

DETERMINATION OF QUANTUM STATE FROM
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We show that the motional quantum state of a particle moving in an arbitrary one-dimensional potential can be determined directly from the time-dependent position distribution. The sampling functions are the derivative of the product of the usual eigenfunctions and the linearly independent (nonnormalizable) solutions of the Schrödinger equation.

1. Introduction

Since the first experimental demonstration by Smithey et al. [1] the reconstruction of the density matrix of an electromagnetic field from the measured quadrature component distributions in balanced homodyne detection has attracted much interest. Several theoretical studies developed algorithms to reconstruct the density matrix elements in the Fock basis directly by sampling the quadrature component distributions with so-called pattern functions, see [2,3,4] and the literature cited there. Recently it could be shown [3,4] that these pattern functions have a quite simple structure. They are just proportional to the first derivative of the product of the usual (normalizable) solution (energy eigenfunction) and a second linearly independent (nonnormalizable) solution of the Schrödinger equation of the harmonic oscillator.

Note that the measured quadrature component distributions are nothing but the time-dependent position distributions of the fictitious harmonic oscillator associated with the quantized electric field. Thus the question arises whether or not this result is restricted to the motion in a harmonic potential. As expected it turns out that the general structure of the pattern functions applies to the motion of a particle in an arbitrary one-dimensional potential as well [5,6], as we now will show. In doing so we generalize our treatment in [6] to nondiagonal pattern functions.

One-dimensional problems are of interest, not only as the quantization of a single

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mode electric field relies on the one-dimensional harmonic potential but also because, after some appropriate manipulations, in a variety of problems one is led to equations of motion which correspond to the one-dimensional Schrödinger equation. As one example we mention the diatomic molecular vibrations [7]. Moreover we note that proposals to measure the time-dependent position distribution of an ion in a trap have been made [8,9].

2. Spectral decomposition of the time-dependent position distribution

Let us consider the wave packet of a particle of mass m moving in a one-dimensional (real) potential $V(x)$. The probability $P(x, t)$ that the particle described by the density operator $\hat{\rho}$ can be found at time t with position x is given by well known expression

$$P(x, t) = \sum_{m,n} \rho_{mn} u_m(x) u_n(x) \exp[i(\omega_n - \omega_m)t], \quad (1)$$

where the functions $u_n(x)$ which can be chosen as real functions [10] form an orthonormal set of energy eigenfunctions of the time-independent Schrödinger equation

$$\frac{d^2}{dx^2} u_n(x) = [U(x) - \epsilon_n] u_n(x), \quad (2)$$

belonging to the scaled energy eigenvalues $\epsilon_n = (2m/\hbar^2)\omega_n$. Here we have adopted the notation $U(x) = (2m/\hbar^2)V(x)$ for the scaled potential. $\rho_{mn} = \langle u_m | \hat{\rho} | u_n \rangle$ are the density matrix elements in the energy eigenstate basis. In all that follows we assume that the potential $V(x)$ is asymptotically increasing on both sides faster than some positive powers of the modulus of the position. This restriction upon the potential 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 [10]. 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 $v_n(x)$ to the same eigenvalue which is, however, not square-integrable. For this reason it must be rejected as a physical state. However, as we will show, the nonnormalizable solutions play an important role when reconstructing the quantum state.

Our object is to determine the density matrix elements ρ_{mn} from the given time-dependent position distribution (1). We note that all parts of $P(x, t)$ are either constant in time or else oscillate harmonically with the difference frequencies $\omega_n - \omega_m$. Moreover, each density matrix element contributes only to one particular difference frequency component. Clearly, a spectral decomposition of the probability distribution $P(x, t)$ reduces the number of density matrix elements we have to determine simultaneously from a given difference frequency component. For this reason we multiply $P(x, t)$ by $\exp[-i(\omega_s - \omega_r)t]$ and average over times T that are large compared with the periods

of all difference frequencies occurring in the expansion (1). Doing this we immediately find

$$\bar{P}(x; \omega_s - \omega_r) = \frac{T}{\hbar} \int_0^T dt P(x, t) \exp[-i(\omega_s - \omega_r)t] = \sum_{m,n} \rho_{mn} u_m(x) u_n(x) \quad (3)$$

for $T \gg \max(2\pi/|\omega_n - \omega_m|)$ with $\omega_m \neq \omega_n$; \sum' indicates that the sum is taken over only those values of m, n which fulfill the frequency condition $\omega_s - \omega_r = \omega_n - \omega_m$. Note that in the case that all difference frequencies are nondegenerate, in principle, after a sufficient long observation time T the nondiagonal density matrix element ρ_{rs} is directly proportional to $\bar{P}(x; \omega_s - \omega_r)$. In general, however, several density matrix elements contribute to $\bar{P}(x; \omega_s - \omega_r)$. In particular, all diagonal density matrix elements contribute to the time-averaged position distribution $\bar{P}(x; 0)$.

3. Pattern functions, biorthonormality relation and differential equations

The reconstruction of the density matrix elements ρ_{mn} from $\bar{P}(x; \omega_s - \omega_r)$ requires a set of pattern functions $f_{kl}(x)$ which is biorthonormal to the functions $u_m(x) u_n(x)$, i.e.

$$\int_{-\infty}^{\infty} dx u_m(x) u_n(x) f_{kl}(x) = \delta_{mk} \delta_{nl}, \quad (4)$$

where m, n take on all values which met the frequency condition $\omega_m - \omega_n = \omega_r - \omega_s$ or equivalently the energy constraint

$$\epsilon_m - \epsilon_n = \epsilon_r - \epsilon_s. \quad (5)$$

As a result the density matrix elements in the energy representation can be determined from the spectral components (3) of the position distribution $P(x, t)$ by the formula

$$\rho_{kl} = \int_{-\infty}^{\infty} dx \bar{P}(x; \omega_s - \omega_r) f_{kl}(x). \quad (6)$$

Next we propose to show that the functions $f_{kl}(x)$ are the first derivatives of the product of the usual energy eigenfunctions $u_k(x)$ and the second linearly independent (not square-integrable) solutions $v_l(x)$ of the Schrödinger equation (2). The proof is based on the fact that the product $Y_{mn}(x) = y_m(x) y_n(x)$ of two arbitrary solutions $y_k(x)$ (square-integrable or not) of the stationary Schrödinger equation (2) obeys the following ordinary differential equation of fourth order

$$L[Y_{mn}(x)] \equiv \left(\frac{d^4}{dx^4} - 2[2U(x) - (\epsilon_n + \epsilon_m)] \frac{d^2}{dx^2} - 6U'(x) \frac{d}{dx} - [2U''(x) - (\epsilon_n - \epsilon_m)^2] \right) Y_{mn}(x) = 0, \quad (7)$$

as can be easily verified. Here we have introduced the notation $U'(x) = (d/dx)U(x)$. The corresponding adjoint equation reads

$$\bar{L}[z_{kl}(x)] \equiv \left(\frac{d^4}{dx^4} - 2[2U(x) - (\epsilon_l + \epsilon_k)] \frac{d^2}{dx^2} - 2U'(x) \frac{d}{dx} + (\epsilon_l - \epsilon_k)^2 \right) z_{kl}(x) = 0. \quad (8)$$

Next we specialize $Y_{mn}(x)$ to the functions in terms of which the quantities $\bar{P}(x, \omega_s - \omega_j)$ are expanded in Eq. (3), i.e. we put

$$Y_{mn}(x) = u_m(x)u_n(x) \equiv y_{mn}(x). \quad (9)$$

Now we multiply Eq. (7) for $y_{mn}(x)$ and the adjoint equation (8) for $z_{kl}(x)$ by $y_{mn}(x)$ and subtract one from the other. Utilizing the shorthand notation $y^{(j)} = (d^j/dx^j)y(x)$, $j = 1, 2, \dots$ we obtain

$$\begin{aligned} & \frac{d}{dx} F_{mn}^{kl}(x) + [(\epsilon_m - \epsilon_n)^2 - (\epsilon_k - \epsilon_l)^2] y_{mn}(x) z_{kl}(x) \\ &= -2(\epsilon_m + \epsilon_n) z_{kl}(x) \frac{d^2}{dx^2} y_{mn}(x) + 2(\epsilon_k + \epsilon_l) y_{mn}(x) \frac{d^2}{dx^2} z_{kl}(x). \end{aligned} \quad (10)$$

Here the function $F_{mn}^{kl}(x)$ is given by

$$\begin{aligned} F_{mn}^{kl}(x) &= z_{kl} y_{mn}^{(3)} - y_{mn} z_{kl}^{(3)} - z_{kl}^{(1)} y_{mn}^{(2)} + z_{kl}^{(2)} y_{mn}^{(1)} \\ &\quad - 4U(x) [z_{kl} y_{mn}^{(1)} - y_{mn} z_{kl}^{(1)}] - 2U'(x) y_{mn} z_{kl}. \end{aligned} \quad (11)$$

Then integrating over all x , in doing so the first integral on the rhs. of Eq. (10) by parts two times, and assuming that the asymptotic behaviour of the involved functions $z_{kl}(x)$ ensures that the boundary values vanish we get

$$\begin{aligned} & [(\epsilon_m - \epsilon_n)^2 - (\epsilon_k - \epsilon_l)^2] \int_{-\infty}^{\infty} dx y_{mn}(x) z_{kl}(x) = \\ & 2[(\epsilon_k + \epsilon_l) - (\epsilon_m + \epsilon_n)] \int_{-\infty}^{\infty} dx y_{mn}(x) \frac{d^2}{dx^2} z_{kl}(x). \end{aligned} \quad (12)$$

In fact, as we will see later on $z_{kl}(x)$, Eq. (19), involves the product of at least one non-normalizable and at most one non-normalizable solution. Thus the structure of the relevant terms even in the most unfavourable case, being the product of three normalizable solutions and one non-normalizable solution, leads to the supposed asymptotic behaviour. Now restricting the integers m, n, k and l such that

$$\epsilon_m - \epsilon_n = \pm(\epsilon_k - \epsilon_l), \quad (13)$$

we immediately obtain

$$0 = [(\epsilon_k + \epsilon_l) - (\epsilon_m + \epsilon_n)] \int_{-\infty}^{\infty} dx y_{mn}(x) \frac{d^2}{dx^2} z_{kl}(x). \quad (14)$$

Clearly, the integral in Eq. (14) can be different from zero only in the case that $\epsilon_k + \epsilon_l = \epsilon_m + \epsilon_n$. Collecting all together we thus find

$$\int_{-\infty}^{\infty} dx y_{mn}(x) \frac{d^2}{dx^2} z_{kl}(x) = 0, \quad (15)$$

provided that (i) the energy constraint (13) is fulfilled and (ii) $\epsilon_m + \epsilon_n \neq \epsilon_k + \epsilon_l$. Obviously under these restrictions the functions $u_m(x)u_n(x)$ which are solutions of the original differential equation (7) are orthogonal to the second derivative of any solution $z_{kl}(x)$ of the corresponding adjoint differential equation (8). But what about the (normalisation) integral

$$I_{mn} = \int_{-\infty}^{\infty} dx u_m(x)u_n(x) (d^2/dx^2) z_{mn}(x), \quad (16)$$

if besides Eq. (13) also $\epsilon_m + \epsilon_n = \epsilon_k + \epsilon_l$ applies. Is it different from zero and what do the functions $z_{kl}(x)$ look like? To answer these questions we differentiate the adjoint equation (8) with respect to x and obtain

$$\frac{d}{dx} [Lz_{mn}(x)] = L[dz_{mn}/dx] = 0. \quad (17)$$

Thus, if $z_{mn}(x)$ is a solution of the adjoint equation (8) then its derivative $dz_{mn}(x)/dx$ is a solution of the original differential equation (7). Vice versa, to each solution $Y_{mn}(x)$ of the equation (7) there exist a solution $z_{mn}(x)$ of the adjoint equation with the property

$$\frac{d}{dx} z_{mn}(x) = Y_{mn}(x). \quad (18)$$

Indeed from $L[Y_{mn}(x)] = 0$ follows immediately that $z_{mn}(x)$ defined by Eq. (18) obeys the equation $L[z_{mn}(x)] = C$, where C is a constant. Actually, z_{mn} is defined by Eq. (18) only up to a constant and can be chosen such that $C = 0$. Now we specialize the solution $z_{mn}(x)$ of the adjoint equation (8) in expression (16) by the requirement

$$\frac{d}{dx} z_{mn}(x) = u_m(x)\phi_n(x), \quad (19)$$

where $\phi_n(x)$ is any solution of the Schrödinger equation (2). In particular, $\phi_n(x)$ can be chosen to be linearly independent of the energy eigenfunction $u_n(x)$ and is then non-normalizable. Substituting equation (19) into (16) yields after partial integration

$$\begin{aligned} I_{mn} &= \int_{-\infty}^{\infty} dx u_m u_n \frac{d}{dx} (u_m \phi_n) \\ &= \frac{1}{2} \int_{-\infty}^{\infty} dx \left(u_m u_n \frac{d}{dx} (u_m \phi_n) - (u_m \phi_n) \frac{d}{dx} (u_m u_n) \right) \\ &= \frac{1}{2} \int_{-\infty}^{\infty} dx u_m^2 \left(u_n \frac{d}{dx} \phi_n - \phi_n \frac{d}{dx} u_n \right) = \frac{1}{2} W(u_n, \phi_n) \int_{-\infty}^{\infty} dx u_m^2. \end{aligned} \quad (20)$$

Here $W(u_n, \phi_n)$ denotes the Wronskian

$$W(u_n, \phi_n)(x) = u_n(x) \frac{d}{dx} \phi_n(x) - \phi_n(x) \frac{d}{dx} u_n(x) = W(u_n, \phi_n)(x_0), \quad (21)$$

which is independent of x for arbitrary solutions $u_n(x)$ and $\phi_n(x)$ of the stationary Schrödinger equation (2) for the same energy eigenvalue ϵ_n and depends only on the solutions involved [10]. The Wronskian $W(u_n, \phi_n)$ vanishes if the two solutions u_n and ϕ_n are linearly dependent and is different from zero if the solutions are linearly independent. Therefore, to get the biorthonormality of the functions $u_m(x)u_n(x)$ and $(d/dx)[u_k(x)\phi_l(x)]$ within the restriction $(\epsilon_n - \epsilon_m) = \pm(\epsilon_l - \epsilon_k)$ the function $\phi_n(x)$ must be chosen as a solution of the Schrödinger equation (2) which is linearly independent of the normalized solution $u_n(x)$ with a proportionality factor in such a way that the Wronskian in Eq. (20) becomes equal to 2. Collecting all together and using the presupposed normalisation of the eigenfunctions $u_m(x)$ we finally arrive at

$$\int_{-\infty}^{\infty} dx u_m u_n \frac{d}{dx} (u_k \phi_l) = \delta_{mk} \delta_{nl}, \quad (22)$$

provided that

$$W(u_n, \phi_n) = 2 \quad \text{and} \quad (\epsilon_n - \epsilon_m) = \pm(\epsilon_l - \epsilon_k). \quad (23)$$

Obviously, an arbitrary multiple of the normalized solution $u_l(x)$ can be added to the nonnormalizable solution $\phi_l(x)$ without changing the biorthonormality relation (22) since the Wronskian remains preserved. Moreover, we note that our proof shows that instead of $(d/dx)(u_k \phi_l)$ we can as well use $(d/dx)(u_l \phi_k)$ as our pattern function f_k in Eq. (4).

In conclusion, we have shown that the density matrix elements in the energy representation can be determined from the spectral components (3) of the position distribution $P(x, t)$ by sampling them with pattern functions which are the first derivative of the product of normalizable and nonnormalizable solutions of the Schrödinger equation in the energy representation.

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