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Phase retrieval in quantum mechanics

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Determination of the wave function from probability distributions for the position and momentum, the so-called phase problem, is studied. An algorithm leading to the local phase reconstruction is given. Illustrative examples are presented and possible generalizations are indicated.

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The phase retrieval problem, i.e., the reconstruction of the complex wave from measurable intensity distributions attracts a great deal of attention in various branches of physics. A well-known example is coherence theory, where the problem is to recover the second-order correlations of partially coherent light. The standard approach to determine the degree of coherence is based on interferometric measurements, e.g., the observation of the visibility of the interference fringes [1]. There are also various noninterferometric techniques developed to reconstruct the cross-spectral density function [2–4]. Very similar problems are also common in every kind of microscopy [5,6]. In light [7] and electron [8] microscopy the task is to determine the incident complex wave from images taken at different planes; e.g., from intensity distributions in the exit pupil and in the image plane. In the domain of microscopy alone the problem has been extensively investigated [5]; despite this, only a few approximate algorithms have been devised. The most successful of them, the Gerchberg-Saxton algorithm [9,10], is based on an iterative scheme and allows an approximate reconstruction. However, certain symmetries in the object result in a twofold ambiguity [11]; in this case a unique reconstruction is not possible. Only recently has a somewhat different phase reconstruction problem been tackled in quantum optics [12]. The authors reconstruct the wave function from the distributions for the quantized optical phase and the photon number. They follow the procedure by Gerchberg and Saxton; however, they restrict their analysis to finite superpositions of Fock states. On the other hand, striking advances in matter-wave interferometry [13,14] have also aroused great interest in methods for reconstructing the atomic wave function (for the center-of-mass motion) from measured data.

As the wave fields in the above-mentioned exit pupil and image plane are Fourier transforms of one another, the underlying mathematical problem consists in determining a complex function from its modulus and from the modulus of its Fourier transform. Just in this form, it also occurs in quantum mechanics. Here the task is to determine the Schrödinger wave function from both the probability distributions for position and momentum. The importance of this problem for foundations of quantum mechanics was, as early as 1933, recognized by Pauli [15], who remarked on the mathematical problem, "whether for given functions, $W(x) = |\psi(x)|^2$ and $W(p) = |\phi(p)|^2$, the wave function ψ, if such a function exists is always uniquely determined... ." The Pauli problem appears implicitly in investigations, both theoretical and experimental, of electron spatial and momentum distributions [16]. It has also been very thoroughly studied in the context of the informational completeness of quantum mechanics [17], being closely related to the problems of an optimal determination of the past of the system and an optimal forecasting of its future behavior [18,19]. In this field, efforts have mostly concentrated on finding counterexamples when no unique reconstruction is possible [20]. It is known, e.g., that for any functions of a given parity, the unique phase retrieval is impossible, as we cannot distinguish between the given function and the function obtained by complex conjugation.

A version of this problem is also of actual interest in modern quantum optics, since the mentioned distributions can be directly measured on a single-mode radiation field with the help of optical homodyning. In this case, the position and momentum must be identified with the quadrature components of the electric field strength. In fact we can measure all "rotated" distributions

$$P_\theta(x_\theta)=\int W(x_\theta\cos\theta-p_\theta\sin\theta,x_\theta\sin\theta+p_\theta\cos\theta)dp_\theta\ , \tag{1}$$

where

$$x_\theta=x\cos\theta+p\sin\theta,\quad p_\theta=-x\sin\theta+p\cos\theta\ , \tag{2}$$

and $W(x,p)$ denotes the Wigner function of the considered quantum state [21]. It can be shown that the complete field determination is possible with the help of the inverse radon transformation if we know *all* marginal distributions corresponding to the various settings of the local oscillator phase θ [22]. This has been experimentally confirmed for a class of optically realizable states [21,23]. In the Pauli problem we know only two of these marginal distributions. Therefore it is clear that *in general* such a reconstruction is impossible. However, if we know *a priori* that the state of the system is a pure state, use of the Gerchberg-Saxton algorithm has been suggested to simplify the problem [23]. Again we have problems with the possible twofold ambiguity.

The purpose of this paper is to show that there is a large class of nontrivial quantum states for which the Pauli prob-

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lem can be *constructively* solved. They are finite superpositions of harmonic oscillator energy eigenstates, which in case of a single-mode electromagnetic field are known as photon-number or Fock states. For these states it is actually sufficient to measure distributions of only two quadrature operators to find the initial state of the field, up to the well-known twofold ambiguity. Let us stress that such finite superpositions are extensively investigated in the framework of cavity quantum electrodynamics. The recent progress in manipulations of single highly excited Rydberg atoms in high-Q electromagnetic cavities opens new possibilities for quantum state engineering. Using methods of cavity quantum electrodynamics, it is possible, in principle, to create arbitrary finite superpositions of photon-number states. Presently, there are at least two different very general methods for the generation of arbitrary finite superpositions. One is based on the carefully controlled interaction of two-level atoms subsequently traveling through a resonant cavity [24]. The cavity is initially in the vacuum state. Atoms are consecutively injected in such a way that there is at most one atom in the cavity at a given time. The interaction of a single atom with the cavity is described by the well-known Jaynes-Cummings Hamiltonian [25,26]. The other method is based on the adiabatic transfer of atomic Zeeman coherence to the radiation field [27]. It involves the passage of atoms with Zeeman substructure through an optical cavity. Strong coupling of the atom to the cavity field makes possible the adiabatic transfer of atomic ground-state Zeeman coherence to the cavity mode. The latter method seems to be useful also for a single photon-number state generation.

We present here a very transparent scheme leading to the constructive phase retrieval for these states. Moreover, it seems to us that our method can be a proper starting point for approximate methods applicable also in the case of infinite superpositions. It is important to note that our method is completely different from the Gerchberg-Saxton algorithm [9,10] and can deal successfully with the mentioned twofold ambiguity. We simply get both solutions directly from calculations. Our method works only for pure states that can be described by wave functions.

In quantum optics, it is natural to choose Hermite functions as a basis in the underlying Hilbert space. So we expand the unknown wave function $\psi(x)$ in the form

$$\psi(x)=\sum_{n=0}^{\infty} c_n h_n(x), \tag{3}$$

where

$$h_n(x)=\pi^{-1/4}(2^n n!)^{-1/2}\exp(-x^2/2)H_n(x). \tag{4}$$

Here $H_n(x)$ denotes the nth Hermite polynomial [28]. Our task is to determine the coefficients c_n from both $|\psi(x)|^2$ and $|\phi(p)|^2$, where $\phi(p)$ is the Fourier transform of $\psi(x)$. Fortunately, the Fourier transform of a Hermite function $h_n(x)$ is also a Hermite function [29]

$$(2\pi)^{-1/2}\int h_n(x)e^{ipx}dx=i^n h_n(p). \tag{5}$$

We thus obtain from Eq. (3) and its Fourier transform after a little algebra

$$|\psi(x)|^2=\sum_n R_{nn}h_n^2(x)+2\sum_{m>n} R_{nm}h_n(x)h_m(x), \tag{6}$$

$$|\phi(x)|^2=\sum_n R_{nn}h_n^2(x)+2\sum_{m>n} U_{nm}h_n(x)h_m(x). \tag{7}$$

Here, the following abbreviations have been introduced:

$$U_{nm}=\begin{cases} R_{nm} & \text{for } m=n \mod 4, \\ I_{nm} & \text{for } m=n+1 \mod 4, \\ -R_{nm} & \text{for } m=n+2 \mod 4, \\ -I_{nm} & \text{for } m=n+3 \mod 4, \end{cases} \tag{8}$$

$$R_{nm}=\tfrac{1}{2}(c_n^* c_m+c_n c_m^*), \quad I_{nm}=\frac{i}{2}(c_n^* c_m-c_n c_m^*)\ . \tag{9}$$

Our further procedure is based on the observation that the products $h_n(x)h_m(x)$ in Eqs. (6) and (7) can be expanded in terms of appropriately scaled Hermite functions, also forming an orthonormal basis

$$\hat{h}_n(x)=2^{1/4}h_n(\sqrt{2}x). \tag{10}$$

Indeed, the modified argument in Eq. (10) gives us the exponential needed for the proper normalization. Therefore any product of Hermite functions can certainly be expressed as a sum of Hermite functions, even when the arguments differ by a factor. Hence we may write

$$h_n(x)h_m(x)=\sum_{\mu=0}^{\infty}\beta_\mu^{n,m}\hat{h}_\mu(x), \tag{11}$$

where the coefficients $\beta_\mu^{n,m}$ are different from zero only when (i) $\mu\leq n+m$ and (ii) both μ and $n+m$ are either even or odd. Nonvanishing values of these coefficients can be calculated analytically

$$\beta_k^{n,m}=\left(\frac{2}{\pi}\right)^{1/4}\sqrt{\frac{n!m!}{k!}}2^{-2q-(k+1)/2}(-1)^q \times\sum_{i=0}^{\min(n,m,q)}\frac{(-4)^i(n+m-2i)!}{i!(n-i)!(m-i)!(q-i)!}\ , \tag{12}$$

where $q=\frac{1}{2}(n+m-k)$. The relation (11) enables us to expand the right-hand sides of Eqs. (6) and (7) in terms of the functions $\hat{h}_n(x)$, and since the latter form an orthonormal basis, we arrive at the following two systems of equations:

$$\psi_\mu=\sum_n R_{nn}\beta_\mu^{n,n}+2\sum_{m>n} R_{nm}\beta_\mu^{n,m}, \tag{13a}$$

$$\varphi_\mu=\sum_n R_{nn}\beta_\mu^{n,n}+2\sum_{m>n} U_{nm}\beta_\mu^{n,m}, \tag{13b}$$

where the coefficients ψ_μ and φ_μ are determined from the measured position and momentum distributions,

$$\psi_\mu = \int |\psi(x)|^2 \hat{h}_\mu(x) dx, \tag{14a}$$

$$\varphi_\mu = \int |\phi(x)|^2 \hat{h}_\mu(x) dx \ . \tag{14b}$$

So far no approximations or simplifications have been made. Equations (13) are quadratic in the unknown coefficients c_k, c_k^* and form, in the general case, a set of infinite dimension. Hence, at first sight, their evaluation seems to be nontrivial. However, a closer inspection reveals that there is a promising procedure: Truncating the expansion (3) at $n' = n_{\max}$, one gets two equations which immediately give us $|c_{n'}|^2$. Since the wave function is quite generally determined only up to a global phase factor, $c_{n'}$ can be chosen real. Then two equations can be selected from the systems (13) which are *linear* in $c_{n'-1}$ and $c^*_{n'-1}$ and, after insertion of $c_{n'}$, yield $c_{n'-1}$. The next step is to select a set of equations which are linear in $c_{n'-2}$, $c^*_{n'-2}$, $c_{n'-3}$, $c^*_{n'-3}$ and, after insertion of previously calculated $c_{n'}$ and $c_{n'-1}$, allow the determination of $c_{n'-2}$ and $c_{n'-3}$. This procedure can be repeated until all the coefficients $c_n (n \leq n_{\max})$ are known. So the mathematical problem actually reduces to subsequently solve blocks of linear equations.

The algorithm works perfectly if $\psi_{2n'} = \varphi_{2n'}$. Otherwise we have a contradiction from the very beginning. However, the mentioned condition is always fulfilled for finite superpositions of $n'+1$ photon-number states. Therefore, for these states, the Pauli problem can be constructively solved. On the other hand, any infinite superposition can be approximated by a finite one. Thus we believe that our procedure, which is exact for finite superpositions, can also be a good starting point for infinite superpositions. Our numerical simulations suggest that for some special but realistic states it is indeed the case.

Let us present two simple illustrative examples, i.e., linear superpositions of the vacuum state $|0\rangle$ with the one-photon state $|1\rangle$ and with two-photon state $|2\rangle$: $|\psi_1\rangle = c_0|0\rangle + c_1|1\rangle$ and $|\psi_2\rangle = c_0|0\rangle + c_2|2\rangle$. In the first case, there is no definite parity and the unique (up to an irrelevant *global* phase) solution is given by

$$c_1 = \sqrt{\frac{\psi_2}{\beta_2^{1,1}}} \ , \tag{15}$$

$$c_0 = \frac{\psi_1 + i\varphi_1}{2\beta_1^{0,1} c_0} \ . \tag{16}$$

The coefficients ψ_i and φ_i should be calculated from measured distributions $|\psi(x)|^2$ and $|\phi(p)|^2$ via relations (14). Of course we have $\psi_2 = \varphi_2$. The second case is more complicated. The corresponding wave function is even and there is no unique reconstruction possible. Solving Eqs. (13) we get

$$c_2 = \sqrt{\frac{\psi_4}{\beta_4^{2,2}}} \ , \tag{17}$$

$$c_1 = 0 \ . \tag{18}$$

From the rest of Eqs. (13) we can uniquely calculate $|c_0|$ and the real part of this coefficient $\mathrm{Re}(c_0)$. Thus the imaginary part $\mathrm{Im}(c_0)$ is given up to the $\pm$ sign. But this is nothing but the twofold ambiguity we should expect in this case. Also here we have $\psi_4 = \varphi_4$.

In summary, we devised a method for phase retrieval in quantum mechanics. It works perfectly well for states that are finite superpositions of photon-number states. In this case, even if the unique reconstruction is impossible for fundamental symmetry reasons, we get explicitly all possible solutions. Our method is completely different from the well-known Gerchberg-Saxton algorithm. It does not rely on any iterations starting from random phases, but is based on solving blocks of linear equations for unknown coefficients in the expansion of the desired wave function into the Fock-state basis. Being *exact* for finite superpositions, it should also be a good starting point for *approximate* reconstruction in more general cases. Work along these lines is in progress and results will be reported elsewhere.

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