

PHYSICAL REVIEW LETTERS

VOLUME 76

18 MARCH 1996

NUMBER 12

Observation of Moving Wave Packets Reveals Their Quantum State

U. Leonhardt* and M. G. Raymer

Department of Physics and Chemical Physics Institute, University of Oregon, Eugene, Oregon 97403

(Received 3 November 1995)

We show how to infer the quantum state of a wave packet from position probability distributions measured during the packet's motion in an arbitrary potential. We assume a nonrelativistic one-dimensional or radial wave packet. Temporal Fourier transformation and spatial sampling with respect to a newly found set of functions project the density-matrix elements out of the probability distributions. The sampling functions are derivatives of products of regular and irregular wave functions. We note that the ability to infer quantum states in this way depends on the structure of the Schrödinger equation.

PACS numbers: 03.65.Bz, 03.65.Db

Quite generally, physics distinguishes between the dynamical law and the state of a system. The state contains the complete statistical information about an ensemble of physical objects at a particular moment, while the dynamical law determines the change of the status quo at the next instant of time. In this general picture, quantum mechanics makes another Cartesian-like separation: quantum states and observable quantities are distinct. There is no way, for instance, to observe directly Schrödinger's wave function $\psi(x, t)$ for a mechanical system at position x and time t . All that quantum mechanics allows us to measure are expectation values, for example, the position probability distribution $|\psi(x, t)|^2$. In a typical pump-probe experiment, for instance, a Schrödinger wave packet is first prepared in a certain initial state, then it is left to evolve according to the dynamical law of the system, and finally the position x is measured at time t . By repeating this procedure many times sufficient statistical information is gained about the position probability distribution.

Can we use the dynamical law to infer the state of a moving wave packet after position measurements have been performed? In molecular emission tomography [1], for instance, the quantum state of a molecular vibration has been determined from its elongation encoded in the time-evolved fluorescence spectrum. The Wigner function of the vibrational state (which contains the same information as the density operator) was reconstructed using the inverse Radon transformation [2]. Also optical homodyne tomography [3] is a method to reconstruct the

state of an electromagnetic oscillator from (positionlike) field-quadrature distributions measured using homodyne detection. In this case the timelike evolution of the system is brought about by phase shifting. So far these methods and other feasible schemes to reconstruct the quantum states of wave packets [4–7] have been restricted to harmonic oscillators or free particles. Only in these cases does the Wigner function evolve in time as a classical phase-space density, i.e., by simple shearing or rotation, and only in these cases the quantum state can be reconstructed by means of classical tomography (known, for instance, from medical computer-assisted tomography).

Can we infer the state of a wave packet moving in an arbitrary potential from position measurements in time? This would be extremely useful for state measurements of anharmonic molecules [8,9], of wave packets in semiconductor quantum wells [10], or of electronic wave packets in atoms [11], to name just a few examples. In case of anharmonic potentials the evolution of the Wigner function does not obey classical laws anymore [12]. The dynamical equation contains infinitely many spatial derivatives which correspond to the complicated reshaping of the Wigner function as quantum-interference effects (wave-packet collapses and revivals [9]) come into play. As a consequence, classical tomography cannot be used anymore to infer the quantum state. However, the very nature of quantum mechanics offers an alternative and truly quantum way of *nontomographic* state recon-

struction. As described in this Letter, the superposition principle combined with the structure of the Schrödinger equation allows us to reveal the quantum state of a moving wave packet from position observations.

Suppose we can measure the position probability distribution $pr(x, t)$ of a one-dimensional nonrelativistic wave packet moving in an arbitrary stationary potential $U(x)$. The case of radial motion in a centrally symmetric potential is considered below. Using the quantum-mechanical superposition principle we express the state of the system at time $t = 0$ in the energy representation ρ_{mn} of the density operator $\hat{\rho}$:

$$\rho_{mn} = \langle m | \hat{\rho} | n \rangle, \quad (1)$$

with $|n\rangle$ being the energy eigenstates of the system. This has the great advantage that the position probability distribution $pr(x, t)$ is spectrally decomposed into terms oscillating at differences of eigenfrequencies

$$pr(x, t) = \sum_{mn} \rho_{mn} \psi_m(x) \psi_n(x) \exp[-i(\omega_m - \omega_n)t]. \quad (2)$$

Here $\psi_n(x)$ denotes the wave function of the energy eigenstate $|n\rangle$. Since the potential $U(x)$ is real, the eigenfunctions can be chosen to be real as well. We assume that only the discrete part of the energy spectrum is excited. Since none of the discrete levels is degenerate [13], Sec. 21, $\psi_n(x)$ is the only normalized solution of the stationary Schrödinger equation with eigenfrequency ω_n

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

(For simplicity the mass and \hbar are set to unity. This can always be achieved by a proper rescaling of physical units. In this Letter a ∂ or a prime symbolizes differentiation with respect to x .)

After watching the motion of the wave packet and measuring the position distribution we should perform a Fourier transformation of $pr(x, t)$ to obtain a spectrally decomposed probability distribution

$$\begin{aligned} & \widetilde{pr}(x, \omega_m - \omega_n) \\ & \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{+T/2} pr(x, t) \exp[-i(\omega_m - \omega_n)t] dt \\ & = \sum'_{\mu\nu} \rho_{\mu\nu} \psi_\mu(x) \psi_\nu(x), \end{aligned} \quad (4)$$

where \sum' indicates a sum restricted to values of μ, ν such that

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

Terms oscillating at one particular frequency difference $\omega_m - \omega_n$ are singled out. Note that there might be many

of these terms. A harmonic oscillator, for instance, has an equidistant spectrum and produces infinitely many terms oscillating at identical frequency differences in $pr(x, t)$. In any case, all eigenstates contribute at least to the zero-frequency component which contains the main-diagonal elements ρ_{nn} of the density matrix.

How can we extract the density-matrix elements? We would like to have functions $f_{mn}(x)$ which are *orthogonal to products of wave functions* $\psi_\mu(x)\psi_\nu(x)$, provided the frequency constraint (6) is given, i.e.,

$$\int_{-\infty}^{+\infty} \psi_\mu(x) \psi_\nu(x) f_{mn}(x) dx = \delta_{m\mu} \delta_{n\nu}. \quad (7)$$

Sampling the spectrally decomposed probability distribution $\widetilde{pr}(x, \omega_m - \omega_n)$ with respect to the functions $f_{mn}(x)$ would then produce the density matrix

$$\rho_{mn} = \int_{-\infty}^{+\infty} \widetilde{pr}(x, \omega_m - \omega_n) f_{mn}(x) dx. \quad (8)$$

Surprisingly, the sampling functions $f_{mn}(x)$ turn out to be very simple. They are just derivatives of regular and irregular wave functions [14,15]

$$f_{mn}(x) = \partial[\psi_m(x)\varphi_n(x)]. \quad (9)$$

What are irregular wave functions? Any linear differential equation of second order such as the Schrödinger equation (3) must have two linearly independent solutions for a given frequency ω_n : one is the regular wave function ψ_n ; the other fundamental solution φ_n is called *irregular*. Since the stationary states $|n\rangle$ are nondegenerate [13], Sec. 21, φ_n cannot be normalizable as ψ_n is, and it must be discarded as a physical state. Nevertheless, irregular wave functions have been used in scattering theory [16], and this Letter shows yet another important physical application of these mathematical constructions [17].

The proof of our key theorem (7) and (9) is inspired by the same principal idea as in the classic orthogonality proof for eigenfunctions of Hermitian operators [13], Sec. 3. As an additional ingredient, we will persistently use partial integration and take advantage of the Schrödinger equation (3) and the frequency constraint (6). First, we derive from the stationary Schrödinger equation (3) two Schrödinger-like equations, one for the product of the wave functions,

$$\partial^2(\psi_\mu \psi_\nu) = 2U_{\mu\nu} \psi_\mu \psi_\nu + 2\psi'_\mu \psi'_\nu, \quad (10)$$

and another for $\partial(\psi_m \varphi_n)$,

$$\begin{aligned} \partial^3(\psi_m \varphi_n) &= 4U_{mn} \partial(\psi_m \varphi_n) + 4U' \psi_m \varphi_n \\ &\quad - 2(\omega_m - \omega_n) W_{mn}, \end{aligned} \quad (11)$$

with the modified potential

$$U_{mn} \equiv 2U - \omega_m - \omega_n. \quad (12)$$

We introduce the generalized Wronskians

$$W_{mn} \equiv \psi_m \varphi'_n - \psi'_m \varphi_n \quad (13)$$

and

$$V_{\mu\nu} \equiv \psi_\mu \psi'_\nu - \psi'_\mu \psi_\nu. \quad (14)$$

It is easy to see from the Schrödinger equation (3) that the derivatives of the Wronskians W_{mn} and $V_{\mu\nu}$ obey the relations

$$W'_{mn} = 2(\omega_m - \omega_n)\psi_m \varphi_n \quad (15)$$

and

$$V'_{\mu\nu} = 2(\omega_\mu - \omega_\nu)\psi_\mu \psi_\nu. \quad (16)$$

To prove the orthogonality of $\psi_\mu \psi_\nu$ and $\partial(\psi_m \varphi_n)$ we abbreviate the scalar product of both functions by

$$G_{\mu\nu}^{mn} \equiv \int_{-\infty}^{+\infty} \psi_\mu \psi_\nu \partial(\psi_m \varphi_n) dx \quad (17)$$

and replace the product of the wave functions $\psi_\mu \psi_\nu$ using the first Schrödinger-like equation (10):

$$2(\omega_\mu + \omega_\nu)G_{\mu\nu}^{mn} = \int_{-\infty}^{+\infty} [4U\psi_\mu \psi_\nu - \partial^2(\psi_\mu \psi_\nu) + 2\psi'_\mu \psi'_\nu] \partial(\psi_m \varphi_n) dx. \quad (18)$$

Then we integrate by parts to move the differential operator ∂^2 to the sampling function $\partial(\psi_m \varphi_n)$ and apply the second Schrödinger-like equation (11). In this way we obtain

$$2(\omega_\mu + \omega_\nu)G_{\mu\nu}^{mn} = \int_{-\infty}^{+\infty} \psi_\mu \psi_\nu (4U\partial - 4U_{mn}\partial - 4U') \times \psi_m \varphi_n dx + H_{\mu\nu}^{mn}, \quad (19)$$

with the additional term

$$H_{\mu\nu}^{mn} = 2 \int_{-\infty}^{+\infty} [\psi'_\mu \psi'_\nu \partial(\psi_m \varphi_n) + (\omega_m - \omega_n)\psi_\mu \psi_\nu W_{mn}] dx. \quad (20)$$

To evaluate $H_{\mu\nu}^{mn}$ we integrate $\psi'_\mu \psi'_\nu \partial(\psi_m \varphi_n)$ by parts; we utilize the frequency constraint (6) and the relation (16) of the generalized Wronskian $V_{\mu\nu}$ to arrive at the

intermediate result

$$H_{\mu\nu}^{mn} = \int_{-\infty}^{+\infty} [-2\psi_m \varphi_n \partial(\psi'_\mu \psi'_\nu) + V'_{\mu\nu} W_{mn}] dx. \quad (21)$$

We integrate $V'_{\mu\nu} W_{mn}$ by parts, use

$$-\partial(\psi'_\mu \psi'_\nu) = -U_{\mu\nu} \partial(\psi_\mu \psi_\nu) + (\omega_\mu - \omega_\nu) V_{\mu\nu} \quad (22)$$

and again the frequency constraint (6) together with relation (15) of the Wronskian W_{mn} to obtain the final result

$$\begin{aligned} H_{\mu\nu}^{mn} &= -2 \int_{-\infty}^{+\infty} \psi_m \varphi_n U_{\mu\nu} \partial(\psi_\mu \psi_\nu) dx \\ &= +2 \int_{-\infty}^{+\infty} \psi_\mu \psi_\nu (U_{\mu\nu} \partial + 2U') \psi_m \varphi_n dx. \end{aligned} \quad (23)$$

We insert this expression for $H_{\mu\nu}^{mn}$ into Eq. (19) and see immediately from the definition (12) that

$$2(\omega_m + \omega_n - \omega_\mu - \omega_\nu)G_{\mu\nu}^{mn} = 0. \quad (24)$$

This means that if the sums $\omega_m + \omega_n$ and $\omega_\mu + \omega_\nu$ are not equal, $G_{\mu\nu}^{mn}$ must vanish. Since the differences $\omega_m - \omega_n$ and $\omega_\mu - \omega_\nu$ coincide according to the frequency constraint (6), $G_{\mu\nu}^{mn}$ must be proportional to $\delta_{\mu m}$ and $\delta_{\nu n}$.

What happens when $m = \mu$ and $n = \nu$, i.e., when $\omega_m + \omega_n - \omega_\mu - \omega_\nu = 0$? First, we note that according to Eq. (15) the Wronskian W_{nn} is a constant (as it is well known for solutions of the Schrödinger equation). We differentiate $\psi_m \varphi_n$ in $G_{\mu\nu}^{mn}$, and use the Wronskian and the normalization of the regular eigenfunction ψ_m to obtain

$$G_{mn}^{mn} = \int_{-\infty}^{+\infty} \psi_m \varphi_n \partial(\psi_m \psi_n) dx + W_{nn}. \quad (25)$$

On the other hand, partial integration in the definition (17) of G_{mn}^{mn} gives

$$G_{mn}^{mn} = - \int_{-\infty}^{+\infty} \psi_m \varphi_n \partial(\psi_m \psi_n) dx. \quad (26)$$

Adding Eqs. (25) and (26) implies that $2G_{mn}^{mn}$ must equal the Wronskian W_{nn} . So if we require that

$$\psi_n \varphi'_n - \psi'_n \varphi_n = 2, \quad (27)$$

the theorem (7) and (9) is proven. Equation (27) plays the role of a normalization for the irregular wave functions φ_n . It indicates that ψ_n and φ_n must indeed be linearly independent since otherwise their Wronskian W_{nn} would vanish. We note that apart from the restriction (27) any irregular wave function φ_n can be chosen as long as it satisfies the stationary Schrödinger equation (3). We also note that we could as well use $\partial(\varphi_m \psi_n)$ instead of

$\partial(\psi_m \varphi_n)$ as a sampling function f_{mn} . We could easily modify our proof to show that $\partial(\varphi_m \psi_n)$ is also orthogonal to the product of the wave functions ψ_μ and ψ_ν . The actual choice of the sampling functions is a matter of numerical convenience.

We have used partial integration to prove our theorem (7) and (9) which means that it is valid if quantities such as $\psi_m \varphi_n U_{\mu\nu} \psi_\mu \psi_\nu$ decay fast enough at the boundaries $-\infty$ and $+\infty$. That this is correct can be seen from the known asymptotic behavior of one-dimensional wave packets [13], Sec. 21. On the other hand, we may extend our state-reconstruction procedure to other systems as long as they are described by one-dimensional Schrödinger equations with proper boundary conditions. This is the case if there is a symmetry reducing both the dynamical law and the quantum state to a quasi-one-dimensional problem. A good example is a radial wave packet moving in a centrally symmetric potential $U(r)$. As it is well known [13], Sec. 32, radial wave functions $R_n(r)$ can be mapped into solutions

$$\psi_n(r) = rR_n(r) \quad (28)$$

of the one-dimensional Schrödinger equation (3) with the potential

$$U_l(r) = U(r) + \frac{l(l+1)}{2r^2}. \quad (29)$$

The additional term $l(l+1)/2r^2$ accounts for the centrifugal energy of the wave packet. In contrast to truly one-dimensional wave packets with position variables x the range of the radius r is restricted to $[0, \infty)$. We may use, however, the known behavior of the regular and irregular wave functions near the origin [13], Sec. 32, to show that they obey the boundary conditions we need. So we can reconstruct the quantum state of radial wave packets as well. For this we should replace the regular and irregular radial wave functions according to the mapping (28) and (29) and integrate with respect to the radius r instead of the position x and from zero to infinity only.

How is our method related to the tomographic state reconstruction for harmonic oscillators? In the harmonic case the position probability distribution $pr(x, t)$ is periodic in time t , so that an integration over one period is sufficient for reconstruction. This integration is usually expressed in terms of an integral over a temporal phase shift. In combination with the spatial integration with respect to the sampling functions f_{mn} this is equivalent to the previously studied sampling version [18] of harmonic quantum-state tomography [3]. Note that in the anharmonic case we must integrate over a sufficiently long time (many quasiperiods) to guarantee good resolution of the different frequency components with $\omega_\mu - \omega_\nu \neq \omega_m - \omega_n$. During this time the system must be iso-

lated from the environment so that Schrödinger dynamics is valid.

In summary, watching a one-dimensional wave packet moving in an arbitrary potential reveals the quantum state of the packet. An experimentalist needs to measure the position probability distribution during a sufficiently long time interval, to perform a temporal Fourier transformation, and to integrate with respect to a set of spatial sampling functions. The sampling functions are derivatives of products of regular and irregular wave functions, as we have shown in a new theorem on the stationary Schrödinger equation. This method could become a powerful tool wherever experimentalists encounter one-dimensional or radial wave packets.

Our theorem depends critically on the structure of the Schrödinger equation. We may as well turn the tables and ask whether this result was a coincidence or a principle. Has nature chosen the Schrödinger equation so that the states of physical objects can be inferred from measurement? Or, in other words, what are the conditions imposed on dynamical laws such that quantum states can be reconstructed?

We would like to thank D. Adkison, H. J. Carmichael, C. Leichtle, I. Leonhardt, Th. Richter, W. P. Schleich, and I. A. Walmsley for help and fruitful discussions. The work of U. L. at the University of Oregon was supported by an Otto Hahn Award of the Max Planck Society. M. G. R. was supported by NSF Grants No. ECS-9212996 and No. PHY-9224779.

*Also at the Arbeitsgruppe "Nichtklassische Strahlung" der Max-Planck-Gesellschaft an der Humboldt-Universität zu Berlin, Rudower Chaussee 5, 12484 Berlin, Germany.

- [1] T. J. Dunn, I. A. Walmsley, and S. Mukamel, *Phys. Rev. Lett.* **74**, 884 (1995).
- [2] J. Bertrand and P. Bertrand, *Found. Phys.* **17**, 397 (1987).
- [3] K. Vogel and H. Risken, *Phys. Rev. A* **40**, 2847 (1989); D. T. Smithey, M. Beck, M. G. Raymer, and A. Faridani, *Phys. Rev. Lett.* **70**, 1244 (1993).
- [4] M. G. Raymer, M. Beck, and D. F. McAlister, *Phys. Rev. Lett.* **72**, 1137 (1994); D. F. McAlister, M. Beck, L. Clarke, A. Mayer, and M. G. Raymer, *Opt. Lett.* **20**, 1181 (1995); U. Janicke and M. Wilkens, *J. Mod. Opt.* **42**, 2183 (1995).
- [5] Schemes to measure the quantum state of a single light mode are reviewed in U. Leonhardt and H. Paul, *Prog. Quantum Electron.* **19**, 89 (1995). For recent developments see M. Freyberger and A. M. Herkommer, *Phys. Rev. Lett.* **72**, 1952 (1994); O. Steuernagel and J. A. Vaccaro, *ibid.* **75**, 3201 (1995); P. J. Bardroff, E. Mayr, and W. P. Schleich, *Phys. Rev. A* **51**, 4963 (1995).
- [6] S. Wallentowitz and W. Vogel, *Phys. Rev. Lett.* **75**, 2932 (1995).
- [7] Quantum-state reconstruction of discrete systems was considered in U. Leonhardt, *Phys. Rev. Lett.* **74**, 4101 (1995), and references cited therein.
- [8] P. M. Morse, *Phys. Rev.* **34**, 57 (1929).

- [9] M.J.J. Vrakking, D.M. Villeneuve, and A. Stolow (to be published).
- [10] K. Leo, J. Shah, E.O. Göbel, Th. Damen, S. Schmitt-Rink, W. Schäfer, and K. Köhler, *Phys. Rev. Lett.* **66**, 201 (1991).
- [11] J.A. Yeazell and C.R. Stroud, Jr., *Phys. Rev. Lett.* **60**, 1494 (1988).
- [12] J.E. Moyal, *Proc. Cambridge Philos. Soc.* **45**, 99 (1949).
- [13] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1977).
- [14] Th. Richter (to be published) was the first who pointed out that the diagonal sampling functions f_{nn} for the harmonic oscillator are derivatives of products of regular and irregular wave functions. Later Th. Richter and A. Wünsche (to be published) generalized independently from our work this result to diagonal sampling functions f_{nn} in arbitrary potentials.
- [15] U. Leonhardt, M. Munroe, T. Kiss, Th. Richter, and M.G. Raymer, *Opt. Commun.* (to be published).
- [16] H. Friedrich, *Theoretical Atomic Physics* (Springer, Berlin, 1990); see also Ref. [13], Sec. 138.
- [17] A semiclassical theory of general irregular wave functions has been elaborated in Ref. [15].
- [18] See Ref. [15], and references cited therein.