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Determination of occupation probabilities from time-averaged position distributions

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We show that the occupation probabilities of the energy eigenstates excited in a wave packet moving in an arbitrary one-dimensional potential can be determined directly from the time-averaged position distribution. The sampling functions are the derivative of the product of the usual eigenfunctions and the linearly independent (non-normalizable) solutions of the Schrödinger equation for the same energy eigenvalue. This is the same structure as those for the harmonic-oscillator case.

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The ultimate goal of measurements in quantum mechanics is the determination of the density operator $\hat{\rho}$ of a statistical ensemble of systems previously produced by some reproducible means. A complete set of measurements should determine all the density-matrix elements. As early as 1933 Pauli asked the question whether the Schrödinger wave function could be uniquely determined from given probability distributions of position and momentum if the quantum system were known beforehand to be in a pure state [1,2]. It is now well known that for any wave function of definite parity the Pauli problem is not uniquely solvable [2]. Somewhat later Feenberg [3] could show that for one-dimensional problems, in principle, the wave function $\psi(x,t)$ can be reconstructed from positional observations; that means from the position distribution $P(x,t)=|\psi(x,t)|^2$. Specifically he proved that the values of $P(x,t_0)$ and $(\partial P/\partial t)(x,t_0)$ at any given time t_0 uniquely determine $\psi(x,t)$ itself apart from a trivial global phase factor. But what can be said if the quantum state is a mixed state described by the density operator $\hat{\rho}$, and even more interesting, does there exist a constructive algorithm for reconstructing the quantum state? This problem has attracted much interest in recent years in quantum optics [4–22].

Following a proposal by Vogel and Risken [5], Smithey *et al.* [13] were the first to determine the density matrix of a single-mode field from the reconstructed Wigner function, which in turn was reconstructed from the measured quadrature component distributions in balanced homodyne detection. A balanced homodyne detector [23] utilizes the interference of the signal field and a strong local oscillator, which has an adjustable phase Θ and measures the probability distributions $w(x_\Theta,\Theta)$ for the quadrature component x_Θ of the signal field, which are just marginal distributions of the corresponding Wigner function. One observes that the measured quadrature component distributions are nothing else but the time-dependent position distributions of the fictitious harmonic oscillator associated with the quantized electromagnetic field [see Eqs. (1,10)]. This experimental work stimulated theoretical studies [14–21] to develop algorithms to reconstruct the density-matrix elements directly from the measured histograms of homodyne data. The quadrature component distribution can be written in the form [19,21]

$$w(x_\Theta,\Theta)=\sum_{mn}\rho_{mn}h_m(x_\Theta)h_n(x_\Theta)e^{i(n-m)\Theta}, \qquad (1)$$

where $h_n(x)$ are the well-known energy eigenfunctions of the harmonic oscillator in position representation described by Hermite functions (e.g., [26]) and ρ_{mn} denotes the density-matrix elements with respect to these eigenstates. Clearly, the reconstruction of the density matrix in the Fock basis from the measured quadrature component distributions requires a set of pattern functions $F_{kl}(x_\Theta,\Theta)$ that is biorthonormal [19]

$$\int_{-\infty}^{+\infty}dx_\Theta\int_0^\pi d\Theta\; w_{mn}(x_\Theta,\Theta)F_{kl}(x_\Theta,\Theta)=\delta_{km}\delta_{ln} \qquad (2)$$

to the set of functions

$$w_{mn}(x_\Theta,\Theta)=h_m(x_\Theta)h_n(x_\Theta)e^{i(n-m)\Theta}. \qquad (3)$$

It turns out that the functions F_{kl} are just proportional to the derivative of the product of (normalized) eigenfunctions with a non-normalizable solution of the Schrödinger equation for the harmonic oscillator [19,20]. If one is interested solely in the photon statistics (diagonal density-matrix elements) the knowledge of the phase-averaged quadrature component distributions alone is sufficient, as has been experimentally demonstrated [18].

In this paper we show that with respect to the diagonal density-matrix elements ρ_{nn} all statements made for the harmonic oscillator are perfectly true also for anharmonic one-dimensional potentials if instead of the phase-averaged quadrature component distributions time-averaged position distributions are used [24]. One-dimensional problems are of interest, not only as the quantization of a single-mode electromagnetic field relies on the one-dimensional harmonic po-

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tential, but also because, after some appropriate manipulations, in a variety of problems one is led to equations of motion that correspond to the one-dimensional Schrödinger equation. As one example we mention the diatomic molecular vibrations [25].

Let us consider the wave packet of a particle of mass m moving in a one-dimensional potential $V(x)$. The time evolution of its wave function is governed by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(x,t)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi(x,t). \tag{4}$$

An arbitrary time-dependent (square-integrable) wave function can be expanded in terms of the stationary solutions

$$\psi_n(x,t)=u_n(x)e^{-i\omega_n t}, \tag{5}$$

where the functions $u_n(x)$ that can be chosen as real functions [26] form an orthonormal set of energy eigenfunctions of the time-independent Schrödinger equation

$$\frac{d^2}{dx^2}u_n(x)=[U(x)-\varepsilon_n]u_n(x), \tag{6}$$

belonging to the scaled energy eigenvalues $\varepsilon_n=(2m/\hbar)\omega_n$. Here we have adopted the notation $U(x)=(2m/\hbar^2)V(x)$ for the scaled potential. We assume throughout this paper that the potential $V(x)$ is asymptotically increasing on both sides faster than some positive powers of the modulus of the position that guarantees the presence of only a discrete spectrum of energy eigenvalues. From a practical point of view it is also sufficient to suppose that for arbitrary potentials only eigenstates of the discrete energy spectrum are excited, so that we may consider these states as a complete basis for our purposes. It is known that the energy eigenvalues belonging to the discrete spectrum of the one-dimensional Schrödinger equation are nondegenerate [26]. Since the Schrödinger equation is a second-order differential equation to each normalized eigenfunction $u_n(x)$ of the discrete spectrum, there exists a second linearly independent solution to the same eigenvalue, which is, however, nonnormalizable. The time-dependent solution of the Schrödinger equation (4) having $\psi(x,0)=\Sigma_n c_n u_n(x)$ as the initial state at time $t=0$ can be represented as a linear superposition of the stationary states (5)

$$\psi(x,t)=\sum_n c_n u_n(x)e^{-i\omega_n t}. \tag{7}$$

Clearly, the composite structure of $\psi(x,t)$ leads to quantum-mechanical interference. Indeed, the probability $P(x,t)$ that the particle can be found at time t with position x is given by

$$P(x,t)=|\psi(x,t)|^2=\sum_{m,n} c_m c_n^* u_m(x)u_n(x)e^{i(\omega_n-\omega_m)t}. \tag{8}$$

Only the terms with $m=n$ are time independent and the expansion coefficient $|c_n|^2$ in front of them determines the probability with which the energy eigenstate $|u_n\rangle$ is excited in the wave packet (7). In the case where the particle is in a mixed state described by the density operator $\hat{\rho}$, formula (8) generalizes to

$$P(x,t)=\sum_{m,n}\rho_{mn}u_m(x)u_n(x)e^{i(\omega_n-\omega_m)t}, \tag{9}$$

where $\rho_{mn}=\langle u_m|\rho|u_n\rangle$ are the density-matrix elements in the energy eigenstate basis.

For the harmonic-oscillator potential to which the quantization of a single-mode electromagnetic field is reduced, we have $\omega_n-\omega_m=(n-m)\omega$ with ω as the angular frequency of the harmonic oscillator, and expression (9) simplifies to

$$P(x,t)=\sum_{m,n}\rho_{mn}u_m(x)u_n(x)e^{i(n-m)\omega t}. \tag{10}$$

Translated into the language of quantum optics $P(x,t)$ is nothing but the quadrature component distribution (1) of a single-mode electromagnetic field. We just have to identify ωt in (10) with the phase Θ of the strong local oscillator in the balanced homodyne detection scheme and the eigenfunctions $u_n(x)$ with $h_n(x)$. This is based on the fact that for the harmonic-oscillator potential the position distributions of the particle at time t may be obtained as marginal distribution from the rotated Wigner function of the initial state $\psi(x,0)$ since the rotated coordinates just reflect the motion of the harmonic oscillator.

Next we follow [18,24] and ask the analogous question: What information can be obtained from the time-averaged position distributions? If we average the position distributions (9) over times T large compared with the periods of all difference frequencies occurring in the expansion (9), we immediately find the expression

$$\bar{P}(x)=\frac{1}{T}\int_0^T dt\, P(x,t)=\sum_n \rho_{nn}u_n^2(x) \quad \text{for } T\gg \max\left(\frac{2\pi}{|\omega_n-\omega_m|}\right), \tag{11}$$

which only depends on the diagonal density-matrix elements. Note that there is a whole class of quantum states that leads to just this form of (time-independent) position probability distributions. These are the states that are described by a statistical mixture (incoherent superposition) of the energy eigenstates, so that the density matrix is purely diagonal. Obviously, in this case all time dependence vanishes. Such distributions are characteristic for particles in thermal equilibrium or, for example, for incoherently excited vibrational wave packets in molecules. But the same also holds true for initially coherently excited wave packets after sufficiently strong purely phase-destroying relaxation.

The reconstruction of the diagonal elements of the density matrix from the time-averaged position distribution (11) requires a set of functions that is biorthonormal to the functions $u_n^2(x)$. The aim of this Rapid Communication is to show that the known structure of the pattern functions for the determination of the diagonal elements of the density matrix in the harmonic-oscillator case holds true for anharmonic potentials as well. The proof is based on the fact that the product $y_n(x)=v_n^{(1)}(x)v_n^{(2)}(x)$ of two arbitrary solutions $v_n^{(1)}(x)$ and $v_n^{(2)}(x)$ of the stationary Schrödinger equation (6) for the same energy eigenvalue ε_n obeys the following anti-self-adjoint ordinary differential equation of third order,

$$\left(\frac{d^3}{dx^3}-4[U(x)-\varepsilon_n]\frac{d}{dx}-2\frac{dU(x)}{dx}\right)y_n(x)=0, \qquad (12)$$

as can be easily verified. Now, by multplication of Eq. (12) by $f_m(x)=u_m^2(x)$, of the adjoint equation for $f_m(x)$ by $y_n(x)$, and subtraction of this equation from the first, which effectively leads here to an addition, we find

$$\begin{aligned}0=\frac{d}{dx}\Bigg\{&f_m\frac{d^2y_n}{dx^2}-\frac{df_m}{dx}\frac{dy_n}{dx}+\frac{d^2f_m}{dx^2}y_n\\&-4\left(U(x)-\frac{\varepsilon_n+\varepsilon_m}{2}\right)f_my_n\Bigg\}\\&+2(\varepsilon_n-\varepsilon_m)\left(f_m\frac{dy_n}{dx}-\frac{df_m}{dx}y_n\right).\end{aligned} \qquad (13)$$

We now specialize in this equation $y_n(x)=g_n(x)=u_n(x)v_n(x)$, where $v_n(x)$ is any solution of the Schrödinger equation (6). In particular, $v_n(x)$ can be a second linearly independent solution to the nondegenerate eigenvalue ε_n, which is therefore a non-normalizable one. Then, integrating over all x and assuming that the asymptotic behavior of the involved functions $y_n(x)$ ensures that the boundary values vanish, we get

$$0=2(\varepsilon_n-\varepsilon_m)\int_{-\infty}^{+\infty}dx\left(f_m\frac{dg_n}{dx}-\frac{df_m}{dx}g_n\right). \qquad (14)$$

In fact, the structure of the relevant terms being the product of at least three normalizable solutions and at most one non-normalizable solution leads to the supposed asymptotic behavior. The integral in (14) can be different from zero only in the case $\varepsilon_m=\varepsilon_n$ and one finds with $f_m(x)=u_m^2(x)$ and $g_n(x)=u_n(x)v_n(x)$,

$$\begin{aligned}&\int_{-\infty}^{+\infty}dx\left(u_m^2\frac{d}{dx}(u_nv_n)-(u_nv_n)\frac{d}{dx}u_m^2\right)\\&=\delta_{mn}\int_{-\infty}^{+\infty}dx\ u_n^2\left(u_n\frac{d}{dx}v_n-v_n\frac{d}{dx}u_n\right)\\&=\delta_{mn}W(u_n,v_n)\int_{-\infty}^{+\infty}dx\ u_n^2.\end{aligned} \qquad (15)$$

Herein, $W(u_n,v_n)$ denotes the Wronskian

$$\begin{aligned}W(u_n,v_n)(x)&=u_n(x)\frac{d}{dx}v_n(x)-v_n(x)\frac{d}{dx}u_n(x)\\&=W(u_n,v_n)(x_0),\end{aligned} \qquad (16)$$

which is independent of x for arbitrary solutions $u_n(x)$ and $v_n(x)$ of the stationary Schrödinger equation (6) for the same energy eigenvalue ε_n (see, e.g., [26]) and depends only on the solutions involved. From (15) it follows by partial integration and by using the presupposed normalization of the eigenfunctions $u_n(x)$

$$\int_{-\infty}^{+\infty}dx\ u_m^2\frac{d}{dx}(u_nv_n)=\frac{1}{2}W(u_n,v_n)\delta_{mn} \qquad \left(\int_{-\infty}^{+\infty}dx\ u_n^2=1\right). \qquad (17)$$

The Wronskian $W(u_n,v_n)$ is vanishing if the two solutions $u_n(x)$ and $v_n(x)$ are linearly dependent and is nonvanishing if they are linearly independent. Therefore, to get the biorthonormality of the functions $u_m^2(x)$ and $(d/dx)[u_n(x)v_n(x)]$ in (17), the function $v_n(x)$ must be chosen as a solution of the Schrödinger equation (6) that is linearly independent of the normalized solution $u_n(x)$ with a proportionality factor such that the Wronskian in Eq. (17) becomes equal to 2, i.e.,

$$\int_{-\infty}^{+\infty}dx\ u_m^2\frac{d}{dx}(u_nv_n)=\delta_{mn} \qquad \left(W(u_n,v_n)=2,\quad \int_{-\infty}^{+\infty}dx\ u_n^2=1\right). \qquad (18)$$

Thus $v_n(x)$ is a non-normalizable solution of the Schrödinger equation (6). Obviously, an arbitrary multiple of the normalized solution $u_n(x)$ can be added to the non-normalizable solution $v_n(x)$ without changing the biorthonormality relation (17) since the Wronskian remains preserved. As a result the diagonal matrix element ρ_{nn} of the density operator in the energy representation can be determined by the formula

$$\rho_{nn}=\int_{-\infty}^{+\infty}dx\ \bar{P}(x)\frac{d}{dx}[u_n(x)v_n(x)], \qquad (19)$$

where $\bar{P}(x)$ is the time-averaged position distribution (11).

In conclusion, we have shown that the known structure of the pattern functions used in the tomographic reconstruction of the photon statistics holds true also for the motion of a particle in an arbitrary one-dimensional potential. Specifically, we proved that the occupation probabilities of energy eigenstates excited in a wave packet moving in an arbitrary one-dimensional potential can be directly sampled from the time-averaged position distribution of the particle. The sampling functions are the derivative of the product of the usual eigenfunctions and the linearly independent (non-normalizable) solutions of the Schrödinger equation belonging to the same energy eigenvalue.

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