix

$$Q(q_i, q_i'; t_i) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{m\omega}{2\hbar}(q_i^2 + (q_i')^2)}$$

Using the expression for the propagator together with this expression for $Q$ in (107) one can easily calculate the resulting Gaussian integrals. In the result the pre-exponential factors combine to unity and one obtains, Ref. [11]

$$F[x(t), x'(t)] = \exp\left\{-\frac{1}{\hbar}\Phi[x(t), x'(t)]\right\} \tag{110}$$

where

$$\Phi[x(t), x'(t)] = \frac{c^2}{2m\omega} \int_{t_i}^{t_f} dt \int_{t_i}^{t} dt' \ [x(t) - x'(t')] \ [x(t') \ e^{-i\omega(t-t')} - x'(t') \ e^{i\omega(t-t')}]$$

$$+ i\frac{c^2}{2m\omega^2} \int_{t_i}^{t_f} dt \ [x^2(t) - (x')^2(t)] \quad (111)$$

The last term in this expression is equivalent to adding $(cx)^2/2m\omega^2$ to the potential of the $x$–part. The first term depends on the difference $[x(t) - x'(t')]$, has both real and imaginary parts and is time non–local. Its physical interpretation is not straightforward and serves as an excellent demonstration of how involved even in the simple exactly solvable case is the influence of one physical system on another.

The reader is referred to the book of Feynman and Hibbs, Ref. [11] for further discussions and more general properties of influence functionals. In realistic systems one can rarely calculate exactly the path integral representing the influence functional $F$ and one must resort to approximations. There exists however a simple limit in which the q–part can be regarded as a "featureless" environment the only effect of which on the x–part *in the classical case* would be the appearance of a *friction force* $-\gamma(dx/dt)$ in the equation of motion for the x coordinate. What happens quantum mechanically to a system in such an energy dissipating environment is a highly non trivial question addressed in many studies which were recently reviewed in the book of Weiss, Ref. [12]. There exist a convenient model of a dissipative environment represented as a (continuum) collection of harmonic oscillators with a certain distribution of frequencies and with the linear coupling to the $x$–part. The Feynman–Vernon influence functional can be calculated exactly for such a model, cf.,Ref. [12].

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