

STATE RECONSTRUCTION IN QUANTUM MECHANICS<sup>1</sup>U. Leonhardt<sup>2</sup>

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The observation of moving one-dimensional wave packets reveals their quantum state. The theory [U. Leonhardt and M. G. Raymer, Phys. Rev. Lett. 76, 1985 (1996)] is reviewed. Additionally, some semiclassical expressions and a concise reconstruction formula are sketched.

## 1. Introduction

A typical experiment in quantum mechanics consists of three steps: preparation, evolution and measurement. First, the object of interest is prepared in a certain state. Then it evolves according to the experimental settings and, finally, some physical quantities of the quantum system are measured. This scenario is repeated sufficiently often on an ensemble of equally prepared objects to achieve statistical confidence in the measurement results. Quite typically, the goal of the experiment is the study of the evolution in terms of the measured quantities.

Suppose, however, that the last two steps of the experimental scenario are well investigated and perfectly under control. In particular, we assume that the system evolves in a known way. Can we use this information to infer the prepared state? Evidently, this could be useful for exploring the preparation process. In a sense, we can consider the combination of the steps evolution and measurement as *one* measurement procedure designed to investigate the initial state. However, there is an important difference between this type of “quantum measurements” and conventional experiments: Observables at different stages of the evolution process do not commute in general. Observing one particular quantity during the evolution may explore the wealth of complementary aspects of a quantum system. If this is possible then we can determine the complete quantum state of a physical object from experimental data.

In fact, in a pioneering quantum-optical experiment [1] the quantum state of a single light mode was reconstructed by means of tomographic imaging [2,3]. This first practical demonstration of state reconstruction stimulated other experiments on light

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[4-6] and diatomic molecules [7] and initiated a series of theoretical papers [8-44]. (It was also one topic of the last Budmerice meeting [42-44].) So far all performed experiments have been restricted to one-dimensional harmonic oscillators (light modes and molecular vibrations). The evolution of the system was harmonic and the position  $x$  (or a position-like quantity) was measured at different times  $t$  (or phase angles).

## 2. State reconstruction

How to infer the quantum state of one-dimensional wave packets from observing their motion in arbitrary potentials? Quite recently, recipes were developed for the reconstruction of the complete density matrix [14] and of the population numbers [29]. How do they work? We assume that only the discrete part of the spectrum is excited. The measured histograms  $\text{pr}(x, t)$  of the position  $x$  evolving in time  $t$  is given by

$$\text{pr}(x, t) = \langle x, t | \hat{\rho} | x, t \rangle = \sum_{\mu\nu} \rho_{\mu\nu} \psi_{\mu}(x) \psi_{\nu}(x) \exp[i(\omega_{\nu} - \omega_{\mu})t] \quad (1)$$

in terms of the (real) wave functions  $\psi_n(x)$  of the stationary states and of the density matrix

$$\rho_{mn} = \langle m | \hat{\rho} | n \rangle \quad (2)$$

in energy representation. The wave functions  $\psi_n(x)$  are the normalizable solutions of the stationary Schrödinger equation

$$\left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + U(x) \right] \psi_n = \omega_n \psi_n \quad (3)$$

with energy (eigenfrequency)  $\omega_n$ . We have scaled all physical units in such a way that the mass and  $\hbar$  are unity.

How to infer the density-matrix elements from the position distribution? What about using Fourier analysis? In this way we can distinguish terms oscillating at particular transition frequency. We obtain for a large observation time  $T$

$$\begin{aligned} \tilde{\text{pr}}(x, \omega_m - \omega_n) &= \frac{1}{T} \int_{-T/2}^{+T/2} \text{pr}(x, t) \exp[i(\omega_m - \omega_n)t] dt \\ &= \sum_{\mu\nu}' \rho_{\mu\nu} \psi_{\mu}(x) \psi_{\nu}(x) \end{aligned} \quad (4)$$

where the summation is restricted by the constraint

$$\omega_{\mu} - \omega_{\nu} = \omega_m - \omega_n. \quad (6)$$

As a second step, we would like to find a set of spatial sampling functions  $f_{mn}(x)$  to project the density-matrix elements out of the Fourier-transformed distribution

$$\rho_{mn} = \int_{-\infty}^{+\infty} \tilde{\text{pr}}(x, \omega_m - \omega_n) f_{mn}(x) dx. \quad (7)$$

For this we must require that the  $f_{mn}(x)$  are orthogonal to products of wave functions

$$\int_{-\infty}^{+\infty} \psi_{\mu}(x) \psi_{\nu}(x) f_{mn}(x) dx = \delta_{m\mu} \delta_{n\nu}, \quad (8)$$

given the frequency constraint (6). Surprisingly, the sampling functions are quite simple

$$f_{mn}(x) = \frac{\partial}{\partial x} \left[ \psi_m(x) \varphi_n(x) \right], \quad (9)$$

as has been recently shown in a new theorem [14,29] on the Schrödinger equation. Here  $\varphi_n$  denotes an *irregular wave function* with the Wronskian

$$\psi_n \frac{\partial \varphi_n}{\partial x} - \varphi_n \frac{\partial \psi_n}{\partial x} = 2. \quad (10)$$

What are irregular wave functions? We know that every differential equation of second order like the stationary Schrödinger equation (3) has two linearly independent solutions with a non-vanishing Wronskian. For most frequencies (energies)  $\omega$  both solutions grow exponentially, but there are cases where one of the solutions decays. As we know very well since Schrödinger's "Quantisierung als Eigenwertproblem" [45], this leads to the quantization of energy. The decaying (normalizable) solution of the Schrödinger equation is the regular wave function. However, the second independent solution, i.e. the irregular wave function, still exists as a mathematical object. Here we see that it is physically useful to reconstruct the quantum state of moving wave packets. We note that the Wronskian (10) takes over the role of the normalization for the irregular wave functions.

## 3. Semiclassical theory

How do the irregular wave functions look? How do the sampling functions behave? Probably the easiest way to answer these questions is studying the semiclassical theory for regular and irregular wave functions. For this we simply apply the standard WKB technique [46]. We introduce the semiclassical momentum

$$p_n(x) \equiv \sqrt{2\omega_n - 2U(x)} \quad (11)$$

for a given energy (frequency)  $\omega_n$ . At the turning points  $a_n$  and  $b_n$  of the motion the momentum vanishes

$$p_n(a_n) = p_n(b_n) = 0. \quad (12)$$

According to the semiclassical quantization rule the phase integral should yield

$$\oint p_n dx = 2\pi \left( n + \frac{1}{2} \right) \quad (13)$$

for a round-trip between the classical turning points. We denote the time-independent part of the classical action by

$$S_n(x) = \int_{a_n}^x p_n(x') dx' \quad (14)$$

The momentum  $p_n$  and, consequently, the action  $S_n$  is real in the classically allowed region between the turning points. On the other hand,  $p_n$  and  $S_n$  are purely imaginary in the forbidden zone. A regular wave function oscillates in the allowed region

$$\psi_n = c_n p_n^{-1/2} \cos\left(S_n - \frac{\pi}{4}\right) \quad (15)$$

and decays exponentially in the forbidden zone

$$\psi_n = \frac{c_n}{2} |p_n|^{-1/2} \exp(-|S_n|) \quad (16)$$

Knowing these results we easily guess the semiclassical formulae for the irregular wave functions. We must only satisfy the Wronskian condition (10) for the  $\psi_n$  given by the expressions (15) and (16) and the irregular wave function. We may readily verify that this is achieved for

$$\varphi_n = 2c_n^{-1} p_n^{-1/2} \sin\left(S_n - \frac{\pi}{4}\right) \quad (17)$$

in the classically allowed region and for

$$\varphi_n = 2c_n^{-1} |p_n|^{-1/2} \exp(+|S_n|) \quad (18)$$

in the forbidden zone. (A more rigorous derivation [40] shows that the guess is indeed the correct result.) We see that between the turning points the irregular wave functions oscillate as well, yet with the opposite phase as the regular ones. Therefore they interfere constructively near the turning points and grow exponentially in the forbidden zone, whereas the regular wave functions decay. For this very reason they are usually discarded as being physically meaningless, except some rare applications in atomic scattering theory [47]. However, the product of the regular and the irregular wave functions is well behaved in the classically forbidden zone, since

$$\psi_n \varphi_n = c_n c_n^{-1} |p_n p_n|^{-1/2} \exp(|S_n| - |S_m|) \quad (19)$$

with

$$\begin{aligned} |S_n| - |S_m| &= \int_a^x \left[ |p_n(\xi)| - |p_m(\xi)| \right] d\xi + c \\ &= \int_{a_n}^x \frac{2(\omega_n - \omega_n)}{|p_n(\xi)| + |p_m(\xi)|} d\xi + c. \end{aligned} \quad (20)$$

[Since the energies  $\omega_n$  and  $\omega_m$  are different in general the classical turning point  $a_n$  differs from  $a_m$  as well. Therefore we obtain a constant  $c$  in eq. (20).] This expression leads to

$$|S_n| - |S_m| \sim (\omega_n - \omega_m) \int_{a_n}^x [2U(\xi)]^{-1/2} d\xi + c' \quad (21)$$

for large  $x$  [with another (unimportant) constant  $c'$ ]. We see that for  $\omega_n \geq \omega_m$  the product of  $\psi_n$  and  $\varphi_n$  decays nicely.

In the classically allowed region we obtain a very simple semiclassical expression for the diagonal sampling functions [40]

$$f_{nn}(x) \sim 2 \sin [2S_n(x)] \quad (22)$$

To find this result we take advantage of the formulae (15) and (17) and neglect the slow variation of the momenta  $p_n$  in the fundamental relation (9) for the  $f_{nn}$ . Formula (22) shows that the diagonal sampling functions are bare oscillations of the action  $S_n$  at twice the frequency as the regular wave functions. Therefore they are able to sense the typical features of the wave functions squared. A sampling function  $f_{nn}(x)$  overlaps perfectly with  $\psi_n^2$  and it is orthogonal to all other  $\psi_n^2$ . This is the reason why the functions  $f_{nn}(x)$  do detect the diagonal density-matrix elements in the time-averaged probability distribution

$$\bar{\rho}(x, 0) = \sum_{\nu} \rho_{\nu\nu} \psi_{\nu}^2(x) \quad (23)$$

We have seen that we can understand the behavior of the irregular wave functions and of the sampling functions with the help of the semiclassical WKB approximation.

#### 4. Summarizing formulae

We have achieved some familiarity with the irregular wave functions. Let us go a step further to summarize our results in a concise and general reconstruction formula. The density matrix  $\rho_{a'a}$  in an arbitrary basis is related to the energy representation by the expression

$$\rho_{a'a} = \sum_{mn} \langle a' | m \rangle \rho_{mn} \langle n | a \rangle \quad (24)$$

The time-dependent regular wave functions  $\psi_a(x, t)$  for the basis states  $|a\rangle$  are given by

$$\psi_a(x, t) = \sum_n \langle n | a \rangle \psi_n(x) \exp(-i\omega_n t) \quad (25)$$

They are solutions of a time-dependent Schrödinger equation with the potential  $U(x)$  and the initial condition  $\psi_a(x) = \langle x | a \rangle$ . We define irregular wave functions  $\varphi_a(x, t)$  as

$$\varphi_a(x, t) \equiv \sum_n \langle n | a \rangle \varphi_n(x) \exp(-i\omega_n t) \quad (26)$$

Using these expressions and the theorem (9) we recombine the separately considered sampling steps (4) and (7) in the final formula

$$\rho_{a'a} = \left\langle\left\langle \frac{\partial}{\partial x} \left[ \psi_a^*(x, t) \varphi_a(x, t) \right] \right\rangle\right\rangle_{x,t} \quad (27)$$

The double brackets denote an average with respect to the experimentally measured  $(x, t)$  data.

The observation of the moving wave packet reveals the quantum state at  $t = 0$ . Of course, for this we need to know the dynamical law of motion, i.e. the potential  $U(x)$  in the Schrödinger equation (3) to calculate the required regular and irregular wave functions. Formula (27) shows how to sample the density matrix from observation of the position  $x$  evolving in time  $t$ .

We may also express the observed quantity, i.e. the probability distribution  $\text{pr}(x, t)$  in a similar way as the reconstruction formula (27). We find

$$\text{pr}(x, t) = \sum_{a'a} \rho_{a'a} \langle x, t | a' \rangle \langle a | x, t \rangle \quad (28)$$

which is

$$\text{pr}(x, t) = \langle \psi_a(x, t) \psi_a^*(x, t) \rangle_\rho \quad (29)$$

Here the brackets denote an average with respect to the density matrix.

The two formulae (27) and (29) summarize concisely the mutual relation between the quantum state and the observed quantity. The probability distribution  $\text{pr}(x, t)$  is a quantum average of the product of the regular wave functions  $\psi_a(x, t)$  and  $\psi_a^*(x, t)$ . On the other hand, the density matrix is a classical average of the derivative of the product of the regular and the irregular wave functions.

Is this result a happy coincidence or could it be a principle of Nature? Are the dynamical laws of quantum mechanics designed in such a way that quantum states can be reconstructed? Everything fits that nicely together — the Fourier transformation (4), for instance, generates exactly the right frequency constraint (6) needed for the orthogonality (8) of the spatial sampling functions. Indeed, we may speculate that there might be a deeper reason behind these mathematical games. Maybe we have just caught a first glimpse of an interesting structure relating quantum states to observations. There is certainly much room for future research.

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